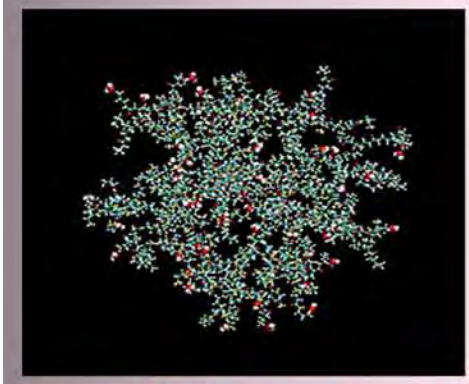

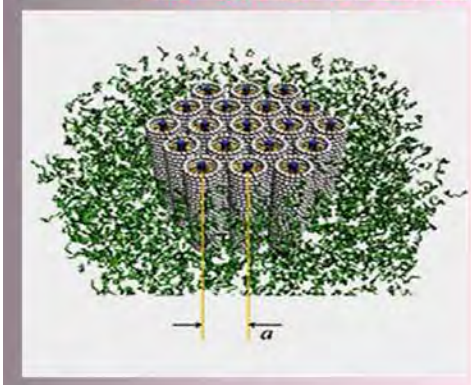

Grand Challenges in Soft Matter

Workshop report University of California Santa Barbara, May 17th-18th, 2014

Organizers: Fyl Pincus (University of California, Santa Barbara) and Matt Tirrell (University of Chicago)

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Sponsored by:

Oak Ridge National Laboratory
Institute for Molecular Engineering, University of Chicago
University of California Santa Barbara, Dept. of Physics
University of California Santa Barbara, College of Engineering

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I. Executive Summary

One of the goals of modern science is to create materials by design with specific functionalities. Soft matter composed of covalently bound molecular building blocks (including polymers, surfactants, nanoparticles, gels,, etc.) provides almost endless complexity and tunability for making new materials to achieve this goal. As the complexity of these systems grows, so do the challenges for developing our fundamental understanding of the materials properties with the ultimate goal of controlling static and dynamic function. In order to identify these challenges for the next decade, a workshop was organized toward this end and to additionally examine how neutrons can play a role in solving these problems.

Neutron scattering has played and continues to play a major role in magnetism (spin dependent interactions associated with the spin of the neutron) and in soft matter (isotopic labeling). Thus it is not accidental that three of the neutron oriented workshops are intimately related to these areas of condensed matter. At the Soft Matter Workshop,39 invited leading researchers (including four NAE members and one NAS member) from 14 different universities, 5 other national laboratories, and 3 industrial research centers, joined 5 participants from ORNL on the UC Santa Barbara campus on May 17-18, 2014. The workshop was organized by Matt Tirrell, University of Chicago, and Fyl Pincus, UC Santa Barbara and included presentations/discussions on experiments, synthesis, theory, and modeling/simulation.

While neutrons are an essential tool for studying soft matter today, in the future, new techniques and new sources will provide even more information on these complex systems. For example, the proposed Second Target Station at SNS will be optimized to provide a high flux of long wavelength neutrons over a wide bandwidth. Such a source will be ideally suited to simultaneously studying multiple temporal and spatial scales, crucial to understanding complexity in soft systems. In order to exploit and to fully interpret the data, a closer coupling between modeling and experiment will be essential. Significantly increased facilities for selective isotopic labelling (primarily deuteration) will be needed. Soft matter has a growing synergistic relationship with molecular and cellular biology in the area of synthetically reproducing and enhancing the functionality found in living systems. Achieving these goals may involve the marriage of synthetic and biological moieties.

The outcome of the workshop was to produce a report on these challenges and to anticipate how to address the challenges with new techniques. While the focus was on the future, the recommendations and discussions represent a graded set of actions from the near term to the end of the decade. Below we list a summary of the challenges and the recommendations for ways to confront them using neutrons.

Areas of Soft Matter where more research is required to develop fundamental understanding:

1. **Response of mechanical deformation**- jamming, glassy materials, gels, and non-equilibrium phenomena in soft matter
2. **Soft/hard composite materials**
    a. How to manipulate particles/dispersions in composites, understand properties to improve functionality
    b. Understand anisotropic (particle shapes or interactions) systems
    c. Behavior of organic shells (application to soft matter hierarchical systems)
    d. Weakly ordered systems

    e. Tissue structure and scaffolds
3. **Transport in soft matter** - Electron/ion/water/phonon transport across large length scales in a multicomponent system – e.g. bicontinuous structures, composites, etc.
    a. Segmental motion -> glass transition (small length scale) relevant to larger scale transport (macro performance).
    b. Ionic movement in gels, flows, brushes
    c. Interplay of convection and charge transport
    d. Interplay of charge transport and humidity

4. **Polyelectrolytes**
    a. Multiple charge states, amphiphilic architectures
    b. Surface structures
    c. Multipolar and polarizibility effects
5. **Complex structures in solution** – hierarchical assemblies
6. **Soft matter under industrial processing conditions** - including the effects of flow, shear, high temperature, high pressure, etc.

7. **Active soft materials**
    a. Steady state morphologies of active systems
    b. Structure and functionality of decorated membranes
    c. Enzyme dynamics
    d. Scattering from whole cells, imagine deuterating say just microtubules or just membranes in a living cell
8. **Expand our ability to make quantitative measurements** such as
    a. Membrane curvature and fluctuations and equilibrium dynamics
    b. Methods to probe non-equilibrium behaviour and dynamics
    c. Providing in-situ, short range local information in soft materials
9. **How do we define interfaces** and set boundary conditions in soft matter/hybrid systems to understand their properties (structure, dynamics, chemistry). How do we design interfaces with defined structures and functions
10. **Polar solvents other than water**
11. **What are the effects of polydispersity** on properties (physics).

