

**FINAL TECHNICAL REPORT**  
**DOE Grant No. DE-0005206**  
**American Conference on Neutron Scattering**

The American Conference on Neutron Scattering (ACNS) is a focus for neutron scattering research in North America, bringing academics, students, post-docs and national laboratory scientists together to communicate the latest developments in all areas of science and engineering that neutron scattering facilitates. There is no other conference/meeting in North America that offers the same breadth and depth of neutron science. The ACNS series of meetings are organized by the Neutron Scattering Society of America (NSSA) in collaboration with various government sponsored neutron scattering facilities. The first meeting took place in Knoxville in 2002. This was followed by meetings in 2004, 2006 and 2008. **The fifth conference in this series was held in Ottawa, ON, Canada, from June 26<sup>th</sup> – June 30<sup>th</sup>, 2010.**

The NSSA views the ACNS as a means to provide a focal point for the national neutron user community to strengthen ties within this diverse group, while at the same time promoting neutron research among colleagues in related disciplines identified as “would-be” neutron users. The ACNS thus serves a dual role as a national user meeting and a scientific meeting. As a venue for scientific exchange, the ACNS showcases recent results and provides forums for scientific discussion of neutron research in diverse fields such as hard and soft condensed matter, liquids, biology, magnetism, engineering materials, chemical spectroscopy, crystal structure, and elementary excitations, fundamental physics and development of neutron instrumentation through a combination of invited talks, contributed talks and poster sessions. As a “super-user” meeting, the ACNS fulfills the main objectives of users' meetings previously held periodically at individual national neutron facilities, with the advantage of a larger and more diverse audience. To this end, each of the major national neutron facilities (NIST, LANSCE, HFIR, SNS and Chalk River in Canada) have an opportunity to exchange information and update users, and potential users, of their facility. This is also an appropriate forum for users to raise issues that relate to their facility. For many of the national facilities, this super-user meeting should obviate the need for separate user meetings that tax the time, energy and budgets of facility staff and the users alike, at least in years when the ACNS is held. We rely upon strong participation from the national facilities. The NSSA intends that the ACNS will occur approximately every two years, but not in years that coincide with the International Conference on Neutron Scattering. The ACNS continues to be held in association with one of the North American neutron centers in a rotating sequence, with the host facility providing local organization and planning assistance. The ACNS, targeting the entire potential neutron North American user community, complements the annual NIST, ANL and LANSCE schools which give hands-on experience primarily to graduate students who anticipate using neutron scattering in their thesis research. The summer schools are promoted at the ACNS and represent a natural path for students to take after being inspired by the activities of the ACNS.



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## ACNS 2010 Meeting Scene 1



Ottawa, ON, Canada  
June 26-30

ACNS 2010



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### DAY 1: Sunday, June 27

Located at the confluence of three major rivers, the Ottawa, the Gatineau and the Rideau, the city of Ottawa is the capital of Canada. This week, it is also the venue of the [2010 American Conference on Neutron Scattering](#), being held at the historic Fairmont Château Laurier hotel. The conference opened Saturday evening with a reception. Two tutorials were held on Saturday as well. An opening plenary session was held Sunday morning with six speakers. Several technical sessions were held during the day, while the first poster session in conjunction with the exhibit was held in the evening.

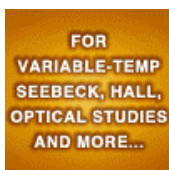


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**MMR Technologies**  
Microcryogenic and  
Thermal Stage Systems



#### ■ Plenary Lectures



The major event of the day was the plenary session in the morning that included six major talks. Conference chair Simon Billinge (Columbia University) opened the session and the conference by welcoming all attendees. He also thanked the various organizers responsible for bringing this conference to fruition. Bruce Gaulin (McMaster University) who is current president of the Neutron Scattering Society of America welcomed overseas visitors to Canada and Ottawa, and recommended attendees spend some time outside of the conference exploring Ottawa.

#### **Fifty Years of Neutron Scattering in Canada - William J. Buyers**



William Buyers of the Canadian Neutron Beam Centre at Chalk River, Ontario, is a well known name in neutron science. It was fitting that Buyers was the first plenary speaker of this conference being held in Canada. In his talk, he overviewed developments in neutron scattering from a Canadian perspective subtitled his talk, from Brockhouse to the 21st century. Bertram N. Brockhouse of course won the 1994 Nobel Prize in Physics "for the development of neutron spectroscopy" along with Clifford Shull. Buyers is originally from Scotland, and came to Canada over 50 years ago. Starting with some of his early work in neutron science, he described specific examples of seminal work done in Canada in this field. He covered cobalt oxide spin waves, perovskite antiferromagnets, quantum He-4 fluid, and solitons in one-dimensional antiferromagnets. He also

described some recent very interesting work including residual stress determination in engineering materials (formed into a commercial entity), polarized neutron beam science, and the orientation of cholesterol molecules in a bio-membrane. Buyers concluded by mentioning the export of talented neutron science researchers to institutions outside Canada including to Oxford, NIST, MIT, Berkeley, and Oak Ridge showing Canada's ability to consistently produce scientific leaders.

#### **Tackling our Energy Challenges in a New Era of Science - Linda Horton**



Linda Horton is Director of the Materials Sciences and Engineering Division of the Office of Basic Energy Sciences (BES) within the U.S. Department of Energy (DOE). In her plenary talk, Horton described opportunities for funding of neutron scattering through the DOE. The energy needs of the world continue to grow at a torrid pace, particularly in Asia. Along with this is the alarming rise in CO<sub>2</sub> levels in the atmosphere accompanied by ice loss in the polar regions. Clearly breakthroughs are needed in various energy areas to be able to supply the energy for such growth, and to do this in a manner that does not disrupt the

current environmental balance, which is already tilting in a negative direction. The DOE is involved in various ways in promoting research on critical energy-related areas, and Horton overviewed these in her talk. She described strategic planning efforts within BES. In particular, DOE invests in science to achieve transformational discoveries, she said. Horton indicated that neutron scattering plays an important role in several research directions supported by the DOE and BES. In addition to core research support, BES also has funded Energy Frontier Research Centers and Energy Innovation Hubs. Further information on all of these topics as well as much more is available on the BES website at <http://www.sc.doe.gov/bes/BES.html>.

