

# American Conference on Neutron Scattering

## PLENARY and PRIZE

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\* Invited Paper

Monday Morning, July 13, 2020  
Live Presentation

**11:00 AM**

### **WELCOME AND INTRODUCTION**

by Peter M. Gehring, National Institute of Standards and Technology/ACNS Conference Chair

**11:05 AM I02.01.01\***

### **PLENARY: Spintronics and Skyrmions in Magnetic Heterostructures**

Kang L. Wang; University of California, Los Angeles, United States

Recent advances in the physics of spintronics have made spin-transfer torque, spin-orbit torque and voltage controlled magnetic memory devices possible. Antiferromagnetic (AFM) and ferromagnetic materials (FRM) offer the speed advantage to THz, allowing for information propagation in the form of spin and skyrmion current. Magnetic skyrmions are swirling topological spin textures in either non-centrosymmetric magnetic bulk compounds or in thin films with broken inversion symmetry. They are stabilized as a result of the balance among the Dzyaloshinskii–Moriya interaction, the Heisenberg exchange interaction, magnetic anisotropy, and the Zeeman energy. Skyrmions can be as small as a few nanometers and behave as particles, which can be created, annihilated and manipulated. They may be a strong candidate for high density and energy-efficient information storage and processing. In this talk, we will discuss the use of magneto-transport and Kerr effect as complemented by neutron scattering, X-ray magnetic dichroism and others for the studies of interface magnetism of heterostructures for room temperature spintronics and skyrmionics. Examples include topological insulator/AFM (MnTe) heterostructures which will be described to show the use of the induced exchange bias via interface proximity effect to control the topological charge number via field cooling. Then, we will discuss the exchange coupling of the two

sub-lattices of FRM and AFM. We will discuss the use of DMI and anisotropy energy, the Zeeman energy to create and control skyrmions in ferromagnetic and antiferromagnetic systems, particularly in insulator heterostructures, which have an advantage of having no electrical charge current. Voltage-control of skyrmions and their dynamics will be also described. Lastly, we will discuss the recent use of 2D spintronics and skyrmionics materials.

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<sup>+</sup> Present address: Hong Kong University of Science and Technology, Hong Kong

**12:05 PM I02.01.02\***

### **CLIFFORD G. SHULL PRIZE: Neutrons and Me—The Long and Winding Road**

Thomas P. Russell<sup>1,2</sup>; <sup>1</sup>University of Massachusetts, United States; <sup>2</sup>Lawrence Berkeley National Laboratory, United States

Neutrons have been an indispensable tool for the characterization of polymers in the bulk and in thin films. Over the past few decades we have seen a tremendous growth in the use of neutrons from their initial use to characterize the configuration of a polymer chain in the bulk using small angle neutron scattering to complex morphologies formed from multi-component systems to probing the surface and interfacial behavior of polymers and block copolymers in thin films and at interfaces to the dynamics of polymers in the bulk using neutron spin echo. From initial experiments at the Oak Ridge Research Reactor to the National Center for Neutron Research and the Spallation Neutron Source, neutrons have been an essential component of my research. Some of the past accomplishments will be discussed but emphasis will be placed on more recent advances we have made in the elucidation of the morphology of mikto-arm terpolymers in the bulk and thin films where the selectively labelling of the components of the terpolymer have been instrumental, in deciphering the morphology, in the deformation of hydrogels that show fully recoverable stress-strain behavior up to very large strains, and in

understanding the unusual characteristics of the interface between two immiscible aqueous solution.

## Tuesday Morning, July 14, 2020 Live Presentation

**11:00 AM**

### **FELLOWS ANNOUNCEMENT**

by Despina Louca, University of Virginia/NSAA  
President

**11:10 AM I03.01.01\***

### **PLENARY: Quantifying Polymer and Additive Density Distributions and Nanoscale Morphology Evolution in Block Polymer Thin Films**