Recommendations to help address these areas of need:

1. **Pursue a reflectometer** (including Grazing Incidence Diffraction capabilities) on a brighter Second Target Station. This could increase the q-range, provide for single shot kinetics measurements, and improve spatial resolution to define interfaces and interface structure.
2. **Advance time-dependent kinetics techniques** and experiments for SANS, USANS, and GI-SANS. Currently limited to minutes, but Second Target Station could achieve 100-fold increase in flux to achieve 1 second to enable new realm for single-shot kinetics measurements.
3. **Advances in neutron lens and mirror technology** are needed. Use to achieve spatial profiling at the micron-scale for neutron imaging, phase contrast imaging neutron tomography, SANS and Reflectometry to obtain fine local structure. Also, use for Very-high resolution SANS (VSANS).

4. **Develop "conventional" spin echo at HFIR** to allow order of magnitude faster measurements with higher dynamic and q-range. Currently, ILL can do 800-1000ns.
5. **Enhance Backscattering instrumental resolution** to cover a broader time range
6. **Develop Larmor precession techniques** such as SESANS to extend spatial resolution to very large length scales
7. **Need wide variety of advanced experimental environments** specific to soft matter research to achieve "lab at the instrument"
    a. For applying fields (e.g. electric, magnet, flow)
    b. Impose extreme conditions (e.g. flow, shear, evaporation, humidity, gas vapor pressure, confinement)
    c. Arbitrary duration, phasing, and spatial configuration for non-equilibrium structures
    d. Need better infrastructure at facilities for sample environment development by external researchers. Europe has this, US doesn't.
8. **Expand capabilities for computationally-involved data analysis**
    a. Integrate with data simulation methods that can be constrained using data and supplementary information
    b. Develop tools for more detailed computation/simulation methods where complex data can be modeled in real time for data where "traditional" analysis fails
    c. Real time data visualization.
    d. Dedicated high speed computers will be required.
    e. Theory combined with experiment – key component to all these challenges is harmonizing both approaches.
9. **Provide facilities for sample preparation and characterization** on site and in close proximity to the instruments, particularly for biological or interfacial samples.
10. **Design and build complementary and simultaneous in-beam characterization** with positional sensitivity (e.g. fluorescence, x-ray reflectivity, Brewster angle, SEM/TEM, AFM, etc.)
11. **New methods to measure local distributions of stress or anisotropy** in soft materials such as homogeneously polarized spins in the sample (stress) combined with labeling materials with nuclear spin probes
12. **Extend the times scales for dynamics measurements far beyond 1 microsecond**. High flux of very long wavelength neutrons coherent beams might be used (neutron speckle)
13. **Provide abundant facilities for specific deuteration** of materials. For example, deuteration of just one peptide sequence in a whole protein such as just one alpha helix of a 7 alpha helix GPCR, or expanded capabilities for isotopic labelling of molecular components of polymers.
14. **Need flexibility with beam time** for iterative experimental design process. This could also serve for training students in neutron scattering. Funding and new paradigms needed to take full advantage of neutron facilities and supply neutron scattering expertise in the future
15. **Broadly advertise and highlight advantages of neutrons** to the Soft Matter Community; make a greater effort to expand the neutron scattering community.

II. Introduction

This report is a summary of a workshop on the Grand Challenges in Soft matter Science held at the University of California Santa Barbara campus, May 17 and 18, 2014. It is the third of a series of workshops sponsored by Oak Ridge National Laboratory to explore future directions and needs of the scientific community. This report is intended to supply input from the scientific community to ORNL management and the Department of Energy (DOE) which will help guide the development of advanced neutron scattering technology in the United States. The workshop was convened and organized by Prof. Phillip Pincus, University of California Santa Barbara and Prof. Matt Tirrell, University of Chicago (see the agenda in Appendix I). The workshop brought together thirty nine researchers from Academia, Industry, and National Laboratories performing research in theory/modeling/simulation, synthesis, and experimental characterization to discuss current topics in Soft Matter Science and to consider what scientific problems in soft matter science may be solved in the coming years. A list of the attendees can be found in Appendix II. A ten year time frame was targeted for discussion since today's scientific understanding may be extrapolated from current state-of-the-art yet it is still a stretch of the imagination to predict problems on that time scale.

The charge to the workshop attendees was to:

1. Identify the ten major challenges relating to the first-principles understanding for the design of broad classes of soft materials and polymers;
2. Identify the missing tools/methods necessary to address these challenges and the steps required to develop the methods using neutron scattering as a standalone technique or in combination with other techniques;
3. Construct a vision for how neutron scattering, theory, computation, synthesis, and other experimental techniques can interact synergistically to discover new materials; and
4. Elaborate the experimental advances and infrastructure needed (particularly with respect to neutron scattering) to enable more effective synergistic interaction.

The workshop consisted of a series of sessions on the topics of Polymers, Lipids/Membranes, Assemblies/ Biomaterials/ Charged Systems/ Colloids, Surfaces/ Interfaces, and Instrumental Needs. In each session a twenty minute invited, keynote talk was presented followed by five minute contributed talks. A general discussion period followed each set of presentations. A list of talk titles and the names of the session chairs, and session scribes are presented in Appendix III. All of the participants were given the opportunity for presentation.

In the afternoon of the second day of the workshop, the attendees broke into working topical sessions to develop a response to the charge of the workshop. The working group reports were then summarized and discussed by all attendees in these summary workshop sessions. The body of this report is organized as follows: for each topical session a summary of the presentations are presented followed by the summary of the discussions following the presentations and then the results from the breakout sessions. The common themes and recommendations were then summarized in the Executive Summary.