#### **Neutron Scattering and Energy - Thomas Mason**

Thomas Mason is Director of the Oak Ridge National Laboratory in Oak Ridge, Tennessee, in the United States. He is also originally Canadian and was involved in neutron research. He was deeply involved in the construction phase of the Spallation Neutron Source at Oak Ridge. Mason presented the plenary lecture on neutron scattering as a crucial tool for scientific breakthroughs in developing advanced energy technologies. The starting point of his talk was world energy consumption, which is expected to increase significantly by 49% from 2007-2035. He emphasized



that economic and population growth results in increasing energy demand. Another important point is that human activity is affecting global climate and the concentration of  $\text{CO}_2$  is progressively increasing in the atmosphere, as also mentioned by the previous speaker.

The main questions to ask are (1) where we are going to get the energy, and (2) what we are going to do to resolve the problem of climate change? It is clear that a new set of transformational discoveries and disruptive technologies are needed involving efficient use of energy and new alternative sources. In this respect, the essential "green" energy technologies include nuclear power, wind, solar, biofuels, and electrically-driven vehicles. Mason also

emphasized that materials form a crucial proportion of the energy equation.

His main focus was on today's neutron facilities which provide capabilities for understanding of structure-dynamics-function relationships of materials leading to the development of clean and sustainable energy technologies. The talk highlighted the use of neutron scattering to explore biomaterials, superconductors, and other engineering energy-related systems. One of the examples Thomas mentioned was developing high-temperature long-lasting materials based on nickel alloys for high-strength and light-weight vehicles. Another example is the investigation of bio-based fuel systems for sustainable energy based on cellulose digestion. One more recent study performed with neutrons focused on the design of next generation batteries with dramatically improved capacities and long life-times.

#### **Magnetic Superconductors: The Perfect Playground for Neutron Scattering - Jeffrey Lynn**



Jeffrey Lynn (NIST) in his talk described the development of superconductors over nearly a century, the connections to magnetism and how neutron scattering plays a crucial role in understanding the connection between the two. He started with a history of superconductors and Cooper pairs recognized to be the mechanism for superconductivity in the original systems. Magnetic impurities disrupt spin pairing and were recognized to be detrimental. However, exceptions to this were found including magnetic sublattices with long range magnetic order and ferromagnets. He discussed the use of small angle neutron scattering to elucidate some of the properties of these materials. Lynn then described cuprate superconductors with high  $T_c$  values discovered in the mid-1980s. In these, the parent 'systems' are

Mott-Hubbard antiferromagnetic insulators with very strong two-dimensional magnetic interactions. These strong exchange interactions survive into the superconducting state yielding highly correlated electrons that participate directly in the superconducting pairing. Finally, Lynn discussed the new iron-based superconductors first discovered in 2008 that are attracting tremendous current attention. Neutron scattering has been used to investigate all of these systems.

Lynn summarized his talk by suggesting that magnetic superconductors have a rich history going from "should not have magnetic spins in the lattice" to "must have magnetic spins in the lattice" for high  $T_c$ . For cuprate superconductors, the Cu spin dynamics provide the needed high energy scale. In these materials, the magnetic resonance is directly tied to the superconducting state for both hole and electron-doped cuprates. Finally, iron-based superconductors exhibit a similar phase diagram as the cuprates. The 'parent' systems exhibit a ubiquitous structural transition below which long range antiferromagnetism is seen. The role of spin fluctuations in the superconducting pair is clear. Lynn suggested that our understanding of this new family of superconductors is better than for the cuprates thanks to neutron scattering, and this might yield the key to a full understanding of both classes of high  $T_c$  superconductors.

#### **Neutron Imaging: The Vision Superman should have had - Muhammad Arif**



There have been tremendous strides made over the last two decades in neutron imaging, that is, using thermal and cold neutrons to image materials that can reveal startling details that cannot be imaged by other techniques. Muhammad Arif of NIST presented various examples of images formed using neutrons in his talk in the plenary session. Currently, a range of imaging techniques including neutron tomography, phase contrast imaging and energy selective imaging are available. Neutrons in particular are very effective for probing low atomic number materials, which are difficult to image using X-rays. Images are captured using high efficiency neutron detectors yielding spatial resolutions of ten micrometers. Arif then presented various examples of using neutron imaging for useful applications.

Polymer electrode membranes are used in current fuel cells. Arif described how neutron scattering can be used to image the flow of water within channels in the fuel cell.



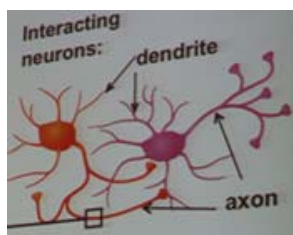
In addition, water distribution within a membrane could also be imaged. Another example was hydrogen storage beds used to store hydrogen for use in vehicles. Neutron imaging was used in real-time to measure H-uptake and the distribution along the length of the storage bed. The H-distribution could also be measured in 3-D to study effects of temperature gradients and bed construction. Another example was Li-batteries wherein both Li and H are energy carriers. Neutron scattering was used to image Li and H-ion transport bottlenecks. Neutron tomography was also used to investigate the growth patterns of ancient (2 billion years old) microbes using buried organic inclusions, using the hydrogenous component. Another fascinating example was imaging the complete 3-D structure of the lung of a rat. Phase contrast imaging has various applications. In a forensic application, phase contrast neutron imaging was used to image the serial number on a car that had been machined out. The number could still be imaged using neutrons. In another study, polarized neutrons were used to image phase transitions in a magnetic system, a PdNi crystal at different temperatures. Clearly, neutron imaging will find a host of useful applications and continue to see rapid growth.

