FINAL REPORT

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The **2009 International Conference on Neutron Scattering (ICNS2009)** was held May 3-7, 2009 in Knoxville, Tennessee at the [Knoxville Convention Center](#). This meeting was under the auspices of the [Neutron Scattering Society of America \(NSSA\)](#). This is the 9th ICNS in the series of meetings beginning with ICNS '82 in Hakone, Japan, and following ICNS 2005 in Sydney, Australia.

As a scientific tool, neutron scattering, with its ability to probe length scales from atomic to microns and time scales down to picoseconds, is ideally suited to the study of a wide range of materials and problems in a variety of areas such as soft and hard condensed matter, biology, magnetism, engineering materials, chemical spectroscopy, crystal structure, and fundamental physics. With the unprecedented number of new and upgrade neutron source projects being undertaken around the world, this is a particularly good time to focus on the many recent advances in the field.

This meeting showcased the breadth of recent scientific results achieved through the use of neutron techniques as well as exciting developments in neutron related instrumentation from software to new source development. In this spirit, all aspects of the technique and applications of neutron scattering were discussed. **General topical areas** meant to be inclusive of the current diversity of the technique included:

- A. [Soft Condensed Matter](#)
- B. [Biological Sciences](#)
- C. [Condensed Matter Physics](#)
- D. [Chemistry/Earth Sciences](#)
- E. [Engineered and Applied Materials](#)
- F. [Neutron Physics](#)
- G. [Instrument Concepts/Techniques/Devices](#)
- H. [Sample Environment](#)
- I. [Software](#)
- J. [Facilities/Source Development](#)
- K. [Plenary](#)
- L. [General](#)

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Proceedings Information

The proceedings of the *International Conference on Neutron Scattering 2009* will be published in the **Open Access *Journal of Physics: Conference Series***. (JPCS) which is published by the **Institute of Physics Publishing** in the UK.

All papers published in JPCS are fully citable and upon publication will be free to download. JPCS is abstracted and indexed in Scopus, Inspec, and elsewhere. Citations to JPCS papers are tracked online using IOP Publishing's citing articles facility in addition to the full citation tracking facilities provided by Scopus. Authors may also like to know that in 2008 JPCS had over 1 million article downloads. ICNS 2009 papers will be peer-reviewed.

The funds provided by this DOE Grant supported:

- ✓ 10 invited speakers with travel awards of \$500/each
- ✓ 10 postdocs with travel awards of \$500/each
- ✓ 30 graduate students with travel awards of \$500/each

The total number of participants was 626, representing the following Countries:

✓ Argentina	1
✓ Australia	22
✓ Canada	17
✓ China	1
✓ Czech Republic	6
✓ Denmark	15
✓ France	39
✓ Germany	67
✓ Hungary	5
✓ Israel	1
✓ Italy	2
✓ Japan	38
✓ Korea	5
✓ New Zealand	1

✓ Norway	2
✓ Russian Federation	2
✓ South Africa	1
✓ Spain	5
✓ Sweden	11
✓ Switzerland	9
✓ The Netherlands	3
✓ United Kingdom	35
✓ United States	338

Scientists from 23 countries converged in Knoxville for ICNS 2009. The conference featured over 660 oral and poster presentations. A strong program of plenary, invited and contributed talks covered topics in biology, chemistry, materials science, engineering, soft matter, condensed matter physics, instrumentation, and fundamental physics – confirming the great diversity of science that is enabled by neutron scattering. During the poster sessions, authors were available for in-depth discussions of their research.

MEETING SCENE

DAY 1

MONDAY, MAY 4

"When nothing else can do the job, neutrons to the rescue...!"

- John H. Root, Keynote Speaker

The [2009 International Conference on Neutron Scattering](#) (ICNS2009) is being held from May 3rd through the 7th, 2009, in Knoxville, Tennessee. This is the 9th ICNS in a series beginning with ICNS 1982 in Hakone, Japan, and following the last ICNS 2005 in Sydney, Australia. The conference started on Sunday with a welcome reception in the evening. Monday morning saw the official opening of the conference with a keynote talk, followed by two plenary lectures. Technical sessions commenced on Monday afternoon with symposia A, C, D and H holding sessions. A visit to the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR) at the Oak Ridge National Laboratory was organized in the evening.

OPENING SESSION

The conference officially opened on Monday morning with a welcoming session. Gregory S. Smith (Oak Ridge National Laboratory), conference chair, first welcomed everyone to Knoxville, Tennessee. Simon Billinge, also a conference chair and vice-president of the National Scattering Society of America (NSSA) then presented a few remarks. He mentioned that there were 616 registered attendees from 29 different countries, with 219 oral presentations and 303 poster presentations scheduled for the week. He also mentioned the significance of neutron science and the broad applications of the field to science. He indicated that it is important to keep the societal impact of neutron science in mind.

(left to right) Gregory Smith, Simon Billinge and Bruce Gaulin

The president of NSSA, Bruce Gaulin, followed with his welcoming remarks. He described the various recent advances in neutron facilities and tools. He mentioned that 1 MW operation of the SNS was now imminent, which the neutron scattering community has been waiting for eagerly. Various facilities around the globe are seeing advances, including newer facilities planned in places such as China. He concluded that there has never been a better time to be a member of this scientific community.