III. Session Reports

A. Polymers

Presentations

Brett Helms, Lawrence Berkeley Laboratory and the Molecular Foundry (keynote)

Brett discussed self-assembly with the goal of understanding polymer structure at polymer inorganic interfaces upon assembly, and energy transduction through those assembled interfaces. This included multicomponent hierarchical assembly and transport across polymer-inorganic interfaces. One challenge is to design both custom-purpose diblock copolymers which adsorb onto open coordination sites as well as nanoparticle "naked" crystals with the proper coordination sites for polymer binding. Challenges in hierarchical assembly that could be addressed using neutron scattering include understanding the design rules for building mesostructured architectures from arbitrary shapes, sizes and compositions; understanding the effects of polydispersity; the effects of kinetic evolution and polymer processing on surfaces with arbitrary chemistry and topography; and how kinetic pathways may lead to reproducible and uniform phases over large areas. Control over the production of these materials can have several use-inspired applications such as energy storage, membranes (e.g. fuel cells), and building efficiency. Challenges for making fuel cells commercially viable include developing membranes for ion transport at high flux in non-aqueous conditions while being impermeable to molecules that limit membranelifetime. Outstanding questions in relating transport to hybrid structures include

- How does the introduction of a nanoscale inclusion of arbitrary shape, composition, or surface charge density perturb the structure of polymer chains in a (mesostructured) composite?
- What is the role of solvation, dielectric medium, etc.? How do we probe, model and validate the heteromaterial interfacial structure at critical length and time scales in situ while transport is occurring?
- How does interfacial structure differ between polymer-nanocrystal composites and mesostructured BCP-nanocrystal composites?
- What effect does interfacial structure have on transport pathways?
- Do we understand defect structure (at all length scales) and its impact on transport?
- What means do we have to intervene and guide interfacial structure? Is it possible to systematize perturbations to yield more efficient transduction paths?

In-situ simultaneous measurements of transport and structural properties would be valuable tools. Similarly, being able to measure structure in an applied field (kHz frequencies help align the structures) or as a result of different processing (e.g. spin coating versus spray coating) to obtain processing information would be a huge help. These effects are all important on the nanoscale since surface charge plays a large role at these length scales, measuring local structure at the interface would be an important tool. Appropriate time scales are from microseconds to seconds which are a challenge for both scattering methods and simulation.

Michael Chabinyc, University of California Santa Barbara

Michael presented a talk on moving electrons in semiconducting polymers. He discussed how processing leads to different structures using the same materials and how chain orientation is critical to electronic transport. Conduction could be through 2-dimensional "sheets or through 3-dimesoional conduction paths depending on the alignment of the conjugated polymers. Also, thermal transport changes as

polymer chains are stretched. It would be useful to supplement the spectroscopic measurements with knowledge of the phonon transport in organic materials as well as information on the local structure. The impact of such studies would include new materials for energy conversion, developing an understanding of the ultimate limits in thermal and electrical conductivity.

Gary Grest, Sandia National Laboratories

Gary talked about the need for accessing long times in polymers and soft matter. These are unique challenges since the microscopic physical phenomena couple strongly to macroscopic length and time scales through multiple mechanisms. Present methods for studying these systems (e.g. neutron scattering and computation) typically only focus on solving problems at a single length and/or time scale. Stronger coupling between neutron scattering and computational efforts are needed to cover wide ranges of length and time scales. The present state-of-the-art in computation includes bead-spring models with no chemical details which are optimized for testing concepts; atomistic models which include multimillion atoms up to 100's ns or tens of thousands of atoms up to microseconds; or coarse-grained methods with reduced numbers of degrees of freedom but can access very large time/length scales. As an example, simulations of an ionic polymer in different solvents were performed up to about 30-50ns at a rate of 1.5ns per day of computation time. The results match scattering results in each of the solvents.

Julie Kornfield Cal Tech

Julie discussed DNA origami which could be mass produced in the next ten years. These structures may be used for controlled release of drugs (e.g. cancer killing drugs) and as such must be perfect in order to control the release to the proper cells. The exact structure of these materials isn't yet known although snapshots are possible. Information is needed on entire assemblies and time-stamped structures with applied fields would provide important information. Also selective deuteration combined with neutron scattering will be essential to unraveling the details. This is one example of the programmable self-assembly of soft materials and the importance of understanding misfolding.

Lynn Walker, Carnegie Melon University

Lynn presented results on neutron scattering from aligned lyotropic liquid crystalline polymers, rod-like micelles, and block copolymers. In each case common themes include multi-length scales from nm-microns and beyond and the coupling of structure and rheology in non-equilibrium, anisotropic soft materials. The challenges for the future will include studying the structure of more complex (realistic in terms of processing) flow fields and combining several techniques and measurements simultaneously. Neutrons will provide tools for these studies. To enable these experiments improved/advanced sample environments, better analytical tools, and tools to connect theory/modeling and simulation to the scattering will all be needed.

Yang Zhang, University of Illinois at Urbana-Champaign

Yang discussed the challenges of understanding slow dynamics and glassy materials. He explained why neutron scattering is a valuable tool for studying these systems which exhibit physical interactions over heterogeneous length and time scales including the matching of neutron energies to fundamental excitations and the Q-dependent information that neutrons yield. Both coherent and incoherent scattering can be used to study the diffusive and collective motions of the molecules through the intermediate scattering functions measured by quasielastic neutron scattering. Understanding glassy behavior is relevant to glass-forming metallic liquids, confined and low-dimensional systems, self-healing ionic glasses, and even geophysics and materials like cement and asphalt. Neutrons will be useful for unraveling the universality of the glass transition and the nature of materials far from equilibrium and

under extreme environments. Understanding slow dynamics in soft materials will give information on such varied topics as viscous liquids, materials degradation, corrosion, protein folding, pattern formation, self-assembly and liquid interfaces.

Post Presentations Discussions

During the general discussion, it was noted that inorganic materials (solid oxides, etc.) seem to have much clearer neutron scattering information due to enhanced ordering. The key aspect in many soft systems is that we must often measure average properties due to the amount of disorder in the system. Sometimes soft matter is organized as crystals in a sea of disordered material. Other times in multiblocks and melts soft matter is completely disordered. This disorder is one of the reasons that it is essential to combine scattering with simulations. It was emphasized that while determining structural organization through scattering of neutrons/x-rays/light are key, measurements of dynamics and transport on the material chemistry side are also essential. Also, processing the data from the measurements in real time is critical.