#### **Tau Protein Directed Assembly in Neuronal Systems - Cyrus R. Safinya**



Understanding interactions of supramolecular assemblies of biological molecules gives important information on structure-function relationships in biological systems and leads to the development of nanoscale functional biomolecular materials. Cyrus Safinya (University of California at Santa Barbara) focused his plenary talk on the elucidation of directed assembly of Tau proteins in neurological systems. Nerve cells provide a rich variety of bundles and networks of interacting neurofilaments, microtubulus, and filamentous actin. In this respect, Tau is an unstructured but fully functional protein which plays a critical role in the nervous system in stabilizing mature neurons and in the outgrowth of axons in developing neurons.

In his talk, Safinya addressed several important questions targeted at understanding microtubule interactions and functions *in vivo*. Some of these involved the effects of Tau proteins on microtubule assembly, the role of counter-ions in bundling, and the significance of bundles in the maintenance of axons in mature neurons. The study is crucial for exploring Tau-induced bundling in axonogenesis and in understanding how unnatural interactions between tau and microtubules lead to neurodegeneration (including Alzheimer's Disease).



Safinya emphasized that a fundamental understanding of interactions between cell cytoskeletal proteins and their associated molecules can be obtained by combining state-of-the-art techniques such as reciprocal space and real space data resulting from X-ray diffraction and scattering, light-microscopy differential-interference-contrast and three-dimensional confocal imaging, and electron microscopy experiments. He demonstrated that synchrotron small angle X-ray scattering (SAXS) and electron microscopy were capable to probe non-crystalline structures of Tau-directed filament assemblies in neurons; while small angle neutron scattering (SANS) is an ideal tool to directly examine the structural nature of distinct Tau

domains on the microtubule surface.



#### **■ Technical Talks**

### Symposium C: Soft Condensed Matter

#### *Dynamic studies of gel network morphology under flow*

Hydrogels as crosslinked polymers networks are very attractive for biomedical applications as they are soft, bio-mimetic, and tissue-friendly. Congqi Yan, a graduate student from the University of Delaware, presented a mechanically robust hydrogel which was prepared by crosslinking of peptides. Remarkably, the peptide was bio-compatible and possessed self-healing properties. She demonstrated that hydrogels were highly responsive to mechanical shear under flow. However, the shear-thin gel solution was restored into a solid stiff gel after stress was removed. A rheometric study was performed to investigate the restoration of gel rigidity with various shear stresses applied. SANS and SAXS were used to investigate the dynamic gel morphology under various flow conditions. This remarkable self-healing capability suggests that the gels are excellent candidates for tissue regeneration, since they can recover after syringe injection.

### Symposium E: Chemistry & Materials

#### *Controlling Zeolite Beta Nucleation and Growth*

Zeolites are a class of crystalline microporous aluminasilicate materials. Their unique 3-D porous structure along with high thermal stability are very attractive for applications in ion-exchange, catalysis, and separation. One outstanding problem is understanding the nucleation mechanism of zeolites which would afford rational design of the high-performance materials. Nathan Hould, a graduate student from the University of Delaware, focused his work on investigating the fundamental aspects of the beta nucleation process and compared the results with the classical nucleation theory. He found that the presence of sodium ions in Al-containing precursor solutions is important to control the density of the zeolite particles. On the other hand, Al controls particle aggregation as it slows down nucleation at low Al concentrations. More importantly, he was able to probe the transition from amorphous to crystalline zeolite by applying neutron scattering.

### Symposium F: Condensed Matter Physics

#### *Polarized Neutron Scattering Studies of Multiferroic $\text{Ni}_3\text{V}_2\text{O}_8$ in an Electric Field*

Ivelisse M. Cabrera of Johns Hopkins University presented a study on using polarized neutrons to investigate multiferroic domains in  $\text{Ni}_3\text{V}_2\text{O}_8$  (NVO), a system that is both magnetic and ferroelectric. Polarized neutron scattering can reveal details on complex magnetic structures. In the present work, polarized neutrons along with electric polarization measurements yielded direct electric control of multiferroic domains in NVO, as suggested by control of cycloidal domains. The study revealed that magnetic and ferroelectric domains coincided in NVO at low temperatures. This suggests that magnetic domains can be controlled by an external electric field. Polarized neutrons provided a quantitative measure of the population of cycloidal domains as a function of the electric field. Interestingly, an unusual memory effect was observed in the multiferroic phase of NVO, where a previously electrically-polarized sample "remembered" its polarization direction on leaving and re-entering the multiferroic phase in the absence of a field. The underlying reasons for this memory effect are still not clear and will be the subject of future investigations according to the speaker.

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#### ■ Scanning the Conference

#### *Reception*





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## ACNS 2010 Meeting Scene 2



Ottawa, ON, Canada  
June 26-30

**ACNS 2010**



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### [DAYS 2, 3: Monday, Tuesday June 28-29](#)

The second and third days of the [2010 American Conference on Neutron Scattering](#), in Ottawa, Canada, included a number of interesting events and activities. The major event on Tuesday morning was the awards session with various prizes of the Neutron Scattering Society of America (NSSA) awarded by the president of the NSSA Bruce Gaulin and vice-president Simon Billinge. This was followed by two of the prize winners presenting talks.