Thomas Epps; University of Delaware, United States

Block polymer (BP) self-assembly is a promising approach to efficiently create nanoscale structures for numerous applications. For example, nanostructured electrolytes offer a balance of performance and stability for next-generation lithium-ion batteries, but to develop these technologies further, it is essential to understand the overall self-assembly behavior and the distinct salt and polymer distributions within the specific nanoscale domains. To this end, we have quantitatively examined the lithium salt and polymer distributions in salt-doped polystyrene-*b*-poly(*oligo*-oxyethylene methacrylate) [PS-POEM] BPs and explored how the presence of salt affects BP chain conformations and thermodynamics. With respect to the lithium salt distribution, neutron reflectometry was leveraged to infer the salt distributions in POEM domains for a series of lithium salts. All salt-doped BP specimens exhibited lithium salt distributions that were strongly correlated with the POEM density profiles. Furthermore, using X-ray reflectometry in combination with strong-segregation theory, we estimated effective Flory-Huggins interaction parameters ( $\chi_{eff}$ ) and the POEM statistical segment lengths ( $b_{POEM}$ ) as a function of salt concentration and rationalized the noted trends in  $\chi_{eff}$  and  $b_{POEM}$  in terms of lithium counterion basicity. As another example, solvent vapor annealing with soft shear (SVA-SS) can directionally align BP thin film nanostructures by exploiting solvent swelling/deswelling differences between the film and a polydimethylsiloxane (PDMS) pad adhered to the free surface. Although studies have demonstrated the potential of SVA-SS to generate well-aligned domains, the restructuring mechanism and effect of key parameters requires investigation to improve control over self-assembly. We conducted *in situ* small-angle neutron scattering experiments to explore the kinetic pathways of nanostructure alignment of poly(*d*-styrene-*b*-isoprene-*b*-*d*-styrene) thin films during SVA-SS. We

compared the results to SVA (without shear) and determined that alignment occurred through domain breakup and reformation initiated by PDMS swelling and deswelling, respectively. Additionally, changes in parameters such as PDMS elasticity and deswell rate resulted in nonlinear trends in domain directionality and ordering that were not apparent by small-area atomic force microscopy analysis. These results have allowed us to transition our approach to more 'continuous' polymer coating systems.

**12:10 PM I03.01.02\***

### **SCIENCE PRIZE: New Tools for SANS in Complex and Extreme Flows**

Matthew E. Helgeson; University of California, Santa Barbara, United States

*In situ* small angle neutron scattering under flow (flow-SANS) has become a critical tool for developing process-structure-property relationships of complex fluids and soft materials. However, sample environments and associated methods for flow-SANS have largely limited these measurements to steady state flows and/or simple rheometric deformations (pure shearing or elongation) that fail to capture the complex, nonlinear and time-varying deformations usually encountered during flow processing. This talk will review our recent efforts to develop new methods for performing and interpreting flow-SANS under complex and extreme flow conditions. This includes the design and validation of new sample environments that overcome challenges in simultaneously optimizing flow control and SANS measurements in a single device. It also includes advanced modeling and analysis tools for the anisotropic scattering of weakly ordered materials that provide more direct access to structural information used in the development of rheological constitutive models. We demonstrate these new capabilities through examples of previously unattainable studies aimed at elucidating important phenomena in polymeric and colloidal materials. These include the flow-induced stretching and mechanical scission of polymers in dilute solution relevant to many lubrication and flow control applications, as well as flow-interaction coupling in orientable particle dispersions that leads to highly nonlinear ordering in complex material processing flows. We conclude with an outlook on how flow-SANS measurements and analysis in complex, extreme and time-evolving flow fields might enable new approaches to rationally engineer processing flows for out-of-equilibrium soft matter.

## Wednesday Morning, July 15, 2020 Live Presentation

**11:00 AM I04.01.01\***

**SUSTAINED RESEARCH PRIZE: Equilibration and Dynamics in Block Copolymer Micelles**

Timothy P. Lodge; University of Minnesota Twin Cities, United States

Block copolymers provide a remarkably versatile platform for achieving desired nanostructures by self-assembly, with lengthscales ranging from a few nanometers up to several hundred nanometers. In particular, block copolymer micelles in selective solvents are of great interest across a range of technologies, including drug delivery, imaging, catalysis, lubrication, and extraction. While block copolymers generally adopt the morphologies familiar in small molecule surfactants and lipids (*i.e.*, spherical micelles, worm-like micelles, and vesicles), one key difference is that polymeric micelles are typically not at equilibrium. The primary reason is the large number of repeat units in the insoluble block,  $N_{\text{core}}$ , which makes the thermodynamic penalty for extracting a single chain (“unimer exchange”) substantial. As a consequence, the critical micelle concentration (CMC) is rarely accessed experimentally; however, in the proximity of a critical micelle temperature (CMT), equilibration is possible. We use time-resolved small angle neutron scattering (TR-SANS) to obtain a detailed picture of the mechanisms and time scales for chain exchange, for systems at or near equilibrium. The dependence of the rate of exchange on the key variables – concentration, temperature,  $N_{\text{core}}$ ,  $N_{\text{corona}}$ , and chain architecture (diblock versus triblock) – will be discussed. Interestingly, almost none of the observed features are captured by available theory. Possible explanations for these phenomena will be presented.