Programmed self-assembly provides a tie between chemistry of materials used, their molecular organization on the single molecule, and then how those assemblies (mimics of biology for example) can be the way forward to approach a series of polymer areas and grand challenges. Kinetic measurements with neutrons are linked to one's ability to look at wide length scales in short time frames (bursts, etc.). To push the area forward, we need to increase neutron capability to routinely go to lower q to probe length scales of 500nm and above. USANS and SESANS are techniques which can provide information at these length scales. Another discussion evolved around understanding particle/polymer matrix interfacial phenomenon on bulk properties (fillers in rubber as an example). "Still don't understand nanoparticle filled polymers after 100 years." Understanding rafting and voiding in these systems is still a challenge and will require larger length scales and dynamical information. Another important area is to probe materials properties near/at the point "point of failure" to understand structure or properties. Need to be able to put samples in different environments and be "violent" with materials in the beam. The sample environments for such studies using combined high pressures, temperatures, and applied fields (electrical, shear, magnetic) currently don't exist or aren't typically used for soft matter studies but are routine for hard matter.

Even if we could realize all these increases in characterization functionality, data interpretation and fitting is critically important to being able to understand what it says. Because of the heterogeneous length and time scales it's very important to have computational and analytic tools to get the most out of the data. Also, a new generation of students must be trained (and funded) to perform neutron scattering experiments and analysis.

Breakout Session Report

Grand Challenges:

1. Understanding the response of mechanical deformation – jamming, and the glass transition
2. How to manipulate particles/dispersions in composites, understand properties to improve functionality
3. Complexities in solutions – surfactants, polymers, interfaces
4. Transport in soft matter - Electron/ion/water/phonon ("small things") transporting across wide length scales in a multicomponent system – e.g. bicontinuous structures, composites, etc.

    a. Segmental motion -> glass transition (small length scale) relevant to larger scale transport (macro performance). Strong link between old polymer problems (fundamental) and applied problems.
    b. True understanding of a host of conducting polymer systems – electron/phonon coupling, etc.
        i. Tons of materials have been made, put into devices – but not truly understand
5. Polyelectrolytes – understanding them in more complex environments (now only well understood in the most simple environments)
    a. Multiple charge states, amphiphilic architectures
    b. Proteins – unstructured (amphiphilic), and it's interaction with other things.
    c. Interactions are never generalized
6. Processing - If we want to use new, multicomponent soft materials for anything beyond thin films, we have to fully understand effects of processing them.
7. Origins of dynamic heterogeneity, how can we use this to improve properties
8. Theory combined with experiment – key component to all these challenges is harmonizing both approaches.

Capability Gaps and Opportunities:

1. Nonequilibrium structure under - Flow, external fields, shear, evaporation
2. Contrast matching not utilized enough in processing effects studies
3. Not limited to RT or water solvents
    - Deeper dive into other polar solvents beyond water
        - Ionic liquids, specifically
    - Relevant processing temperatures (high T)
4. Effect of polydispersity on properties (physics) – fact of life, how do we use it to our advantage or understand how to work with it

B. Lipids/Membranes/Assemblies

Presentations

Oleg Gang, Brookhaven National Laboratory (keynote)

Oleg presented work and challenges in programmable matter and its transformations at the nanoscale from idea→design→smart-ingredients→smart-assembly. He presented the idea of the inverse problem of self-assembly: how do I need to design systems to get a desired structure? Oleg posed the question: what is needed for self-assembly by design which includes understanding nanoparticle systems from packing to programming. In multicomponent nano systems, how does one make the bonds for nanoparticles to drive from individual nanoparticles to well defined clusters to large scale organizations? The approach is to decouple the driving forces of assembly from the material specificity. Since these are multicomponent systems, neutrons are better suited for investigation of the soft shell around the nanoparticles and x-rays are better probes of the particle cores (due to electron density). A method for

DNA guided 3D ordering of nanoparticles (X-ray BCC structure determined in situ) was shown. In these materials, molecules and nano-objects are comparable in size (analogous to two guys very close to each other fighting with swords bigger than separation between them) and the interplay between curvature and number of linkers is important. Another example was shown of DNA ribbon assembly can be achieved via collective chain interactions.

In multicomponent systems one can build pathway dependent multifunctional materials. The challenge is to grow large-sized, regularly-shaped particles and then assemble with soft linkers. Neutron scattering can allow one to study shape compatibility, non-specific interactions, shell softness. Also, compositional lattice disorder (which increases with shell thickness) can be studied with neutrons taking advantage of the contrast. Liquid ordered clusters is a challenging thing to study. Shell softness and compositional order in multicomponent systems are where neutrons add to the information but neutrons don't have the ability to probe electron density differences.

Two ways to achieve the desired clusters and lattices of nanoparticles is to use engineered isotropic interactions or to make anisotropic (patchy) particles to drive the symmetry. To design clusters and lattices the goal is to make a library of multivalent linkers. This work includes using nanocubes as linkers as well as clusters with DNA frames (origami). It's very hard to describe such structures by scattering. One would also like to create non-periodic structures via modular assembly. One challenge is how to probe disordered and cluster systems? SAXS gives just average distances between particles, not much more than that. Can methods similar to pdf's be used to get the local structure? A small beam is needed to probe local environments and this requires a beam size that is comparable to the cluster size to probe the local coordination number from the angular autocorrelation. Combining scattering with X-ray microscopy permits local probing by soft X-rays. Can neutron beams be focused to these dimensions? There was a brief mentionof system transformations. Neutrons can provide a lot of info on shape changes (especially for the soft shells) and how interactions shift phase transformations.

Questions and discussion following the presentation included: How to focus neutron systems- can sub mm sized beams be produced and/or whether it is possible to scale up the systems to be able to use neutrons without focusing? Another challenge would be to probe defects in systems which include controlled defects to see how they propagate. New methods may have to be developed. Other scientific questions about these systems include: How robust are the clusters? What are the differences between bulk and surface adsorbed materials? How are chains really attached, especially in shape diverse particles? It's very hard to probe particle shells if they are not spherical.