*Some of the new Fellows of the Neutron Scattering Society of America*

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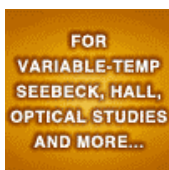
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#### ■ [Neutron Scattering Society of America Awards](#)



*Herbert A. Mook (second from right) receiving the 2010 Clifford G.*





**MMR Technologies**  
Microcryogenic and  
Thermal Stage Systems



*Shull Prize. (l to r) Simon J.L. Billinge, Jaime A. Fernandez-Baca, Herbert A. Mook and Bruce D. Gaulin.*



*(right) Collin Broholm receives the 2010 Sustained Research Prize, and (right) Craig M. Brown receives the 2010 Science Prize of the NSSA.*



*Gregory Smith (second from left) and Steven Shapiro (second from right) receiving special NSSA service awards*

#### **Student Poster Awards**



**First Prize: Suanne Mahabir**  
Mechanism for the growth of "bicelles"



**Second Prize: Christopher Metting**  
Characterization and modeling of off-specular neutron scattering for analysis of two dimensional ordered structures

**Third Prize (Honorable Mention): Ping-Yen Hsieh**  
The gas adsorption behaviors in chiral holmium metal-organic framework materials

#### ■ **Prize Lectures**

**The Edge of Magnetism**  
**Collin Broholm, 2010 Sustained Research Prize**

*"Science is what happens while you are busy making other plans." Collin Broholm paraphrasing John Lennon*





Collin Broholm of Johns Hopkins University is the recipient of the 2010 Sustained Research Prize of the NSSA. He gave a talk on Tuesday morning on "The Edge of Magnetism." He started by stating that in his research career thus far, the dominant theme has been exploring magnetism at its limits. Starting from a system of interacting spins in an insulating solid, how can we suppress the development of long range magnetic order and which phases may be found in its place if we succeed, were the questions he posed. Neutron scattering studies have been at the heart of his research at the edge of magnetism.

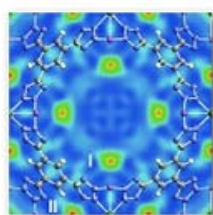
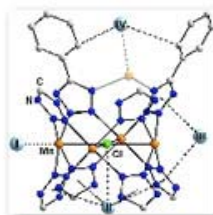
In his talk, Broholm discussed materials driven to the edge through reduced dimensionality, through competing interactions and through interactions with conduction electrons. He described the potential for novel cooperative phases such as superconductivity emerging at the edge of magnetism. He suggested that instrumentation development formed a parallel narrative in his research and in this talk. Following the thread towards the edge, he also described progress in instrumentation that have opened up new windows on magnetism at the atomic scale. This has yielded higher efficiencies, higher energies, higher resolutions and extreme sample environments. Finally, though he did not speak directly of applications, he said that history has shown that qualitatively new states of matter are necessary input to fuel technologies of the future. This body of work could conceivably yield important applications in the future as has been shown time and again by fundamental scientific research.

#### **Understanding How Hydrogen Interacts With Materials Using Neutrons** **Craig Brown, 2010 Science Prize**



Hydrogen, the most abundant element in the universe, has great potential as an energy source. Unlike petroleum, it can be easily generated from renewable energy sources. It is also nonpolluting, and forms water as a harmless byproduct during use. Yet it is so difficult to store that its use as a fuel has been limited. Craig Brown (Center for neutron science, NIST) focused his plenary talk on new hydrogen storage materials based on metal-organic frameworks. He emphasized that new materials must achieve higher gravimetric and volumetric densities than those currently available to afford a viable storage systems that can be reversibly refueled.

Despite the fact that capacity of these hydrogen-storage materials has improved over the last decade, there are still many technological challenges that limit optimizing their performance. He highlighted the main obstacles, involving low hydrogen adsorption enthalpy and the lack of understanding of surface packing density. There are a number of mechanisms he discussed to increase the operating temperature, from strong-binding (less than 'Kubas' though), engineered nanospaces, spillover mechanisms, and substitution of hetero-atoms in carbon frameworks. Brown showed several examples of how he has relied in his research on various neutron methods including powder diffraction and quasi-elastic scattering as well as vibrational and rotational spectroscopy to advance understanding and improve system performance.



<http://www.ncnr.nist.gov/staff/craig/>

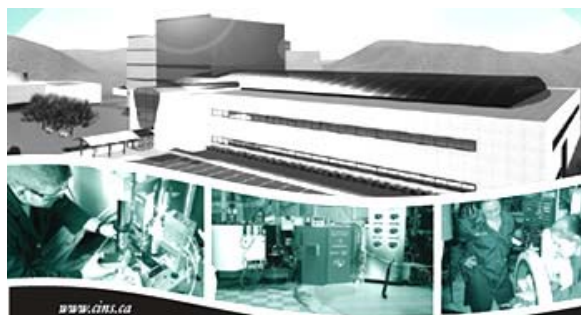
■ [The Future of Neutron Scattering in Canada - Panel Discussion](#)



The main idea of the panel discussion on Monday was to discuss the perspectives of neutron scattering in Canada to ensure that the Canadian scientific community has access to neutron-based experimental facilities in the coming decades. The session was moderated by Dominic Ryan, president of the Canadian Institute of Neutron Scattering (CINS), and Danial Wayner, vice-president of the National Research Council Canada in Physical Sciences. The six panelists included Bruce Gaulin (current president of the Neutron Scattering Society of America and Director of the Brockhouse Institute for Materials Research at McMaster University), Thom Mason (Director of Oak Ridge National Laboratory), Denise Carpenter (President of the Canadian Nuclear Association), Basma Shalaby (President of the University Network of Excellence in Nuclear Engineering, and Professor of Engineering Physics at McMaster University), Ben Rouben (Executive Administrator at the Canadian Nuclear Society), and Dean Chapman (representing the proposed Canadian Neutron Source at the University of Saskatchewan).

The session moderators first overviewed the history of neutron scattering in Canada with a focus on the National Research Universal (NRU) reactor at Chalk River which was built 52 years ago to produce isotopes. However, the reactor is showing its age and has been shut down for over a year for repair. The main questions posed were whether Canada needs its own neutron source and what will be the mission of the re-built reactor?

