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The 8th American Conference on Neutron Scattering

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The 8th American Conference on Neutron Scattering

he 8th American Conference on Neutron Scattering (ACNS) was held July 10-14, 2016 in Long Beach California, marking the first time the meeting was held on the U.S. west coast. The unique venue for the conference was the Queen Mary hotel, attracting 285 attendees. The meeting was coordinated by the Neutron Scattering Society of America (NSSA) led by conference chair Patrick Woodward (The Ohio State University) and NSSA president Stephan Rosenkranz (Argonne National Laboratory) together with the local committee chair, Brent Fultz (California Institute of Technology). The overall conference organization was supported by the Materials Research Society.

The meeting schedule consisted of a morning common session containing an award presentation/ seminar and a plenary lecture. The remainder of the scientific program was made up of four parallel sessions including invited and contributed oral contributions together with poster sessions in the afternoon and evening. The science program was coordinated by program co-chairs Despina Louca (University of Virginia) and Alexi Sokolov (University of Tennessee) and included contributions in the following research areas: Sources, Instrumentation, and Software; Hard Condensed Matter; Soft Matter; Biology; Materials Chemistry and Materials for Energy; Engineering and Industrial Applications; Neutron Physics. Overall the program consisted of 8 award/ plenary talks, 33 invited talks, 168 contributed talks, and 65 posters.



Figure 1. Chuck Majkrzak receives the 2016 Clifford G Shull Prize from Patrick Woodward and Stephan Rosenkranz. © Mark Lumsden. Reproduced by permission of Mark Lumsden. Permission to reuse must be obtained from the rightsholder.

On the opening day of the meeting, there were two tutorials: "Neutrons in Biology" and "Discovering Diffuse Scattering Signatures—Means to Measure, Process Data and Pathways to Analyzing It" followed by a welcome reception.

The Monday morning session started with the presentation of the Clifford G. Shull Prize in Neutron Scattering to Charles F. "Chuck" Majkrzak (National Institute of Standards and Technology (NIST)) with the citation "For leadership in the development, application and establishment of neutron reflectometry as an essential measurement tool for nanoscale materials" (Figure 1). Majkrzak's presentation was entitled "Whatever have we learned from all those neutrons?" and started with a history of what led him into neutron scattering. He planned to become a high school Physics teacher and attended Montclair State Teachers College. There, he was encouraged by his mentors to attend graduate school where he enrolled at the University of Rhode Island with initial interest in physical oceanography. At Rhode Island, they had a small 2MW reactor where Majkrzak worked with Suren Malik and was soon hooked on neutron scattering, optics and instrumentation. He then moved to a post-doctoral position at Brookhaven National Lab (BNL), joining a research team that included Larry Passel, John Axe, and Gen Shirane studying the coexistence of magnetic order and superconductivity, critical phenomena, and graphite



Figure 2. The 2016 class of NSSA Fellows. Present at the meeting were (L to R): John Copley, Pengcheng Dai, Jaime Fernandez-Baca, Brent Fultz, Aaron Krawitz, Jaroslaw Majewski, and John Root. Not present were Michael Crawford, Timothy Lodge, Ramanan Krishnamoorti, and Stephen White. © Mark Lumsden. Reproduced by permission of Mark Lumsden. Permission to reuse must be obtained from the rightsholder.

intercalation. At BNL, Majkrzak was again encouraged by his mentors to develop his own area of specialization and began working on supermirrors and supermirror polarizers. At the same time researchers at Bell Labs and Juelich were creating some of the first high quality superlattice films. Majkrzak partnered with those researchers and began his studies of thin films and interfacial magnetism. He also started to combine neutron and x-ray studies to develop full understanding of magnetic multilayers using both low and high angle scattering. This led him to study coupling of magnetic moments across rare earth interfaces, which was explained in terms of the RKKY interactions.

Later Majkrzak moved to his present position at the NIST Center for Neutron Research (NCNR) where he began to build a dedicated neutron reflectometer. A measurement of the neutron reflectivity as a function of the wavevector transfer can yield the in-plane average of the scattering length density. While the Born approximation used in many scatter-

ing applications breaks for reflectivity, the profiles can be understood in terms of a 1-d Schrodinger equation. Over the years several reflectometers were built to improve and refine the technique leading to the most recent NIST instruments ANDR, used to study biological systems, and CAN-DAR, using a polarized polychromatic beam and optical imaging. Along with Norm Berk at NIST, Majkrzak also pioneered the use of reference layer films to provide information about the scattering amplitude which in turn may be used to invert the reflectivity data. The techniques that he pioneered have enabled advances in many diverse fields such as polymer science, magnetism in magnetic multilayers, biology, electrochemistry, and photovoltaic materials. Even with the advances in other techniques such as fluorescent optical microscopy and synchrotron x-ray techniques, there are many remaining problems where neutron reflectometry provides unique and complementary information.