<u>Monica Olvera de la Cruz, Northwestern University</u>

Monica gave an update on work with lipid membranes. In lipid membranes the non-local forces (electrostatic and elastic) are very hard to model. A grand challenge is that there are many continuum models, but how do we include these into membrane models with molecular detail, especially when the shape of the particle is involved? When simulating lipids, atomistic MD captures mechanisms which promote lipid crystallization. Implicit solvent interactions provide a driving force for assembly and continuum models describe the interactions which drive vesicle shape. Regular shapes exist in nature, for example in the crystalline, closed membranes in certain bacteria and in carboxysomes. A study of ionic nanocontainers was presented where modelling from MD through continuum mechanics was applied to get structural information from the surfactant structure through the mesoscopic assemblies. X-rays are able to give the tail packing symmetry and TEM can give the overall shape. Neutrons would be useful with deuterium labelling to understand the in-plane superlattices. The elasticity of the membranes will depend on the vesicle shapes. Also, there are shape transitions which can be modelled

and observed that change from vesicles to ribbons and back to vesicles as a function of pH as a result of the competition between electrostatic forces and elasticity. These are difficult systems to model due to the effects of the non-local forces involved. Again in these systems neutron scattering could help determine super lattice structure through selective deuteration.

Chris Santangelo, University of Massachusetts Amherst

Chris gave a talk on the growth of macroscopic form (e.g. ribbons and sheets) from the microscopic structure. Do we understand enough to design soft materials from sheets? Chris quoted Richard Feynman "What I cannot create I cannot understand." Growth in nature of organized structures ranges from mitochondria, to tissue shape (e.g. chicken gut). In these cases, the relevant scales are vast. To measure growth and buckling of polymer gels ~500 μm scale is too large for scattering, but maybe something could be learned with imaging. People have used graphene as a model system for these shapes to study folding and with that you get 200 nm systems. Another example: assembled DNA origami in sheets that then fold. To control and design these systems an understanding is needed of small length scale fluctuations, larger scales to drive the assembly, and scale independent issues such as the system being robust to errors and metastable structures.

Ting Xu, University of California, Berkeley

Ting gave a presentation on peptide proteins for synthetic polymers and even for use as micromachines. The challenges in using homopolymer/protein-peptide/hybrid biomaterials are whether we can mimic complex proteins using peptides and can we process proteins using organic media and direct protein assemblies? Using peptides to create biomaterials, the material has to interface with cells to communicate within nature. Here the challenge is to understand materials structure at length/time scales in real environments. On the other hand, we can make hybrid materials for non-biological applications such as catalysis and sensing. To understand these systems we need to understand their structure, function, dynamics, and self-assembly. The "R" groups on proteins can be used to drive function, conformation, etc. in the synthesis of new polymeric materials. The question remains what are proteins and how can we reduce their properties to things we can handle like hydrophobic interactions, etc.? By building a database of synthetic protein-like blocks, we can learn more about how to make these into functional materials.

Margie Longo, University of California, Davis

Margie described how fluorescence microscopy has been a powerful tool to study model membranes to investigate large scale phase separation but interesting biology happens at the 10 nm scale (e. g. nanodiscs or phase separated domain formation in a 50 nm scale). So, they are always looking for techniques to resolve structures at the smaller length scales. Examples of the types of problems and systems which could be studied included diffusion in crowded membranes to test conjectures of the dynamics and structures, curvature directed nanopatterning where mechanical energy gradients drive patterns and dynamics, and sol-gel entrapped nanolipoprotein particles. It was emphasized that one of the key bits of information needed to understand these systems is *simultaneous* information about the structure, dynamics, and kinetics of these.

Post Presentations Discussions

Pattern protein/phase separation: can neutrons look at the size scale that is important for the phase separation? What methods do you use to fold sheets into macroscopic material? One way is to make tri-layers of polymers combined with photolithography. What is the goal of making such beautiful folded arrangements? Use folding to make materials by programming. Membranes reflect the shape they

assembled on time scale for tracking? Often, the pertinent time scales for assembly are milliseconds to sub milliseconds. What can neutrons offer to membrane science? It's hard to deuterate all materials and it's hard to make a lot of materials so synthetic techniques will be needed.

The folding-of-sheets problem is interesting since one needs to access other length scales than just molecule self-assembly alone. Folding sheets under external conditions can be become very interesting moving into the future. Neutron reflectometry can give a lot of information where fluorescence is the majority method being used presently. We normally determine structure from dynamics and vice versa but neutron scattering can offer a way to measure both things combined. What about measuring the homogeneity of samples? Lateral homogeneity is possible to determine with scattering. Modelling and its connection to scattering data is however a missing component in this context and would be essential to analysing the data. Another question is how assembly occurs in well-designed building blocks? How to avoid kinetically trapped systems and how to tackle a variety of timescales are other key pieces of information needed. There is the issue of coherence but besides that can one do something analogous to speckle scattering with neutrons? Can we build a "neutron laser"? Unfortunately, the answer is no. But with neutron spin echo, and ultra-high resolution backscattering you can perform measurements with nanosecond resolution up to 100's of ns. With X-ray correlation spectroscopy you can resolve seconds to microseconds but there is an information gap in between. It would be good to close this gap.

Breakout Session Report

The group's discussions are listed below numbered under major areas with bullet points of specific examples of the types of problems that could be addressed.

Grand Challenges:

1. Biologically active systems
    - Interplay of constituent molecules-active systems. For example, phase transformations driven by ATP.
    - Embedded membrane systems: Segregation of constituent molecules (by proteins, probing local environment). In other words, the interplay between membrane constituent molecules to invoke complex biological processes under physiologically relevant conditions.

2. Transition states→Mesodynamics, Nonequilibrium with external fields and gradients (and molecular stimuli)

3. Protein Conformation Dynamics
    - Protein structure
    - Protein structure in membranes
    - How do proteins locally change membrane conformation and composition. In other words, the interplay between membrane constituent molecules to invoke complex biological processes.