The panel claimed an urgent need for a new type of neutron source in Canada which would significantly contribute to many spheres of society including academia, industry, and healthcare. It was emphasized that Canada's future depends on the ability to train new scientists and to retain existing expertise and knowledge. The domestic neutron source would support not only basic science experiments but would also provide new resources for medicine and R&D perspectives to the Canadian nuclear industry and the North America neutron community. For example, neutron scattering is essential for materials research and engineering to provide improved understanding of novel systems and high-performance materials. Canada's leading role in advanced materials is evidenced by Bertram Brockhouse's Nobel Prize in Physics in 1994. A new multi-purpose research reactor would encourage the entrepreneurial spirit of innovation and would ensure the continued development of highly qualified scientists and engineers. Overall, the reactor would help in securing Canada's role as a world leader in science and technology and radioisotope production.



*The proposed new multi-purpose research reactor in Canada*

In summary, according to the panelists, neutron scattering in Canada is at a historic turning point and actions should be taken now to ensure that the next generation gets to use the enormous capabilities of neutron-based multipurpose facilities. The recent failure of the NRU reactor shows the urgent need to develop an orderly succession plan so that Canada's investment in nuclear research and engineering is not lost and Canada's leadership in neutron science can continue well into the future.

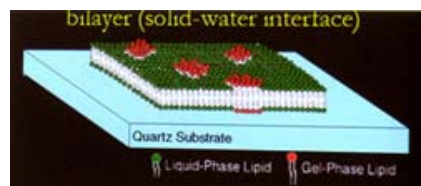
#### ■ Technical Talks

#### **Symposium C: Soft Condensed Matter**

*Dynamic Light Scattering Investigations of Nanoparticle Aggregation Following a Light-Induced pH Jump*

There are many important processes where the stability of nanoparticles can change in response to the solution environment. These changes are challenging to study under controlled conditions. In his poster, Vivek Prabhu (NIST) illustrated the use of dynamic light scattering (DLS) to study the initial kinetics of aggregation of carboxylated polystyrene nanoparticles after well-defined pH jumps using aqueous solutions of photoacid generator. He demonstrated that using this approach, the pH of solutions was controlled by exposure to UV light. He found the aggregation kinetics to be very sensitive to solution pH. Particle aggregation was induced by decreasing pH as a result of decreasing the electrostatic repulsion between the particles. Overall, Prabhu demonstrated that the novel pH jump provides access to challenging time-scales (sub 5 sec) in the absence of mixing flows. Importantly, the ability to tailor pH changes via optical exposure affords investigating complex systems like gels and multicomponent mixtures when traditional methods cannot be used.

#### ***Early Stages of Oxidative Stress-Induced Lipid Membrane Permeabilization: A Neutron Reflectivity Study***



A lipid membrane composed of a bilayer of phospholipids deposited on solid water interfaces is widely used as an attractive model system to mimic cellular membranes. Still, a number of open questions remain in cell membrane behavior. In his invited talk, Jaroslaw Majewski (Los Alamos National Lab.) addressed the topic of membrane stability and described how oxidative stress induced by mild UV irradiation affects properties of lipid membranes such as morphology and structure. He emphasized that oxidative damage of the cell membrane is a very important point to investigate as in the case of apoptosis and Alzheimer's disease. Majewski described a bilayer of DPPC and POPC phospholipids exposed to UV light wherein the structure was examined by neutron reflectivity. The irradiation of membranes results in a decrease in membrane coverage along with the formation of micropores within the membrane. The unique feature of the membrane to reorganize and form of hydrophilic channels was then confirmed with spectroscopy and microscopy techniques.

#### ***Structure Of Lipid Bilayers On Polyethylene Glycol (PEG) Cushions: Fact and Fiction Of PEG Cushioned Membranes***

Erik Watkins (University of California, Davis) continued the topic on using lipid bilayers as systems mimicking cellular membranes. In contrast to previous studies which were mostly focused on deposition of bilayers on solid templates, Watkins presented a polymer cushion to support lipid bilayers in a liquid environment. The cushion is made of a highly hydrated and biocompatible PEG grafted to a solid template. The cushion separates the lipid membrane from the solid template thus providing bio-mimicking physiological conditions for the self-supporting membrane. What is more important, in contrast to the conventional surface-tethered films, the cushion-supported system eliminates problems associated with protein denaturing and restricted protein mobility induced by direct binding of lipids to the solid templates. Watkins demonstrated precise structural quantitative characterization of the membranes with the application of neutron and X-ray reflectivity. The hybrid system was shown to be stable with time and allows liquid access to the lipid bilayer on both sides. The highly hydrated nature of the polymer support is very attractive for applications in developing biologically relevant cellular-like membranes. Overall, the system is robust, easily prepared, tunable, and proposed to mimic extracellular matrix, which is crucial for membrane-based biosensors.

### **Symposium E: Chemistry & Materials**

#### ***Hydrogen Diffusion in Potassium Intercalated Graphite Studied by Quasielastic Neutron Scattering***

Hydrogen is of course being seriously investigated as a future clean and renewable energy source. One option for hydrogen storage is physisorption, and graphite is being investigated as a medium to store hydrogen. Surface adsorption in graphite is low at 4 kJ/mol and hence researchers are considering separating the graphite layers using intercalated guest species to increase interlayer adsorption. Potassium, rubidium and cesium are being investigated as guest species to tailor the pore width between graphite layers. Justin Purewal (California Institute of Technology) in his invited talk on Monday described an investigation using quasielastic neutron scattering (QENS) to study hydrogen diffusion in MC24 graphite intercalation compounds (M=K, Rb, Cs) with focus on KC24. The QENS spectra were analyzed with a two-dimensional honeycomb lattice jump diffusion model. Molecular dynamics simulation was also used to correlate with experimental data. Hydrogen diffusion in KC24 was found to be similar to that in zeolites with molecular sized pores but an order-of-magnitude slower than diffusion in other carbons. Steric diffusion barriers were the determining factor for the magnitude of the diffusion coefficient.