ORNL Director Thomas Mason

Thomas Mason, Director of ORNL, then presented a welcoming talk. He said that the present group is at the heart of neutron science and makes things happen at the facilities end, though the various users are from the broader scientific community. He emphasized the obvious importance of energy today for society, which he described to be an over-constrained problem. Most of the issues of concern in the energy arena are materials problems. For ORNL, this is the essence of all the funding that has been put in place. The neutron scattering community is a critical part of the energy solution and he urged the community to reach out to the broader scientific community. He mentioned the heritage of the SNS and HFIR which go back to the original graphite reactor at ORNL, the first operational reactor after the "Chicago pile." He concluded by indicating that by doing difficult things, we not only accomplish a lot but also in unexpected areas and ways.

Roger Pynn, Bruce Gaulin and John Root

KEYNOTE LECTURE - JOHN H. ROOT

Reflections on the International Neutron Scattering Community

John Root, Director of the Canadian Neutron Beam Centre at Chalk River Laboratories, presented the Keynote lecture of the conference. He said that the purpose of his talk was to start a discussion within the neutron scattering community - those gathered here. He first overviewed the neutron scattering facilities around the globe including recent advances and enhancements. He then said that all this progress was quite encouraging. However, let's take a step back and be sure we are seeing the whole picture, said Root. He mentioned that this was a chance for some audience participation. First, several facilities have been closed in recent times. He asked those whose primary neutron laboratory was closed, from 1998 up to now to stand up. He then asked those who were concerned that resources are not adequate and may be frequently asked to

compromise the original vision for their facility to stand. Finally, he asked those concerned about the health of neutron scattering in the coming decade to stand. At the end of this exercise about 30-40% of the audience was standing. He asked everyone to look around and let the message sink in. The challenge now, he said, is how to identify those possibilities that can build and sustain a strong international neutron scattering community for decades to come.

Root then asked the question, "How can we make the value of neutron scattering into 'common knowledge'?" He asked audience members to describe in a sentence their expectations for people/facilities, impact on science, and impact on society, outreach and global networking. One comment for example was "Science is an investment and not an expenditure." Several people urged members to communicate the field more broadly to the general public in order educate them that neutron science affects them in many ways that they may not know about. He concluded by posing the questions: "How can we make the value of neutron scattering into 'common knowledge'? What "common knowledge" would we like to see ...? How shall we position our facility missions for maximum impact? What can we do to rejuvenate and strengthen neutron scattering competencies outside our facilities?" He urged everyone to talk about these during the course of the conference.

PLENARY LECTURE - TONYA KUHL

Neutron and X-ray Reflectometry and Grazing Incidence Diffraction Studies of Single Phospholipid Membranes

Understanding the nature of living cell membranes gives important information on cell interaction with the environment. Tonya Kuhl of the University of California, Davis, focused her plenary talk on supported lipid bilayers as model systems for cellular membranes. The amphiphilic properties of lipids facilitate their organized assembly into bilayer structures in aqueous environments. One of the interesting properties of the membranes is their ability to provide diffusion of individual components which create functional microdomains and accommodate membrane-interacting protein complexes.

Kuhl demonstrated that precise structural characterization of the membranes allows for a comprehensive understanding of the membrane organization and properties. In this respect, neutron reflectivity is a unique tool for probing membrane structure and mechanism of protein-lipid interactions as a critical step toward understanding protein-lipid interactions at a sub-nanometer resolution. With the help of neutrons, she found that the supported single membranes are identical in structure to lipid multilayers. X-rays were also utilized as a complementary technique to investigate the molecular arrangements and correlation length within the membranes.

Kuhl was also interested in probing the internal structure of polymer-cushioned bilayers. She found that the polymer cushions can be made of pH or temperature responsive polyelectrolytes such as PAA or PNIPAM. Moreover, she illustrates patterned polymer cushions as templates for lipid bilayers. Finally, she demonstrated that supported membranes are potential materials for bio-sensor applications. For example, the designed membranes on responsive cushions might direct protein diffusion to a specific location in response to an applied trigger, such as an eclectic field, followed by protein crystallization at the location.

PLENARY LECTURE - OMAR YAGHI **Reticular Chemistry**

Reticular chemistry is the stitching together of molecules via strong bonds to form networks. Omar Yaghi (Univ. California, Los Angeles) described using reticular chemistry to form metal-organic frameworks (MOFs) wherein inorganic joints are linked together by organic struts to yield various structures (nanoparticles) which can have very large surface areas within. For example, a 25 Angstrom cuboctahedron can be constructed from twelve $\text{Cu}_2(\text{CO}_2)_4$ paddle wheel units forming porous metal-organic polyhedral. The system is very versatile and one can form 3-D networks.

He then described MOF-5 [$\text{Zn}_4\text{O}(\text{O}_2\text{C}-\text{C}_6\text{H}_4-\text{CO}_2)_3$] which is formed from zinc acetate, and which is permanently porous forming iso-reticular series. The material yields a surface area of $3300 \text{ m}^2/\text{g}$. One of the motivations for the present work is hydrogen storage and this porosity level and volume available make this class of materials a strong candidate for this application. This has been demonstrated in several of these materials using volumetric and gravimetric measurements. Yaghi also presented kinetic profiles of hydrogen uptake and release proving that this is a viable possibility. He also described methane storage. Finally, he discussed the interesting possibility of CO_2 capture from a power plant or factory using MOF materials. He closed his talk by describing a new class of Zeolitic Imidazolate Framework (ZIF) materials. These allow for isorecticular covalent functionalization. In other words, a crystal can be used as a molecule.