The Shull prize presentation was followed by a plenary lecture by

Alan Tenant, Oak Ridge National Laboratory (ORNL) who presented his outlook for the next 10 years in neutron scattering in North America and in the world. It is challenging to plan the needs of the future in an environment where everything is evolving so rapidly, from the scientific problems to sources and instrumentation. Four recent national workshops on quantum materials, biosciences, energy materials and soft matter have helped in identifying the scientific challenges of the future. Workshop reports can be downloaded from http://neutrons.ornl. gov/grand-challenge-workshops. It is clear that neutrons are absolutely essential to address these challenges and new sources like the European Spallation Source and the proposed Second Target Station (STS) at the Spallation Neutron Source (SNS), ORNL will play a crucial role. Tennant explained the ORNL three source strategy to address these forefront problems. This consists of optimizing instruments for the strength of the facility: HFIR for applications which take advantage of the highest



Figure 3. Yun Liu receives the 2016 NSSA Science Prize from Patrick Woodward and Stephan Rosenkranz. © Mark Lumsden. Reproduced by permission of Mark Lumsden. Permission to reuse must be obtained from the rightsholder.

time-averaged flux, the first target station at SNS to take advantage of the sharp pulses and high brightness beams of thermal to epithermal neutrons, and the proposed STS to be optimized for high brightness of cold neutrons and a large dynamic range. Specifically, STS will provide the bandwidth and cold neutron intensity needed to address the challenges of complex hierarchical and mesoscale materials. An additional key component for neutron scattering in the future, particularly in cases of increased complexity, is integration with high-performance computing, simulation and modeling.

Prior to the prize/plenary lectures on Tuesday, 11 new Fellows of the Neutron Scattering Society of America where introduced and presented with their fellow certificates (Figure 2). This was followed by the presentation of the NSSA Science Prize to Yun Liu (NIST/University of Delaware) with the citation "For the discovery of dynamic cluster ordering in complex colloidal systems using neutron scattering" (Figure 3). In his award lecture, Liu gave an overview of his work applying neutron scattering to probe the dynamic and complex colloidal structures formed by proteins in relatively concentrated Understanding solutions. these structures is critical to formulating and delivering biopharmaceuticals, as well as describing the behavior of proteins in the cell. However, they present challenges due to a number of complicated colloidal phenomena including complex shape and internal degrees of freedom, both specific and non-specific intermolecular interactions and structuring over a hierarchy of length scales. He gave a brief history of experimental observations in concentrated protein solutions that pointed to the formation of so-called "dynamic cluster" phases, in which proteins form coherent, collective aggregates with finite size and lifetime over a range of conditions. A collaborative team including Liu as well as university and industrial partners has been successful in more deeply characterizing the important features of these cluster phases using a combination of small angle neutron scattering and neutron spin echo measurements. Remarkably, Liu's work has shown that many of these features and behaviors can be captured by a simple model for spherical colloids with isotropic interactions possessing a combination of short-range attraction and long-range repulsion. Specifically, the former drives the formation of clusters, whereas the latter suppresses phase separation and gives rise to their finite size. The resulting balance of interactions produces complex temperature-dependence of cluster formation. More recently, he has investigated the effects of electrostatic screening in these systems, and in particular the ability of multivalent ions that produce bridging interactions between proteins. Such interactions produce interesting "reentrant" behavior, in which low ion concentrations "melt" the clusters into a low-viscosity state, but then lead to gelation at higher concentrations. The conceptual understanding of protein solutions provided by Liu's work allows for more rational formulation of protein therapeutics such as monoclonal antibodies, and also provides model colloidal systems in which to study the formation and behavior of complex colloidal structures including clusters, gels and glasses.

Tuesday's plenary lecture was a passionately given and lively lecture from Julia Kornfield, California Institute of Technology on how "Neutrons get to the heart of Soft Matter" (Figure 4). Through four vignettes, she demonstrated the crucial scientific information afforded through carefully designed and executed neutron diffraction measurements. Her research targets have both significant scientific importance as well as potential for broad technological applications. For example, cleverly designed contrast variation SANS measurements of flow crystallization in polyethylene debunked the conventional wisdom that high molecular weight polymer chains are incorporated into the crystals that preferentially nucleate in their presence. In a highly visual demonstration, she described how molecularly designed ultra high molecular weight supramolecular complexes can suppress misting of fuel and thereby prevent catastrophic explosions of great concern in transportation crashes. These molecular engineered self-assembled complexes are robust in turbulent flows and