4. Synthetic/Hybrid Systems
    - Understand **anisotropic** systems
    - Behaviour of organic shells (application to soft matter hierarchical systems)
    - Weakly ordered systems (modelling and simulation)

5. Quantitative measurements

- Helfrich Free Energy (curvature and fluctuations)→Equilibrium dynamics
- Need methods to probe non-equilibrium behaviour and dynamics
- Local information vs. global averaging

Grander ideas that may not be feasible on a short time scale:

6. Focused beam in-plane, Neutron holography, Phase contrast Imaging (free standing membranes)

7. Molecular detail information by paramagnetic peptides/amino acids as local probes or by using specific deuteration.

8. Scattering from whole cells, imagine deuterating say just microtubules or just membranes in a living cell.

Capability Gaps and Opportunities:

1. Focused neutron beams – high flux on small area
2. Deuteration facilities that would be highly specific (imagine deuteration of just one peptide sequence in a whole protein, e.g. just one alpha helix of a 7 alpha helix GPCR)
3. Ancillary fields
4. All preparation facilities in close proximity
5. Complementary characterization (e.g. fluorescence, x-ray and neutron reflectivity, Brewster angle, SEM/TEM, AFM, etc.)
6. **Simultaneous characterization while in the beam** with positional sensitivity
7. Better data analysis and **Integrated** and co-refined modelling systems. Big data management
8. Physiological conditions relevant for real cells (CO_2…etc.)

C. Biomaterials/Charged Systems/Colloids

Presentations

Juan de Pablo, University of Chicago (keynote)

Juan explained that understanding disordered peptides and peptide aggregation has relevance to both understanding disease (peptide aggregation is linked to more than 15 neurodegenerative diseases) and aggregation of industrially produced proteins (for example insulin). For example, oligomers and dimers are very toxic to brain tissue at small concentrations and small differences between rat amylin and human amylin mean that humans get diabetes where rats do not. SANS is a very useful tool for looking at folding and misfolding of proteins and has been used to study insulin solutions, but still the structure of the nucleus or the dynamics isn't understood. Misfolding in proteins induces misfolding in other proteins. How do we understand this? In particular, when one models dimerization of an alpha helical structure with a beta hairpin, the free energy maps are strongly dependent on which force fields are used. The challenges are to determine the structure of isolate proteins, small aggregates at early stages, aggregates near bilayers and surfaces, and counterions. This information could be used to validate the models.

In another study, de Pablo described modeling of polyelectrolyte complexation and coacervation. This process involves several free energy contributions (entropic release of counterions, electrostatic energy, configurational entropy, and non-electrostatic forces). Question is how does chirality effect structure in aggregates and what aggregates show precipitation versus coacervation? Simulations show that homochiral polyglutamate forms beta sheets where achiral molecules do not. Simulations show beta-sheets form with increasing the length of homochiral sections of the molecules. The challenges are to develop design rules for these materials and theory for structural evolution in hybrid precipitate – coacertive systems, and to understand the structure of coacertives and precipitates, the dynamics of assembly (equilibrium or non-equilibrium), and their assembly and reactions. A third study was presented on spherical nucleic acid based assemblies (SNA's). Gold nanoparticle/nucleic acid assemblies are examples of these materials. An important aspect is to understand the ion cloud around the SNA. Simulations of stepwise hybridization of SNA dimers were shown. The design of molecules with DNA linkers shows how to build a phase diagram. Also, programmed self-assembly was proposed with molecules that can sense the polymer environment (e.g. curvature) and go to a particular environment (e.g. the location of histones). Challenges were summarized including what is the nature of the structure and dynamics of early assembly, where are the counterions, what happens in non-aqueous environments, what happens during non-equilibrium assembly or in external fields, how can we control and understand pattern recognition and programmable assembly beyond hybridization?

The final part of the talk described how the topology of nematic liquid crystalline (LC) drops on the order of 5 microns in diameter) is very sensitive to small amounts (~1000 molecules per drop) of added molecules such as endotoxins. The challenges for understanding these systems include the structure of the LC interfaces; the ionic species at the water LC-interface; the dynamics and coupling to the bulk; the effects of strain, flow, magnetic and electric fields; and the design rules for LC-nanocomposites as a materials design platform.

Some of the discussions centered around the ionic structure. Knowing where the ions are is important and neutron scattering (NS) is a good technique to determine that. Both the ion distribution at an air-water interface and ion distribution at oil-air interface would be interesting and could be measured with NS. The ion distribution around a protein would be interesting to measure since it determines the local charge on the protein. If possible, obtaining the state of the charge would also be useful. It was also pointed out that access to large amounts of beam time is needed to solve these types of major problems.

Matt Helgeson, UC Santa Barbara

Matt described out-of equilibrium states of materials through arrested states of arrangements of colloidal particles. The topic of programmable materials properties through well-defined surface interactions of nanoparticles (e.g. particle shape or asymmetric forces) was one of the running themes for the workshop (Helms, Gang, Helgeson). These include "designer colloidal gels." The goal is to answer the questions: If you know the arrested non-equilibrium state, can you design a particle to achieve that state? The variables in these materials include different particle shapes and different particle

interactions including long range and possibly field induced interactions. The grand challenge is to develop an understanding of the dynamics of gelation at the mesoscale. The time scales involved in these systems range from miliseconds to minutes and the length scales from 10's microns to 10's of nm. Neutron scattering provides the structural details using USANS and SANS. Analytical and phenomenological models lack the complexity for de novo design. The need is to connect more sophisticated simulations with neutron experiments to understand rheological structure.

Tonya Kuhl, UC Davis

Tonya presented work on biomembranes and scattering. One of the big challenges for neutrons is to make the measurements that are interesting to biologists (e.g. studying biologically and medically relevant systems). Many measurements of single bilayer systems can be performed with x-rays so the problems using neutrons should be selected carefully. For example, the in-plane structure of membranes containing integral proteins which don't have x-ray contrast. Protein crystallography is another example. Moving beyond biophysics to biology is a grand challenge.

Michael Rubinstein, University of North Carolina

Three grand challenges were presented. First, can non-DNA-based self-replication be developed to make useful objects (e.g. nanowires, nanotransistors, or nanomotors)? The systems replicated could be chemical groups, colloids, or particles. A fundamental recipe for replication was presented for obtaining growth from a "soup of letters" composed of blocks of materials (e.g. polymers) bound in a particular sequence with strong physical bonds. This template would be used to create duplicate sequences which could be reproduced exponentially. The second challenge would be to add a container (membrane or micelle) to encapsulate such a polymer system. As the system grows it would split into identical daughter particles. The third challenge is the creation of active polymer gels from networks of motile colloidal pairs with either temporary or permanent bonds. The motion of the gels could be driven through the control of external (e.g. magnetic) or internal (e.g. local chemical) activity.