TALKS

Symposium C: Condensed Matter Physics

Experimental and Theoretical Studies of the 4f Hybridization Across the (La,Ce)In₃ and CeRhIn₅-xSn_x Series

Olivier Gourdon (Juelich and SNS) described an investigation on 4f Hybridization Across (La,Ce)In₃ and CeRhIn₅-xSn_x Series. Using a combination of high resolution neutron and X-ray diffraction, refinements of the crystal structures of a series of $\text{La}_{1-x}\text{Ce}_x\text{In}_3$ ($x = 0.02, 0.2, 0.5, \text{ or } 0.8$) intermetallic compounds emphasize atypical atomic displacement parameters (ADP) for In and the rare-earth sites. These deformations have been understood by theoretical techniques based on band theory and are the result of hybridization between conduction electrons and 4f-electrons.

Symposium D: Chemistry/Earth Sciences

Negative Thermal Expansion and Local Structure in Ultra-Flexible Framework Materials

Andrew Goodwin of Cambridge University described highly flexible framework structures using extended linear molecules as bridging ligands and the unusual phenomena demonstrated by these, with specific focus on the negative thermal expansion (NTE) characteristics. While there is interest in such materials for applications such as in spacecraft, Goodwin suggested that there is more interest in the basic science. He described the ZrW_2O_8 and the $\text{Zn}(\text{CN})_2$ linkages in the framework structures. The total scattering technique using neutrons is very useful and the pair distribution function (PDF) can be calculated. This has been

shown to be used to calculate EXAFS and TEM structures accurately. In NTE cyanides, peak widths in the PDF contain information on interaction energies between neighboring atoms. Goodwin then focused on the $\text{Ag}_3[\text{Co}(\text{CN})_6]$ compound. He concluded by indicating that in thermodynamics of flexibility, extreme flexibility can amplify the role of low-energy interactions, the dominant thermodynamic energy scale can be orders of magnitude lower than in "normal" materials, and these results allow for design of materials with attractive thermomechanic and elastic properties.

Negative Thermal Expansion in a Coordination Framework

Vanessa Kate Peterson (The Bragg Institute, ANSTO, Australia) continued the theme of negative thermal expansion for the 3-dimensional coordination framework $[\text{Cu}_3(\text{btc})_2]$ where $\text{btc} = 1,3,5$ -

benzenetricarboxylate. This structure consists of octahedral supramolecular cages that link through their vertices to form a cubic framework with a Pt_3O_4 net containing distorted square units (paddlewheels) and regular planar triangular units. The NTE behavior was thought to involve transverse vibrations of the btc units coupled with rotation of the paddlewheels. Inelastic neutron scattering along with molecular dynamics simulations indicated that NTE in this material arises from local relief of framework frustration through distortion of the paddlewheel units leading to a distribution of paddlewheel arrangements. While the undistorted paddlewheel arrangement is the lowest overall energy arrangement, some groups of energy levels are lower in the distorted arrangement. In summary, the NTE in this material is more complex than for other known systems.

Towards High Impact, High Throughput Chemical Crystallography With Neutrons

Alison J. Edwards (The Bragg Institute, ANSTO, Australia) in her talk first described chemical crystallography as those materials included in the Cambridge crystallographic database (CCDC) which continue to grow at an increasing rate. However, neutron single crystal studies in the CCDC have been decreasing recently. She speculated that perhaps there are a large number of unpublished results as for X-ray determinations. She also discussed trends in papers published in journals and suggested that there are fewer chemists routinely pursuing neutron diffraction studies. She then discussed the new Laue diffractometer KOALA in her facility. The first data collection was done in June 2008. She described using the instrument to determine the "simple" structure of $\text{Zn}(\text{CN})_2$.

VISIT TO THE OAK RIDGE SPALLATION NEUTRON SOURCE FACILITY

Some of the attendees visiting the Oak Ridge Spallation Neutron Source (SNS) facility

DAY 2 **TUESDAY, MAY 5**

The [2009 International Conference on Neutron Scattering \(ICNS2009\)](#) completed its second full day of technical sessions in Knoxville, Tennessee. The day's activities included the poster session

and reception in the evening, the exhibit and the presentation of the 2009 Walter Hälgl Prize of the European Neutron Scattering Association (ENSA) to Dieter Richter in the evening.

PLENARY LECTURE - ALBERTO PODJARNY

New Biological Perspectives for Neutron diffraction: X+N studies of Perdeuterated Aldose Reductase and Antifreeze Protein “tiny” Crystals

Alberto Podjarny (Structural Biology and Genomics, IGBMC, CNRS, France) presented the first plenary talk of the day, and the third of the conference, on protein neutron crystallography. Protein neutron crystallography is a potent tool for the visualization of hydrogen (or deuterium) atoms and water orientations, which is crucial for many biological processes. However, it has historically been limited by the need for large crystals. Recent advances and improved sources now allow for smaller crystals ($\sim 0.1 \text{ mm}^3$) to be measured with shorter exposure times. Podjarny then presented two specific examples.