Also, the rate of  $H_2$  adsorption slowed at larger  $H_2$  compositions likely due to site blocking. The barrier to  $H_2$  rotation in  $KC_{24}(H_2)_x$  was found to be many times larger than in other carbon adsorbents due to confinement between the graphite layers, thus affecting diffusion behavior.

#### ***Evidence of Enhanced Hydrogen Storage in Pt-Impregnated Activated Carbon by the Spillover Effect***

High hydrogen storage levels are critical for future mobile fuel cell vehicles. While various porous materials are under consideration for hydrogen storage, none of them yet satisfy the targets set, in particular by the U.S. Department of Energy. One potential option is using the "spillover" effect to enhance room temperature hydrogen storage capacity. In the spillover effect, in the case of Pt-doped activated carbon, atomic hydrogen is first generated by dissociation of hydrogen molecules on Pt particles, for instance. The atomic hydrogen then migrates onto the carbon by surface diffusion and is then adsorbed. The spillover effect is still rather poorly understood. Yang Zhang speaking on behalf of Cheng-Si Tao of MIT described the use of small angle neutron scattering (SANS) to study the spillover effect on Pt-impregnated activated carbon. The methodology involved transmission measurement combined with SANS. Inelastic neutron scattering was also used to study the state of the hydrogen and its interaction with the carbon adsorbent and carbon-supported metal particles. The results provided some evidence though not entirely conclusive for the spillover effect. However, the methodology used appears to be very useful for further studies to investigate the spillover effect.



#### **Symposium F: Condensed Matter Physics**

##### ***Ferromagnetism Induced at the Interface Between Paramagnetic and Antiferromagnetic Perovskite Thin Films***

Controlled interfaces between two materials can give rise to novel physical phenomena and functionalities. For instance, when epitaxial  $LaMnO_3$  films were grown on  $SrTiO_3$  substrates, magnetism was induced at the interface by doping or charge transfer. A method to probe the magnetism of a buried interface is therefore important. Valeria Lauter (Oak Ridge National Laboratory) and her colleagues used polarized neutron reflectometry with off-specular scattering to investigate interfacial structures. Upon cooling from 300K to 5K under  $H=1T$ , splitting of lines was observed. This was due to a structural phase transition, wherein reflections on laterally coherent tilt domains were obtained. Thus, there was evidence of a reversible temperature-dependent structural modulation of an  $LaMnO_3$  film. In summary, a new type of negative magnetostriction not reported previously was obtained. Reversible temperature-dependent structural changes in  $LaMnO_3$  films were observed. PNR experiments revealed the appearance of laterally coherent tilt domains in the  $LaMnO_3$  film below  $T=95$  K. Magnetization distribution in an  $LaMnO_3$  film was not uniform and was enhanced towards both interfaces.

##### ***Study of $TiO_2$ Nanotube Structures Using SANS***

$TiO_2$  is currently used in a number of fascinating applications, including as photocatalysts. In particular, there is great interest in using  $TiO_2$  nanotubes because of the added surface areas available. Nitrogen doping has been found to reduce the bandgap of  $TiO_2$  bringing it within the visible light range for photocatalysis. Also the use of  $TiO_2$  nanotube arrays yields new and interesting properties. In a new study, described by Lisa DeBeer-Schmitt of Oak Ridge National Laboratory, SANS was used to characterize  $TiO_2$  nanotube arrays to understand their structure and to investigate the effect of nitrogen incorporation into the nanotube structure. While the pure  $TiO_2$  was found to have a disordered structure with crystallites formed between the nanotubes, the nitrogen doped specimens were found to be more ordered with no crystallites between the nanotube arrays. This was evident from the additional peaks in the SANS data for the nitrogen doped specimens. The results suggest that the morphology of the nanotube array could be manipulated by varying the growth conditions.

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■ [Scanning the Conference](#)



#### ■ ABOUT THE MEETING SCENE

The Meeting Scene e-newsletter of the Materials Research Society (MRS) presents news from MRS and other conferences directly from the conference venue.

The Meeting Scene is edited and compiled by [Dr. Gopal Rao](#), Web Science Editor, Materials Research Society. Additional contributors include Dr. Eugenia Kharlampeva, Georgia Institute of Technology.

Eugenia Kharlampeva, under the Apprentice Science Reporter program, is supported by the IMI Program of the National Science Foundation under Award No. DMR-0843934, managed by the International Center for Materials Research, University of California, Santa Barbara, USA.

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## ACNS 2010 Meeting Scene 3



Ottawa, ON, Canada  
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ACNS 2010



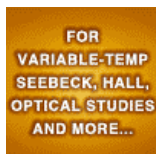
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### [DAYS 3, 4: Tuesday, Wednesday June 29-30](#)

The [2010 American Conference on Neutron Scattering](#) (ACNS 2010) concluded on Wednesday, June 30, in Ottawa, Canada. The conference banquet was held Tuesday evening. The major event on Wednesday morning was a plenary session including four talks. After the conclusion of the conference, a tour of Chalk River Laboratories was organized for attendees.



*Banquet*

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*Ottawa's majestic Fairmont Château Laurier hotel, venue of ACNS 2010. Born in the age of grandeur in 1912, it has hosted a number of well-known people over the years. With its commanding presence in downtown Ottawa next to the parliament building and displaying a green copper roof line, it has been dubbed the "Third Chamber of Parliament" of Canada.*

#### ■ Plenary Lectures

##### **45 Years of Neutron Scattering at ORNL**

**Herbert A. Mook, 2010 Clifford G. Shull Prize Lecture**



The first plenary lecture on Wednesday was presented by Herbert A. Mook Jr. of Oak Ridge National Laboratory (ORNL), one of the pioneers in the field of neutron scattering. The talk was in recognition of his 2010 Clifford E. Shull Prize awarded by the Neutron Scattering Society of America (NSSA) in June 2010. The prize is named in honor of Clifford E. Shull, the 1994 co-winner of the Nobel Prize in Physics, and to recognize high-impact neutron science research, as well as leadership in promoting the North America neutron scattering community. Mook completed his doctorate at Harvard University under the supervision of Clifford Shull (1994 Nobel laureate in physics). In his talk, he emphasized that Shull was wonderful to work for, had great insights and could get more physics out of a piece of data than anyone else.