Cecilia Leal, University of Illinois

Cecilia discussed biomimetic materials. Nature exhibits many functions that we would like to copy synthetically, but they must first be understood. Previously, work they had done was to understand artificial mitochondria composed of cubic phases of lipids and short interfering RNA (siRNA). These could be systems for delivery of siRNA to "silence" malfunctioning genes. More recently, in addition to gene delivery, other functions of biomaterials are being pursued including understanding super-hydrophobic surfaces and antifouling surfaces. The in-plane dimensions of the surface structures of these materials are on the order of a few tens of nm. The challenge is to study these structure and kinetics of these systems during assembly and disassembly in biological media. One needs to understand both the equilibrium and non-equilibrium kinetics of these materials. To understand the non-equilibrium meso-dynamics one needs time-resolved, in situ, experiments which can resolve structures in crowded/complex systems as a function of external stimuli. Data analysis including readily available line shape analysis would also be required.

Post Presentations Discussions

There are still many questions about extracellular matrices that are important with little experimentation performed as of yet. How to prepare biologically relevant realistic samples may be an issue. As a community we need to think about how far we need to go to into the details to determine the fine detail. Biologists know where the ions are in their materials so this may not be a problem. They have been labeling them for years. How ions are interacting with materials may be important for their behavior. It is important for industry to understand the mechanism. Industry has been putting nanoparticles into material for years and still doesn't know where the particles are and this is important. Another point was made that the need for experiments to be relevant to biology, industry, etc. is just one aspect, but everything we do doesn't need to be immediately relevant. Basic research is very important!

One question came up as to whether we can we make a neutron laser so we can get the flux up by orders of magnitude? The answer was no, but increasing flux by a couple of orders of magnitude at say the second SNS target station is possible. Currently it takes too long to do an experiment on a biological system. Need long wavelength neutrons to make a neutron microscope that would be relevant. Analysis is a real bottleneck in understanding the neutron experiments. There is a strong need for computational models to couple with data analysis especially for researchers who are not primarily neutron scatterers. Also, DOE needs to put people power into these resources – people to run and help. A new model for doing experiments and especially for training students at the facilities may be needed.

Breakout Session Report

Discussions preceded the determination of the list of challenges. With high magnetic fields new states of matter can be organized. This is peripherally related to neutrons. What techniques can be applied to a trajectory of counterions in electric fields? You can study a specific ion (e.g. plus ion vs. minus ion). Ionic movement in flows is nice, oscillatory flow in simple ionic systems would be interesting. Water penetration into a polymer brush is important in concentration profiles. Ionic liquids are important – polysalts.

By selective deuteration you can ask important questions about protein folding. Some proteins are better for NS – such as unfolded proteins and misfolded proteins. Protein-membrane interactions would be a good target. Want to look at very small aggregates that are 2 or 3 molecules in nucleation of an aggregate. NS has been used to do this sort of thing. Chirality invoking solid phase precipitation is another interesting topic. By selective labeling you can see the distribution of structure, vs. crystalline or non-crystalline and order at interfaces on scale of 10 nm is important. Foam structure is of interest to P&G but they are not using scattering as of yet. How well the foams drain is of interest. One doesn't get good scattering contrast with x-rays on soft surfactant assemblies. We need better methods for labeling. Oak Ridge has a nanocenter that could help with labelling methods and they have some people who do this, but they need more. Another industrially relevant question is how do micelles change

structure when you introduce additives and how do these the structural changes relateto dramatic changes in the rheology. New sources need to have ability to use other techniques such as microfluidics, lab on a chip.

What is the status of standing x-rays for neutrons? If you can label one specific amino acid, this is one of the most non-destructive ways to label. Do deuterated proteins hydrogen bond the same way? The idea of measuring strain at a molecular level would be important. Organic-inorganic composites such as hydroxyapatite and bone morphogenic proteins should be of interest to NIH. This would be of interest in lubricants and coatings on artificial hips. These things will become important with an aging population. With neutron tomography one can look at what is happening to the squishy materials around the hard material. ILL has facilities where you can deuterate the whole protein, but deuterating selective amino acids easily should be a high priority.

Grand Challenges:

- Ionic movement in gels, flows, brushes,…
  - What ions carry current?
  - Eddies?
  - Dependence on H2O content?
- Ionic liquids
  - Solvents and additives
- Proteins/glycoproteins/polysacharides
- Misfolded proteins
- Polyelectrolyes complexes
  - Structure of solids
  - Layer by layer deposited systems
- Ordered liquids
  - Interfaces, dynamics, structure
- Surfactant Assemblies
- Microbiome
- Corrosion
- Biocomposites
- Tissue structure
  - esp. hard-soft interfaces
  - Scaffold labelling

Capability Gaps and Opportunities:

- Neutron tomography
- Labelling methods
  - Need greater support
  - Need specific labelling for proteins
- Need auxillary equip
  - Microfluids

– Rhelology

D. Surfaces/Interfaces

Presentations

Dvora Perahia, Clemson University (keynote)

Dvora discussed simple systems such as homogeneous, structured or nanoparticle-incorporated polymers containing a variety of surfaces and interfaces in thin films and bulk. All of these are affected by processing conditions and confinement effects. One important, challenging area is in ion containing polymers where the ionic and backbone interactions provide competing interactions. Important interactions may be at liquid/air interfaces, at internal interface between the polymer and liquids, or at the interface between ionomers and non-ionic polymers. In thin films of these materials, in-situ, time-dependent neutron reflectivity studies of rigid ionomers reveals information about the time-dependent diffusion profiles. This would allow one to connect the diffusion properties to the heterogeneous structure and ionic motion. A large q-range is needed to capture the structure over all of the required length scales. Short runs over a limited q-range were shown that took one minute each to collect. The results of the diffusion of alcohols into a film surface were also presented. It was found that there is a non-uniform distribution of alcohol in the films and that the diffusivity was orders of magnitude lower in molecularly thin films than in polymer membranes. To further understand these phenomena one needs the ability to probe kinetics (need higher intensity and proper instrumental configuration); larger q ranges; and in-plane changes, all with an in situ instrument environment for shear, and controlled evaporation.