The first example was human Aldose Reductase, which is a redox enzyme involved in complications related to diabetes. The enzymatic reaction catalyzed by the Aldose Reductase involves a hydride donation from the NADPH coenzyme and a proton donation from the enzyme. The enolate is reduced by the proton from the enzyme to $-\text{CH}_2\text{O}$. Determination of the residue donating this proton is essential for understanding the catalytic mechanism. Ultra high X-Ray resolution structure determination provided a very detailed description of the ordered part of the protein but hydrogen visibility remained weak, especially for mobile ones. *Ab-initio* full deuteration allowed for neutron diffraction at a useful resolution ($2.2 \text{ \AA}$) with a radically smaller crystal (0.15 mm^3). Joint refinement of the X-ray and neutron data (X+N) improved the quality of the neutron diffraction maps. The neutron diffraction structure determination validated the presence of a neutral Lys77, a key feature for the quantum analysis of the enzymatic mechanism (PNAS, **105**, 1844-1848, 2008).

The second example described by Podjarny was an antifreeze protein (AFP) in fish. *Macrozoarces Americanus* is an arctic fish which produces a type-III AFP that lowers the freezing temperature of its blood fluids by binding to ice crystal nuclei. This binding is defined by the interactions, either H-bonds or van der Waals (VDW) bonds, of the protein with the water molecules in ice faces. While several models have been previously proposed for these interactions, it turns out that neutron crystal structures can provide accurate positions and orientations of water molecules interacting with AFP. This is work still very much in progress. Podjarny indicated that complete deuteration of AFP highlights the possibility of collecting accurate neutron data from small crystals ($V : 0.13 \text{ mm}^3$). They observed an ice-type tetrahedral water (W) cluster (W-W distance $\sim 2.7 \text{ \AA}$), forming both H-bonds and VDW contacts with the ice binding surface (IBS), in clear distinction with other

water clusters away from the IBS (W-W distance ~ 3.3 Å). The researchers are currently analyzing the implications for the ice binding mechanism.

Finally, Podjarny presented some perspectives for the near future. Protein Neutron Crystallography is now able to produce high quality structures with smaller crystals. However, long exposure times (in comparison with synchrotron X-Rays) are still limiting access for the biological community. This will evolve with the upcoming high flux spallation sources and associated beam lines, which should reduce the exposure times by another order of magnitude. These new instruments will also allow measurements of crystals of larger proteins with larger unit cells. In this case, Protein Neutron Crystallography should become the tool of choice for biological problems involving protonation states and/or water position and orientation. Another important use of neutron crystallography is H/D labeling, which offers unique capabilities for locating specific components in a crystal. This has already been done, notably for membrane proteins, and its use should increase as more instrument time becomes available.

PLENARY LECTURE - CHUN LOONG

The Future of Neutron Scattering in China: Meeting Increasing Demand with New Facilities?

Chun Loong (Sun Yat-Sen University, Guangzhou, China) described current and near term efforts relating to neutron scattering facilities in China. He first described progress since ICNS 2005, current status, and future directions for China's three neutron-source projects. He then discussed user development and community outreach efforts, and finally the role of international interactions for the advancement of neutron research and development in China.

The first neutron facility described is the China Advanced Research Reactor (CARR) located just outside Beijing in Fang Shan. It has multiple purposes but the primary one is as a user facility for fundamental R&D and neutron scattering. It is expected to go critical in 2009. However, one issue is that the cold source is not ready and will take two years to be completed. The second facility is the China Spallation Neutron Source (CSNS), which will be located in Dongguan in Guangdong province. It has the staunch support of the Guangdong government and the Chinese Academy of Sciences and has received generous international assistance. There are several issues of concern including a very tight budget (low contingency, funding only available for 3 instruments), lack of expertise in Guangdong, requiring the dispatch of a sizable committed workforce from Beijing (at least in the beginning years), and a relatively under-developed neutron user community (especially in south China). The third facility described by Loong was the Tsinghua Hadron Accelerator Research Center (THARC) that includes a Compact Pulsed Hadron (Neutron) Source (CPHS) in Phase I, expected to be completed in three years. This will be located near Beijing close to Tsinghua University.

Loong discussed user development and community outreach activities. In terms of potential users, about 30 research groups from universities and labs have been identified, including their neutron-related research topics, priority of desirable neutron instruments, etc. The estimated user utilization of the CSNS at the time of completion with 3 instruments is 30-40 groups, ~60 expts/year with a full suite of 17+ instruments with ~500 experiments/year. In terms of international cooperation, as the 3 neutron-source projects progress, they look forward to expanding international interactions, particularly accepting Chinese graduate students (short stays and PhD studies), accommodating university researchers from China to engage in neutron experiments and instrument development, working to establish a 'China Neutron Science Society' and then to join the Asia-Oceania Neutron Scattering Association (AONSA).

Finally, he touched upon the topic of recruiting young talent. After the boom in expansion of academia in the nineties, most university and government lab positions are currently filled. Many overseas Chinese scientists are discouraged by the difficulty in getting a faculty position in China. However, this is not the case in the field of neutron/accelerator research, said Loong. The construction, operation, and continuing upgrade of the neutron/accelerator facilities, and more importantly the growth of academic research using neutrons, will create ample employment opportunities. They, in particular, are attempting to recruit overseas Chinese researchers in the field.