**12:00 PM I04.01.02\***

**PLENARY: Understanding and Enhancing Li-Ion Transport in Solids and at Interfaces for All-Solid-State Electrochemical Energy Storage**

Linda Nazar; University of Waterloo, Canada

All-solid state lithium-ion batteries (ASSBs) have emerged as attractive alternatives to conventional liquid electrolyte cells for electrochemical energy storage, owing to their enhanced safety and higher energy densities. ASSBs are founded on high performance fast-ion conducting electrolytes, where the important search for new materials hinges on understanding their intrinsic nature. Currently, a comprehensive knowledge of the factors that dictate facile Li-ion transport still remains elusive, as does mastering the interface of the solid electrolyte with

the electrode materials. Here, neutron diffraction provides an absolutely essential tool in elucidating structure and ionic transport pathways in both crystalline and glassy materials, and correlating these with superionic conductivity. The presentation will cover an overview of the state-of-the art in the field, followed by a focus on recent findings in our laboratory focused on neutron scattering that are complemented by analysis using the maximum entropy method, ab initio molecular dynamics simulations and solid state NMR studies. We correlate structure with ionic conductivity in a range of newly developed fast ion Li conductors to understand how cation disorder and a frustrated energy landscape impacts conductivity and activation energy. These considerations lead to an overarching understanding for design concepts for ion transport and electrolyte-electrode interfaces in solid state batteries, which serves as the theme for the presentation.

## Thursday Morning, July 16, 2020 Live Presentation

**11:00 AM I05.01.01\***

**OUTSTANDING STUDENT RESEARCH PRIZE: Structure-Property Relationships in Soft Materials via Rheo-SANS and Recovery Rheology**

Johnny C. Lee<sup>1</sup>, Kathleen M. Weigandt<sup>2</sup>, Elizabeth Kelley<sup>2</sup>, Lionel Porcar<sup>3</sup> and Simon Rogers<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign, United States; <sup>2</sup>National Institute of Standards and Technology, United States; <sup>3</sup>Institut Laue-Langevin, France

Soft materials, when reacting to dynamic shearing, tend to generate complex material responses. The link between macroscopic flow properties and molecular-level microstructural rearrangements plays an important role in numerous industrial processes such as coating and printing. We show, via time-resolved rheo-small-angle neutron scattering (rheo-SANS) and dynamic shearing, that the recoverable strain is linearly correlated to the temporal evolution of microstructure in both velocity-gradient and velocity-vorticity planes even under nonlinear conditions, forming remarkable structure-property relationships. Investigating two distinct polymeric materials of wormlike micelles and fibrin network, we demonstrate that, in addition to the nonlinear structure-property relationships, the shear and normal stress evolution is also dictated by the recoverable

strain [Lee et al. *Phys. Rev. Lett.*, 122, 24, 2019]. We further apply the understanding into a step strain experiment, which is known to provide important information about constituent dynamics. However, if a material has experienced a complex shear history, the underlying physics is not straightforward to access. We use the recovery rheology and rheo-SANS techniques to probe the nonlinear dynamics of an entangled wormlike micelle solution by applying step strains after complex shear histories enforced. We show that a universal relaxation modulus can be obtained from step strain tests with complex shear histories, only when the modulus is defined in terms of the recoverable strain. The structural alignment of micellar segments and the shear history, are shown to be completely correlated with the recoverable strain [Lee et al. *AIChE J.*, 65, 12, 2019]. This work provides a straightforward path to further explore the structure-property relationships of soft materials under dynamic flow conditions, and lays the foundation of how to accurately probe out-of-equilibrium dynamics in a consistent manner.

**12:00 PM I05.01.02\***

**PLENARY: Competing Phases and Functional Properties from First Principles**

Karin M. Rabe; Rutgers University, United States

In the last decade, there has been a revolution in the generation, organization and use of data for materials design and discovery. In particular, first-principles calculations of the properties of known and as-yet hypothetical materials are now systematically used to augment crystallographic databases. Drawing on the unique capability of first-principles calculations to identify low-energy metastable states in addition to the experimentally observed equilibrium phase, we can predict phase transitions and functional properties "de novo": that is, without prior experimental clues. Further, we can study the evolution of competing phases in applied electric fields to explore switch ability, using a new highly efficient method for the first-principles prediction of switching polarization. Results will be presented for systems including perovskite oxides, (Hf,Zr)O<sub>2</sub> and hexagonal ABC compounds. The challenges and promise of theoretical materials design and theoretical-experimental integration will be discussed.

**1:00 PM**

**POSTER AWARD ANNOUNCEMENT**

by Peter M. Gehring, National Institute of Standards and Technology/ACNS Conference Chair