His talk illustrated his outstanding contributions to the study of magnetism, superconductivity, and quantum phenomena in matter using neutrons. Mook started his career at ORNL in 1965, where he applied neutron scattering to investigate the interaction of magnetism and superconductivity. Over the years, he worked at the forefront of neutron scattering utilizing neutrons to study the nature of the magnetic structure and fluctuations in high-temperature superconductors using ORNL's High Flux Isotope Reactor. His research covers a variety of topics. In his talk overviewing 45 years of neutron scattering at ORNL, he discussed his results on magnetic excitations in transition metals and transition from magnetic to superconducting properties in rare-earth rhodium borides. He also highlighted his work on the nature of magnetic structure and fluctuations in '214' and 'Y123' high-temperature superconducting materials.

Mook served as the first scientific director of the Spallation Neutron Source from 1995-2000 and was the director of the Center for Neutron Science from 2000-2004. He was a recipient of the DOE Award for Outstanding Scientific Accomplishments in Solid State Physics, in 1982 and 1998. He has authored over 225 papers with a total of 9000 citations, holds several patents for neutron instrumentation, two of which have received R&D 100 Awards.

##### **Broken Symmetries of the Cuprate Pseudogap Phase Visualized by Spectroscopic Imaging STM and Detected by Inelastic Neutron Scattering**

**J. C. Seamus Davis**

Cuprate high temperature superconductors were discovered in the 1980s and over the past nearly 25 years have seen significant research and development. A detailed understanding of their electronic structures remains incomplete. In particular, a pseudogap phase is observed in the electronic phase diagram of the cuprates close to the superconducting regime, and it is essential to understand this pseudogap phase to get a clear understanding of this class of materials. In the second plenary talk on Wednesday morning, J.C. Seamus Davis of Cornell University described the use of scanning tunneling microscopy (STM) to visualize the pseudogap phase as well as the use of inelastic neutron scattering to investigate the pseudogap phase in cuprate superconductors. In particular, it is important to understand which electronic



symmetries are broken (nematic phase: rotational symmetries are broken; smectic phase: rotational and translational symmetries are broken) and what the associated order parameter might be.

Typically, STM cannot see the wave function in a material. Davis described a method that can be used to see the wave function using STM (spectroscopic imaging STM or SI-STM). He described the determination of an order parameter representing intra unit cell nematicity within each  $\text{CuO}_2$  unit cell. Focusing on the  $\text{BiSrCaCu}_2$  system, in the underdoped material, he demonstrated evidence for electronic nematicity of the states close to the pseudogap energy. He show how the methodology could be used to show that these phenomena arise from electronic differences

between the two oxygen sites within each unit cell. The excitations seen by inelastic neutron scattering and SI-STM in the pseudogap phase have the same origin, and they represent weakly magnetic states at the oxygen sites whose electronic structure breaks the  $90^\circ$  rotational symmetry. Thus, these investigations by Davis demonstrate that the pseudogap energies (states) can indeed be visualized and quantified yielding a much clearer understanding of the electronic structures of cuprate superconductors. Also, the study represents the first time topological defects, essentially dislocations in the electronic structure, have been viewed.

#### **Beauty Is Only Skin-Deep: Probing The Surface and Beneath by Neutron Reflection** **Charles Majkrzak**



The third plenary talk of the morning was presented by Charles Majkrzak (NIST). His talk was focused on phase-sensitive reflectivity to resolve the structures of nanometer scaled layered and patterned films. In contrast to conventional specular reflectivity which limits accuracy and special resolution, the phase-sensitive method yields a real-space picture without fitting or any parameters. In his talk, he discussed advanced neutron reflectometry and the theory for polarized neutron reflectometry which has led to the development of important new methods of data analysis. He illustrated how he designed, optimized, and made use of supermirror polarizers, integrating them into neutron instruments that attain very low backgrounds and consequently the highest signal-to-noise ratios. This point is crucial in achieving the widest possible wave vector range of data, thereby providing the highest spatial resolution and thus the most detailed and reliable structural information available.

He also highlighted his work on Gd/Y rare-earth multilayers that revealed an oscillatory exchange coupling spanning non-magnetic layers. This research provided the basis for interpreting similar effects in transition metal multilayers that exhibit giant magnetoresistance (GMR), which is now at the heart of present-day magnetic read heads in hard disk drives. His research on neutron reflectometry was also extended to surface-induced ordering of block copolymers and to the structures of biological and biomimetic membranes. In recognition of his extraordinary contributions to the field of neutron reflectometry and diffraction physics and for his pioneering work in the exploration of many issues in interface science, Majkrzak was awarded the Warren Award at the American Crystallographic Association Annual Meeting in Honolulu in 2006.

#### **Brighter and better... The Future of Neutron Sources and Instrumentation** **Ferenc Mezei**



For all the wonderful experiments carried out by neutron scientists, a critical aspect is the neutron source itself and the associated instrumentation. Ferenc Mezei, in the final plenary talk of the conference, described the development of neutron sources from a historical perspective and more importantly, current and future directions. Very recently, Mezei joined the European Spallation Source (ESS) secretariat, which will be constructing the next generation source in Lund, Sweden. Mezei is the originator of the ESS design concept, the long pulse spallation source. Starting with the neutron research universal

(NRU) reactor in Chalk River, Canada, which was the first dedicated neutron source, there has been tremendous progress, culminating in the recent achievement of 1 MW power by the spallation neutron source at Oak Ridge. However, this represents an instantaneous peak flux, and the time-averaged brightness remains lower than those of other sources.