TALKS

Symposium A: Soft Condensed Matter

Structural Studies of the Adsorption of Macrocyclic Ligands at the Air-water and the buried Oil-water Interface Using Neutron Reflectometry

Water-oil interfaces present significant interest for both fundamental and application studies. Research on this topic involves various phenomena, such as transport properties of cell membranes, stabilization of emulsions, mixed surfactants-cold water cleaning, and protein adsorption. Understanding the fundamental aspects of the processes at liquid-liquid interfaces is crucial for a number of applications, for example in phase-transfer catalysis and extraction-based techniques. In his talk, Ali Zarbakhsh (University of London, UK) focused on examining structural conformations of macrocyclic ligands upon their adsorption at air-water interfaces. The cationic macrocyclic ligands such as crown ethers and their derivatives have been used as transport carriers in extraction-based techniques. What is more important, he was able to probe the structure of the ligands at the buried oil-water interfaces by applying neutron reflectivity.

Breathable Polymer with Tunable Hydration Cushions Model Biomembrane

Michael Jablin (Los Alamos National Lab) presented a polymer cushion as a temperature responsive template to support lipid bilayers in a liquid environment. The cushion is made of a

temperature-responsive pNPAM capable of a reversible five-fold change in thickness in the 25-37°C temperature range. In addition, the content of water within the cushion can also be tuned *in situ* between 65-93 vol%. The swelling-deswelling nature of the polymer support is very attractive for applications in developing biologically relevant cellular-like membranes. Also, the hybrid system was shown to be stable for more than two weeks and allows liquid access to the lipid bilayer on both sides. Overall, the system is robust, easily prepared, tunable, and proposed to mimic extracellular matrix, which is crucial for membrane-based biosensors.

Determining the response of surface-bound polymers under shear via neutron reflectivity

The goal of this research by Leslie Sasa (Univ. California Los Angeles) is to use a cone and plate neutron stroboscopic rheometer and neutron reflectometry to test the de Gennes grafted polymer theory, which describes the coupling between the dynamic response of the grafted polymer to that of the bulk material under shear. This principle can be explained by the entanglement and disentanglement of the grafted polymer from the bulk material depending upon the shear rate. Preliminary results using both PDMS and PS are qualitatively in agreement with the de Gennes theory, and provide new information on the structure and dynamic behavior at the molecular and nanoscales of grafted polymers under shear stress.

Symposium B: Biological Sciences

Making sense of order and disorder in a transcription factor

The problem of plasmid replication is of great interest in biophysics, as described by David Jan Scott (University of Nottingham, UK). The transcription factor KorB is central to both transcription repression and partition in IncC plasmids. Still, the investigation of KorB structure is a very challenging task because the dimeric protein has zones of order and intrinsic disorder along its length. Scott demonstrated that applying SANS and SAXS makes it possible to resolve the structure not only of the full length protein but also of its interaction with other biomolecules. He found the constructs to be monodisperse and have unfolded character. However, KorB changes its conformation in the presence of an activator KorA and upon interaction with DNA. In particular, KorB has a compact structure, but it tends to extend when forming a complex with KorA. Scott mentioned that the next step would be to study molecular dynamics of the protein-protein interactions. The presented results significantly contribute to the understanding of the dual role of the protein in repression and partition.

Mechanistic insights into the Phosphotriesterase mechanism from the neutron structure of DFPase

Diisopropyl fluorophosphatase (DFPase) from *Loligo vulgaris* is an enzyme capable of detoxifying a wide range of organophosphorus compounds. Despite the importance of the process, the exact mechanism is poorly understood. The main focus of Julian Chen's (Institute of Biophysical Chemistry, Germany) talk was to clarify how DFPase works. He applied neutron crystallography

and successfully resolved the protonation states of amino-acids and solvent molecules in the active site of DFPase. He found the absence of metal-assisted water activation in the reaction and that amino acid 229 as a nucleophile to play a critical role in the reaction. He also studied H/D exchange and found it to be very pronounced in the amide backbones and in the tunnels but very poor in beta strand amides. The main outcome from his finding is that they allow engineering an improved version of DFPase with enhanced anti-toxic activity.

Symposium C: Condensed Matter Physics

Neutron Scattering Studies of Graphene

Discovered in 2004 by physicists at the University of Manchester, graphene has proved to be a material with extraordinary and very unusual electronic, optical and mechanical properties. Graphene is a two-dimensional crystalline form of carbon that combines properties of semiconductors and metals, creating a new class of materials. Its interesting properties (unusual electronic spectrum, very high mobility/low resistivity at RT, unique half-integer quantum Hall effect, high stability) translates into potential applications, from replacing silicon in electronic devices, spintronics, to reading the sequence of chemical bases in a DNA. The first detailed measurements of the vibrational spectra of both graphene and graphite using INS were presented by Alice (Acatrinei) Smith (Los Alamos National Laboratory) along with a neutron scattering study of hydrogen adsorbed on graphene. Graphene samples were produced in-house by thermal exfoliation, and characterized by means of XRD and TEM. FTIR and IINS measurements were collected for graphite, graphite oxide and graphene.