also have potential as drag reducing agents in oil pipeline transport. Here again, contrast variation SANS experiments afforded critical measurements of molecular nano to mesoscale structure. These two examples have appeared in the journal Science. The third vignette explored the molecular conformation in bottlebrush polymers, a molecular topology of great interest to the field, and provided confirmatory evidence for recent molecular models of this novel class of polymers. Finally, Kornfield closed by highlighting how kinetic USANS measurements are providing critical insight into the formation mechanism in functional polymer membranes. This enthusiastically received lecture highlighted groundbreaking, fundamental research on hierarchical polymers where neutron scattering methods provide unique,



Figure 4. Julia Kornfield presents her plenary lecture, "Neutrons get to the heart of Soft Matter". © Mark Lumsden. Reproduced by permission of Mark Lumsden. Permission to reuse must be obtained from the rightsholder.

critical measurements necessary for molecular engineering and design of potentially revolutionary functional materials.

The conference banquet was held on Tuesday evening in the Queens Salon on the Queen Mary. Attendants were treated to an entertaining and thought-provoking banquet speaker in Adam Steltzner from the Jet Propulsion Laboratory, NASA's lead engineer for the Mars Science Laboratory and Curiosity Rover Entry, Descent and Landing (EDL) phase. His presentation "The Right Kind of Crazy: A True Story of Teamwork, Leadership and High Stakes Innovation," summarized the ten-year project that culminated in the Curiosity Rover's successful landing on Mars on August 5, 2012. His message highlighted technical innovations and their impact, maintaining a careful balance between risk and reward, and persevering through setbacks. As a key tenet, he stated the three thousand men and women involved in the project were "unusually capable of collaborating". Thanks to the Curiosity Rover (and to Steltzner's team), we now know that Mars once had environmental conditions favorable for microbial life. In closing, Steltzner hinted that we explore to find "the edge of us," that curiosity is in our genes, that the curious mind stays agile, innovative and competitive, and that collaboration is innate to our humanity. These messages are ones that neutron scatterers can truly share with scientists of every age and discipline.

On Wednesday, the NSSA Sustained Research Prize was awarded to Pengcheng Dai (Rice University) with the citation "For his sustained and foundational contributions which have elucidated the magnetic properties of iron-based supercon-



Figure 5. Pengcheng Dai receives the 2016 NSSA Sustained Research Prize from Patrick Woodward and Stephan Rosenkranz. © Mark Lumsden. Reproduced by permission of Mark Lumsden. Permission to reuse must be obtained from the rightsholder.

ductors, cuprates, and other correlated electron materials" (Figure 5). He presented a lecture entitled "Antiferromagnetic Order and Spin Dynamics in Iron-Based Superconductors". Dai gave an overview of some of the important neutron scattering contributions he has made during his career in high temperature cuprate superconductors, heavy fermion materials, and colossal magnetoresistive oxide systems. He then concentrated on work on iron-based superconductors which has been the focus of his research efforts since their discovery in 2008. Dai and his collaborators carried out some of the first measurements of the magnetic and crystal structures as a function of composition, mapped out the electronic phase diagram of several types of these systems, and then followed this work by investigations to elucidate the spin dynamics of the parent,

magnetically ordered systems. These first data showed that the spin dynamics turn out to be very energetic, with a band width of several hundred meV, much higher than represented by the antiferromagnetic ordering temperature of typically 150 K (~15 meV) found in the undoped 'parent' materials, but quite similar to the very large energetics exhibited by the other class of high temperature superconductors, the cuprates. The superconducting transition temperatures are not quite as high as the cuprates, but these new materials exhibit much more flexibility in terms of site substitutions on all the crystallographic sites, which enables careful tuning of the magnetic order, spin fluctuations, and superconductivity both to illuminate the essential physics of these materials and to tailor properties for applications. One of the very interesting aspects

is that the iron superconductors exhibit a very strong magnetic resonance that tracks the superconducting order parameter, again similar behavior as the cuprates as well as the heavy fermion superconductors, which ties the superconductivity and spin fluctuations directly together. The detailed inelastic neutron investigations carried out by his group and collaborators have revealed the basic physics of the magnetism and its association with the electron pairing in the superconducting state. Following the extensive previous work on the cuprates, the pace of research on the iron-based superconductors has been extremely rapid, and Dai's neutron research has made him a leader in the field. Indeed, after reviewing work in the field, he then presented his very new polarized inelastic neutron measurements demonstrating how itinerant electrons play an important role in the materials, and how strong spin-orbit coupling and anisotropic spin dynamics break the tetragonal symmetry.