Mezei described recent efforts in refining the source technology mainly by exploiting opportunities of complementarities and interplay between accelerator design and instrumentation approaches. He focused on the use of advanced mechanical neutron beam chopper systems to shape pulses, rather than through the use of accumulator accelerator rings and extensive, delicate neutron absorber structures in the target-moderator assembly. The advanced long pulse source ESS will be the first example of this next generation breakthrough in neutron source power, according to Mezei. The 5 MW ESS will have a linac+target station+100 neutron choppers. Also, a 15 MW long pulse source at the ESS is feasible if crucial issues such as cooling of the target and heat recovery can be solved. If realized, such a source will deliver 2 orders of magnitude greater flux compared to the highest flux reactors available currently.



#### ■ Chalk River Laboratories Tour



On the last day of the conference, Wednesday afternoon, attendees were invited to visit Chalk River Laboratories. The Laboratories accommodate major Canadian neutron facilities used for neutron research performed at the neutron research universal (NRU) reactor located there. The Laboratories are situated on the banks of the Ottawa River, in the upper Ottawa valley, Ontario. Approximately a 2 hour drive up river from Ottawa, the tour started at noon and took about 8 hours in total. The facilities consist of 100 buildings covering a square kilometer and employ 2,000 people.

Originally built after World War II for continued allied atomic research, the labs were a part of the National Research Council. In 1952 the laboratories' organization became a crown corporation "[Atomic Energy of Canada](#)." Today, the National Research Council - Canadian Neutron Beam Centre ([NRC-CNBC](#)) is a unique national science facility, and is a major resource for scientists. It has a strong international reputation and connects Canadian scientists to international collaborations with over 100 institutions in more than 20 countries during a typical five-year period. Since the 1950s, many hundreds of neutron scattering experiments have been carried out to solve practical problems for industry sometimes with multi-million dollar impacts, and pushing back the frontiers of human understanding of the world around us. Those experiments have contributed to the education of many hundreds of highly qualified people across the spectrum of science.

The major attraction of the tour was the [NRU Reactor](#), Canada's largest and most productive science facility. As well as the neutron scattering activities that CINS represents (pioneered by Canadian [Nobel Laureate Bertram Brockhouse](#)), the NRU reactor is the world's largest producer of medical isotopes, used to treat more than 21 million people in 60 countries each year. It is also the test-bed for Canada's nuclear electricity industry. Overall, the NRU reactor has made substantial contributions to the science, technology, energy, health and economy of Canada. However, built in 1952, the reactor is showing its age and has been shut down for a year for repair. Tremendous efforts have been carried out for the reactor to be up and running, and the reactor is expected to start an operational cycle at the end of July.

Visitors had also a chance to see the four neutron scattering spectrometers attached to beam lines at the NRU for experiments. NRU enables hundreds of experiments to be conducted every year on materials from ceramics to biological tissue, from steel to superconductors. At the end of the tour, NRU testing facilities were demonstrated to the visitors. The facilities are used in nuclear research and development, helping to build better electricity-producing reactors. Knowledge gained from the [test facilities](#) at NRU has been an essential foundation for developing the current fleet of CANDU power stations in Canada and abroad. These power stations are an important source of electricity for Canada.



#### ■ Technical Talks

##### Symposium C: Soft Condensed Matter



### *Neutron Reflectometry: From Model Biomembranes To Living Cells*

Understanding the nature of living cell membranes gives important information on cell interaction with the environment. Hillary Smith, who worked under supervision of Yaroslav Majewski (Las Alamos National lab), focused her talk on adhesion of living cells on surfaces followed by probing their structure with neutron reflectivity. The main questions to ask are if it is possible to measure a highly complex living biological systems with neutrons and if it is achievable to visualize the interface between the living cell and solid templates with a sub-nanometer resolution. Measuring living cells is challenging because of the complexity, disordered and inhomogeneous nature of the system, and difficulty to control and obtain the consistent surface coverage. Despite those challenges she demonstrated for the first time the feasibility to perform such experiment which thus providing a unique information about organization of protein in cell membrane which is not affordable with other techniques.

### **Symposium G: Engineering Applications**

#### *In Situ Deformation Studies of Nanocrystalline Materials*

It is now understood that nanocrystalline materials deform very differently from conventional materials that contain larger sized crystalline grains. In conventional crystalline materials, the Hall-Petch relationship is valid, wherein the yield stress increases with decreasing grain size due to reduced dislocation movement. Beyond a critical grain size in the nanoscale regime, however, an inverse Hall-Petch relationship is observed. Sheng Cheng of Oak Ridge National Lab and the University of Tennessee described *in situ* X-ray and neutron investigations to examine this deformation cross-over in Ni. Results showed little intergranular strains in nano-Ni under tensile deformation due to the lack of dislocation slip. However, a significant build-up of intergranular strains was observed in the nano-Ni influenced significantly by twinning. The results clearly confirm the cross-over behavior. In a separate investigation on fatigue deformation, Cheng described how fatigue deformation of nanocrystalline materials is different from that of conventional materials as well as computer simulation predictions. Significant grain growth was seen associated with fatigue cracks. This was speculated to be due to nano-grain rotation and consolidation.

#### *Effects of Overload, Underload During Fatigue-Crack Propagation*

An overload or underload introduced during cyclic loading can significantly retard or accelerate crack growth rate. Peter K. Liaw of the University of Tennessee described the use of neutron and electric potential measurements to investigate the effects of overloading and underloading (5 different loading conditions) of a Hastelloy (56Ni-23Cr-16Mo) alloy during fatigue loading. Neutron measurements were carried out with *in situ* loading. After a single overload or underload-overload, compressive stresses around the crack tip yielded large crack-growth retardation. After a single compressive underload, instantaneous acceleration of crack-growth rates occurred. Thus, distinct residual stress-strain profiles around the crack tip are closely related to different crack-growth behaviors under varying loading conditions. Neutron strain measurements and simulated lattice strain evolutions near the fatigue crack tips are in qualitative agreement.

### ■ Scanning the Conference