Symposium D: Chemistry/Earth Sciences

Structural and dynamical properties of Hydrazine Boranes and their use as hydrogen storage materials

The structural and dynamical properties of the promising hydrogen storage material hydrazine borane ($\text{N}_2\text{H}_4\text{BH}_3$) as well as several derivatives of it ($\text{N}_2\text{H}_4(\text{BH}_3)_2$, $\text{N}_2\text{H}_4\text{BF}_3$, $\text{N}_2\text{H}_4(\text{BF}_3)_2$) have been investigated using neutron powder diffraction and incoherent inelastic neutron scattering, as well as computational methods, as described by Thomas Huegle (Freie Universität, Berlin) in symposium D. Hydrazine boranes have remarkable hydrogen storage capabilities, and are interesting materials due to their hydrogen network and are a good example of donor-acceptor complexes. An insight into their electronic structure, based on charge density calculations, will provide useful information on the mechanism of hydrogen release.

Symposium E: Engineered and Applied Materials

Study of a New Promising Hydride Based on the Cu-Li-Mg System

A small addition of Li changes the orthorhombic structure of CuMg_2 (Fddd) to hexagonal $\text{CuLi}_x\text{Mg}_{2-x}$ ($x = 0.08$, P6222). In a presentation by Maria H. Braga (University of Porto, Portugal), the results obtained using two neutron powder diffractometers (NPDF and HIPPO) were compared with XRD data, and with first principles calculations performed to obtain the most stable composition of the ternary compound. Neutron diffraction data for CuMg_2 and Cu_2Mg were also obtained. Inelastic Neutron Scattering (INS) showed that cycling has a strong effect on the hydrogen absorption site in the lattice.

Next Generation Moderator Materials

A talk on new moderator materials was presented by Monika Hartl (Los Alamos National Laboratory), reporting on experimental total cross sections of potential moderator materials in comparison with theoretical calculations. First steps have been taken to develop more suitable scattering kernels for the new materials. Real life moderator tests have been carried out on several materials.

2009 WALTER HALG PRIZE

Every two years the European Neutron Scattering Association, ENSA, awards the prestigious Walter Hlg Prize to a European scientist for an outstanding programme of research in neutron scattering with a long term impact on scientific and/or technical neutron scattering applications. The Prize of 10,000 Swiss Francs is donated by Professor Walter Hlg, the founder of neutron scattering science in Switzerland. The 2009 Walter Hlg Prize was awarded in a special evening session to Professor Dieter Richter of the Research Center Jlich, Germany, in recognition of his coherent work towards understanding the dynamics of polymers and biological macromolecules using high-resolution neutron scattering techniques. Richter then presented an overview of his work over the years in his talk titled "Interdisciplinary Soft Matter" discussing soft matter dynamics. He specifically focused on the discovery of Neutron Spin Echo and the quest for higher

resolution. His take home message was "Science drives instrumentation and instrumentation drives science."

DAYS 3, 4

WEDNESDAY, THURSDAY, MAY 6,7

The [2009 International Conference on Neutron Scattering \(ICNS2009\)](#) concluded on Thursday, May 7, 2009, in Knoxville, Tennessee, after a successful run of five days of activities and technical sessions. The final event was a mixer followed by a closing plenary talk by Sunil Sinha (University of California, San Diego). The next American Conference on Neutron Scattering (ACNS) will be held in Ottawa, Canada, in 2010, while the next International Conference on Neutron Scattering (ICNS) will be held in Europe in four years.

PLENARY LECTURE - DAVID MANDRUS

A Materials Overview of the New Iron-Based Superconductors

Gold is for the mistress -- silver for the maid --
Copper for the craftsman cunning at his trade.
"Good!" said the Baron, sitting in his hall,
"But Iron -- Cold Iron -- is master of them all."
- Rudyard Kipling

The new class of iron-based superconductors has been very much in the news over the past year or so. David Mandrus (Oak Ridge National Laboratory) presented an excellent overview of these materials. Fe-based superconductors are very exciting because they represent a new family of high-T_c superconductors, they are the best model systems for unconventional superconductivity, and they represent a large materials space to look for new superconductors. Mandrus presented a brief history of these materials leading up to the report in early 2008 of 26 K superconductivity in F-doped LaFeAsO. The key feature of these materials is the square nets of tetrahedrally coordinated iron. Mandrus first discussed the 1-1-1-1 materials including the structure, theoretical density functional theory studies, and magnetic order. He then talked about 1-2-2 materials such as BaKFeAs. He finally discussed FeTe_(1-x)Se_x materials. He ended by indicating that lots of new materials will emerge in this broad class of superconducting Fe-based materials and the whole field has lots to offer to researchers involved in it.

PLENARY LECTURE - COLLIN LESLIE BROHOLM

Exploring Quantum Magnetism Through Neutron Scattering

Collin Broholm presented the plenary lecture on Thursday morning, on the last day of the conference. The subject of his talk was Quantum Magnetism; where do we find it, and why is it interesting? Ferromagnetism essentially is a fundamental and collective phenomenon. Quantum magnetism is inter-atomic singlet formation, macroscopic singlet formation, strong correlations without static order, emergent quantum particles. Broholm indicated that the fundamental question for the field is what types of collective phases are possible, and what are the corresponding quasi-particles. The elements of the research include materials synthesis (both bulk and nano-structured), advanced characterization and of course theory. In terms of applications, these systems represent model systems for quantum correlated physics. Other potential applications include sensors and filters via strong collective response and quantum computing by manipulating emergent quasi-particles. Neutron scattering plays an important role in many of these studies, as Broholm showed using a few examples. To summarize, quantum magnetism goes beyond spin to collective quantum correlations. It is stabilized by low dimensionality, frustration, and proximity to metal insulator transitions.