The Wednesday plenary lecture was given by Takeshi Egami, University of Tennessee and was entitled "Real Space Analysis of Dynamics in Liquid and Glass". In this lecture, he discussed the development of Dynamic Pair Distribution Function (PDF) techniques as an approach to gain deeper understanding of the dynamics in liquids and glasses. Key to this approach is the broad range of momentum and energy space now being routinely mapped out in timeof-flight spectrometers. In analogy with conventional PDF, Dynamic PDF represents a measure of $g(r,\omega)$ a single Fourier transform of the measured $S(Q,\omega)$ while the van Hove function, g(r,t) is the corresponding double Fourier transform. What is required for such an approach is reli-

able measurements of $S(Q,\omega)$ over a sufficient range of Q and w. In general, this approach has advantages in the study of liquids as all the scattering is dynamic and treating all the energy integrated scattering as elastic can lead to problems when there is coupling between Q and ω . Egami described the value of this approach by considering two examples. First, he discussed Dynamic PDF studies of superfluid ⁴He (data obtained using CNCS at SNS) where the proper incorporation of the dynamics of the system leads to an alternative explanation of prior measurements of the "static structure factor". He ended by discussing data collected on the ARCS instrument at SNS using the Neutron Electrostatic Levitator on a metallic glass, Zr₅₀Cu₅₀ and inelastic x-ray scattering data from water where the van Hove function was obtained. This seminar provided a compelling case that the use of inelastic neutron scattering together with analysis of either Dynamic PDF or the van Hove function can provide unique information which can lead to increased understanding of a diverse range of liquids and glasses.

On Thursday, the final prize presentation was for the Outstanding Student Research Prize which was awarded to P. Douglas Godfrin (University of Delaware) with the citation "For the discovery of dynamic cluster ordering in complex colloidal systems using neutron scattering" (Figure 6). He highlighted the importance of competing interactions in antibody solutions used in advanced biotherapeutics for oncology and other diseases. His work, as part of a collaboration with Genentech, utilized small angle neutron scattering and spin echo neutron spectroscopy to map the balance of repulsive and attractive interactions that drive the



Figure 6. Doug Godfrin receives the 2016 NSSA Outstanding Student Prize from Stephan Rosenkranz and Despina Louca. © Mark Lumsden. Reproduced by permission of Mark Lumsden. Permission to reuse must be obtained from the rightsholder.

formation of loosely bound aggregates that form a "clustered fluid". The formation of these clusters dramatically affects the viscosity and rheology of these formulations in ways that can be useful or detrimental to manufacturing and use. That careful balance is highlighted by insights into the work that map the phase space for which cluster fluids are likely to exist. Using these techniques, the team identified the effects of particular types of clustering on the viscosity, providing a roadmap for more effective manufacturing of this important class of therapeutics.

The final plenary talk of the conference was presented by Russell Hemley, Canegie Institute of Washington, and was entitled "Materials in Extreme Environments—New Opportunities for Neutron Scattering". He started by explaining the cosmic importance of high pressure, from the geology of gas giants and their icy moons, to materials with energy application and even biological life that could survive at extreme pressures. He illustrated this through a series of examples that showed how high pressures can affect the chemistry of even the simplest of materials with the simplest element, hydrogen, used as an example. In most cases, extreme pressures of up to a megabar (=100 GPa) and beyond are required. Hemley gave an overview how these conditions were first achieved in the late 1980s at xray synchrotron sources using very small samples in diamond anvil cell devices and small focused beams of x-rays. In more recent years, this capability has also been extended to neutron diffraction. Due to the availability of dedicated instruments such as SNAP at SNS, and the recent development of large volume diamond anvil devices, it is now possible to perform neutron scattering at 1 Mbar.

This opens up an entirely new realm of complimentary neutron and x-ray measurements, where often effects and new phases are seen by x-rays and structural details are revealed by neutrons. Using these high pressure scattering techniques, a number of new materials have been discovered such as new high Tc-superconductors or diamond nanothreads. This new structure of nanophase carbon. expected to yield ultra-high strength fibers, is formed following compression of benzene through polymerization into fully sp³-bonded carbon nanothreads. He then discussed another cosmic example: Recent experiments have demonstrated that biological systems are much more resistant to extreme pressures than previously thought, suggesting that it is possible for simple life to exist in the oceans of the Jovian moon Europa. These examples clearly demonstrate Hemley's final conclusions that high pressure is a powerful tool to identify new materials and phenomena with technological applications as well as elucidate the basic understanding of nature, and that high pressure neutron measurements will play an integral part in solving many outstanding problems.

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