CLOSING PLENARY LECTURE - SUNIL SINHA

Neutron Scattering: Accomplishments, Challenge and Outlook for the Future

Sunil Sinha (University of California, San Diego) presented an outstanding closing lecture outlining the current state of the field of neutron scattering. There have been tremendous accomplishments in the field such as antiferromagnetic structures, rare earth spirals and spin structures, magnetism and superconductivity etc., as well as in soft matter. More recent accomplishments include quantum phase transitions, magnetic order and magnetic fluctuations in high-Tc cuprates etc. He then presented the competition - synchrotron X-rays, scanning probe microscopies, direct imaging. He strongly made the point that though several of the advances and accomplishments in neutron scattering are tremendous, it is very difficult to convey this visually to the scientific community and to the general public as compared to other techniques yielding beautiful images and videos. He noted that synchrotron X-rays and neutrons can be complementary rather than competing because of their unique advantages in different ways. He

presented the example of nanomagnetism with X-rays, imaging and neutrons all yielding different but significant information.

Sinha then made the connection to usefulness of the field to society including in areas such as energy, environment, health, security, culture. In terms of training young scientists in the field, he suggested that it is better to have several smaller neutron sources in addition to one "supersource," where they get a chance to try out different techniques and instruments before going on to the large sources. Finally, he reiterated the point made on the first day of the conference in needing to "sell" neutron scattering to the general public. This was an appropriate plenary talk by a stalwart in the field to end the conference on a high note.

TALKS

Symposium A: Soft Condensed Matter

Structure and Dynamics of Polymer Electrolytes

Lithium-ion batteries are extremely popular today -- they are some of the most energetic rechargeable batteries available. They can be found everywhere - in iPods, laptops, and cell phones. Janna Maranas from Pennsylvania State University presented an investigation on the solid polymer electrolyte PEO/LiClO₄ which can be used as a conductive material in lithium-ion batteries. PEO is a wonderful choice since it is non-toxic, highly flexible and mobile at room temperature. In the talk, Maranas discussed the relationship between PEO structure, mobility and ionic conductivity. At the eutectic point composition in PEO/LiClO₄, fluctuations occur which introduce a configuration reminiscent of the PEO6 crystal structure. This structure has high conductivity at low PEO molecular weight, although the formation of a lamellar morphology at high molecular weight disrupts long range transport of lithium ions. She showed that this structure formed via fluctuations, and contributes to conductivity. If the fluctuations are stabilized, either by a small amount of the pure PEO crystalline phase, or by nanoparticles, the conductivity is enhanced. Both of these modifications do not influence segmental dynamics of the polymer, which is normally associated with lithium transport. Instead, rotation of the PEO6 structure is altered in the presence of pure PEO crystals or nanoparticles.

In-Situ Structural and Rheological Investigation of Fully Hydrated Fibrin Gels formed in D2O buffers

Fibrinogen is a protein crucial to the formation of blood clots. In the presence of the protein thrombin, fibrinogen is converted into fibrin which then self assembles into a network of interconnected fibers. Like other biopolymer matrices the resulting hydrogel exhibits unique mechanical properties, for example the fibrin gel stiffens upon application of sufficient shear stress. Kathleen Weigandt, a graduate student from the University of Washington demonstrated

that using a combination of small angle neutron scattering and various rheological techniques, she can determine the origin of the strain dependent rheological properties of fibrin gels. She also showed in her talk that the strain-hardening of silk is reversible and very sensitive to the protein concentration.

The Couette configuration of the Neutron Stroboscopic Rheometer for the investigation of entangled polymers in the bulk under shear via small-angle neutron scattering

The Couette configuration of the Neutron Stroboscopic Rheometer (CNSR) has been constructed at the Los Alamos Neutron Science Center (LANSCE) to examine the molecular steady-state and dynamic responses of entangled polymeric materials in the bulk to the application of shear stress via small angle neutron scattering (SANS). This was described in a talk by Eric Yearley (Los Alamos National laboratory). The SANS measurements along with the implementation of the CNSR will provide new information on the structure and dynamic behavior at the molecular and nanoscales of polymers under shear stress. SANS results of the highly viscous sample, bulk polystyrene, are presented. The tube model for entangled polymers in the bulk suggests that the disentanglement and elongation of polymer chains due to external stress may be responsible for their unique rheological properties including shear-thinning. The observed anisotropic neutron scattering pattern of the polystyrene melt above entanglement provides evidence that the conformation of the chains are elongated in the direction of the melt flow in agreement with the current tube theories concerning linear polymers in the bulk.

Symposium B: Biological Sciences

Collective Molecular Dynamics in Membranes and Proteins

Understanding of molecular dynamics and mechanisms of functioning of biological membranes is one of the important questions in molecular biology and biophysics. Indeed, a cell membrane has a very complex structure and presents a primary side of interactions. In this respect, Maikel Rheinstadter from McMaster University (Canada) presented new fundamental insights into membrane functioning and protein-protein interactions. He addressed several important questions in his talk. For example, he described dynamics between molecules in membranes to be “multi-scale” with a large range of length (from microscopic to mesoscopic) and time scales. He also illustrated how membrane composition determines dynamics and membrane properties. Applying inelastic scattering measurements he studied membrane permeability and elasticity. Based on his study he found that even in simple models, biological systems present an array of units interacting through coherent interactions indicating that coherence is a fundamental property in molecular biology.

Symposium C: Condensed Matter Physics

Neutron Diffraction Studies of Negative Thermal Expansion in Metallic Conductor ReO₃

Metals generally have high coefficients of thermal expansion. Conversely, highly covalent materials such as diamond show low thermal expansion, and other insulating materials such as ZrW₂O₈ even exhibit negative thermal expansion (NTE). ReO₃ appears to be unique in that it is the only known 'simple metal' which exhibits isotropic NTE behavior. The metallic conductor ReO₃ exhibits both negative and positive thermal expansion, and past studies have varied significantly on the temperature regime at which NTE or PTE are observed. Time-of-flight (TOF) neutron diffraction and specific heat studies of various samples of ReO₃ were presented in this report by Efrain Rodriguez (University of California, Santa Barbara) to explain the observed discrepancies in past studies.

Local and Average Structures of the spin Glass Pyrochlore Y₂Mo₂O₇ from Neutron Diffraction and Neutron Pair Distribution Function Analysis

Pyrochlore oxide was investigated by means of temperature dependent neutron diffraction and neutron pair distribution function in order to solve the issues of positional disorder and frustration in the compound, as described by Delphine Gout (Oak Ridge National Laboratory). The measurements showed no crystallographic phase transition over the temperature range studied, the principal source of disorder comes from the Y-O1 atom pairs instead of the previously considered Mo-Mo pairs, data fit improves significantly as anisotropic displacements for all sites are considered, and becomes worse as temperature decreases.

Symposium D: Chemistry/Earth Sciences

Hydrogen Storage in Microporous Materials

Energy is obviously a major issue currently and in the near-term. Hydrogen of course has been touted to be an important solution to the problem, and in fact hydrogen-fueled automobiles are already making an appearance. The US Department of Energy has placed a grand challenge in terms of targets for hydrogen storage materials FOR 2010, 2015 and beyond including gravimetric and volumetric capacities. Craig Brown (NIST) in his talk on Tuesday described microporous materials for hydrogen storage and ways to improve storage capacities. These include optimized pore size (high specific areas), catalytic spillover of hydrogen, exposed metals and substituted/dopant materials. Brown showed that neutron methods are crucial for these attempts at understanding the performance of materials, including powder diffraction, vibrational and rotational spectroscopy and quasi-elastic scattering. Some of the materials discussed included MIL-53, Mn-BTT and the metalorganic framework, MOF-74. Flexible frameworks provide interesting new avenues for optimized pore sizes. Also, for MOFs with coordinative unsaturated metal centers, the metal is the primary hydrogen absorption site and the hydrogen tends to lie down on the metal, the rotational dynamics are quasi-2D and there is no H-H bond elongation, and the enhanced interaction is primarily Coulombic. The presentation clearly validated the advantages of using neutron-based techniques for microporous materials.

Symposium E: Engineered and Applied Materials

Revealing the Unseen: Residual Stress Characterization of a Fabrication Weld from the Victoria-Class Submarine Pressure-Hull

The HMCS Victoria is a Canadian Navy Victoria-class submarine that was obtained from the British Navy and was formerly the HMS Unseen. When the submarine reached Canadian docks, a largish dent was observed in one panel. This section was removed in the dry dock and this section contained a length of circumferential-seam closure weld. This has allowed for the rare opportunity for detailed characterization of the as-fabricated condition of this common weld type from the original vessel assembly. Ron B. Rogge (Canadian Neutron Beam Center, Chalk River,

Canada) described neutron diffraction studies to study this weld structure. Neutron diffraction is able to yield 3-D characterization of the weld and surrounding structure. The data indicated that the as-formed hull plate (no weld) showed internal tensile stress peaks of around 35% yield stress in both axial and circumferential directions. The circ-seam weld yielded near-surface peak tensile stress values of up to 80% yield stress with a slight dominance of transverse direction stresses. In addition, Rogge described new 3D visualization methods to help guide modeling activities and efforts to attenuate stresses by improved fabrication techniques. In a demonstration he asked the audience to view two dots cross-eyed so that they merge into three and then look at the visualization underneath allowing for 3-D visualization. He termed this his attempt at audience participation. The results of this study will be incorporated into numerical models supporting submarine mission-ops.

In-Situ Electric-Field Studies of Ferroelectric Ceramics Using Time-Resolved Neutron Diffraction on WOMBAT

Ferroelectrics can couple mechanical and electrical displacements as a result of their spontaneous polarization. They are used in a number of electromechanical applications. Many of these applications involve applied fields that are dynamic, with time-dependent dielectric displacement in response to a cyclic stress. The objective of the present study, described by Jacob L. Jones (University of Florida) was to evaluate a new commercial PZT material, EC-65, under the application of dynamic electric fields, in particular using neutron diffraction measurements. These were carried out using WOMBAT which is a high-flux neutron powder diffractometer at the new OPAL reactor at ANSTO, Australia, ideal for time-resolved studies, with stroboscopic data acquisition with 31 microseconds resolution. Ferroelectric/ferroelastic domain switching, tetragonal to rhombohedral phase switching and lattice strains were also measured. The response times of these microstructural mechanisms were found to be faster than the minimum acquisition window indicating that the ferroelectric material exhibits a very soft character with high domain wall displacement. Also domain and phase switching were found to be possible origins of macroscopic nonlinear piezoelectric coefficients in this material.

ABOUT THE MEETING SCENE

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