SANS was used to examine the internal interfaces between ionomers and water. Based on the structures, a study of the dynamics of these systems was undertaken. In a dry membrane at room temperature and at elevated temperatures, the local diffusive motions are examined with backscattering spectroscopy. In that case there is little evidence for polymer motion i.e. the membrane is stationary. However, if water is protonated and the polymer deuterated, clear quasielastic scattering is observed due to the internal motion of the water. The analysis shows that there are two time scales associated with the water motion which implies that there is slowly moving water associated with the polymer and free water. In this case an extended q- and time-range for both backscattering and spin echo spectroscopy would help describe the system further in terms of the dynamics of the various components over different length scales. Further, any methods which can be developed to measure the dynamics in thin films would also further these scientific studies. The final section of Dvora's talk described how computation and neutron scattering can be coupled to understand dynamics and kinetics at an ionomer surface. As has been shown in the past by Russell et al, neutron reflectometry can be used to measure a surface density profile of two non-ionic polymers which can be interpreted in terms of the diffusion of one polymer into another. In recent studies in Dvora's group, similar studies were conducted on ionic polymers which showed that the ionic groups act as a barrier and slow down the interdiffusion. To understand this phenomenon, large scale atomistic simulations were performed to understand the details of the interfacial interdiffusion. It is key to combine both the neutron experimental studies and the computational studies to be able to quantitatively understand the diffusion at the interface.

Paul Nealey, University of Chicago

Paul discussed the need for four dimensional characterization of nanostructured, soft materials. Directed self-assembly (DSA) was discussed as a promising strategy for scalable manufacturing at the nanoscale for applications in electronics, data storage, energy applications, etc. An example was shown for how DSA can be used with diblock copolymers to obtain nanolithographically patterned structures on surfaces. The grand challenges in such systems include the characterization of the three dimensional structure of these films with 1nm resolution or better, characterization of the time evolution of these structures during the assembly process, and understanding such heterogeneous systems from microns down to nm dimensions. Quench times are ~ 1 sec and the process is non-reversible. An example was given of how to start with a patterned surface and multiply the structure (number of lines in a grating for example) by a factor of 2 or 3X. These can be made on large wafers (e.g. 300mm diameter) with small (5mm X 8mm) processed areas. The challenge is to make tools that can survey all of the areas for structural information. There is an opportunity to combine experiments with modeling and simulation to understand and develop these systems. Examples were shown of how the in-plane structure is being measured successfully with x-rays and compared to simulations. The question is whether neutrons can be used to take advantage of contrast.

Chris Soles, NIST

Chris began by discussing how interfacial dynamics influences many applications of thin films including chemically modified photoresists, fuel cell membranes, batteries, filtration, interfacial adhesion, etc. The dynamical landscape contains time scales from 10^{-15} seconds to seconds and a broad range of techniques are needed to understand the dynamical processes. The dynamics are important on disparate length scales. For thin films the challenges are limited sample volumes, the measurement time is often long and only over-simplified models are available to interpret the data. Also, a variety of structural questions can be asked about the film morphology, molecular orientation, phase behavior, thickness, etc. which require a detailed molecular picture. Since the measurements take long times they are often slow and labelling is often required. An example was presented where data interpretation of small angle and surface x-ray scattering was reasonable but lacked molecular detail, but when coupled with simulation, important insights were gained at to structural details. The challenges are to integrate multi-modal characterization into simulation inputs for both structure and dynamics information. Similarly, neutron data must be integrated with other techniques to be fully useful.

Igal Szleifer, Northwestern University

Igal presented a talk on coupling between molecular organization, physical interactions, and the chemical state in soft materials. The inspiration for these studies comes from the desire to understand the chemical and biological processes in living cells where the competition between chemical reaction equilibrium and physical interactions drives the cells' functions. The nature of these processes is such that they are highly inhomogeneous and there are several competing physical interactions while chemical reactions are occurring. Several examples were presented of calculations of systems expressing this competition. In the first example, the calculated morphology phase diagram for a surface-grafted, weak polyacid showing different in-plane surface structures. In a second example, the structure of weak polyelectrolyte thin film hydrogels was discussed. In these systems, the local, internal pH was calculated as a function of distance from the grafting surface for various salt concentrations. A third example presented calculations on membrane pores showing how the potentials of mean force vary on model particles to understand the driving force across the membrane. The last example showed how one may achieve enhanced binding to target cells by varying the physical and chemical interactions between binding receptors and model particles (either polymer coated nanoparticles or micelles). In all of the examples, experimental measurements of the local structure and chemical state are needed.

Post Presentations Discussions

There are several candidates for use in fuel cells. However, most of the companies producing fuel cells are going out of business. The membranes need to be cost effective, durable and reliable, but this hasn't been achieved. Alkaline membranes are cheaper, but reliability is still an issue. One of the grand challenges in these materials is understanding behavior far from equilibrium. Boundary conditions need to be defined properly for the development of theory. Internal interfaces in multicomponent systems such as fillers and nanocomposites are another challenge as well as interfaces between biological systems and materials. A lot of contrast matching is needed to sort out the various components. Another topic for surfaces is to understand the change during the glass transition at interfaces in multicomponent systems. This is part of the bigger challenge of understanding dynamics in thin films and at interfaces. The kinetics of materials at interfaces is also important. The challenge would be to measure structural changes during microseconds (now 1 second is possible). Focusing optics might be able to help in this case. Another technique which would be useful is neutron imaging at short time scales with high resolution. A general topic of importance is materials aging. Since x-rays are a destructive probe for soft materials, it can be difficult to repeat measurements over long periods of time. For these kinds of measurements the challenges include developing proper samples and calibration standards. It's akin to the problem of measuring CAT scans over periods of years.

Breakout Session Report

Grand Challenges:

Interfaces are hard to define. It really is a grand challenge. What defines the interface is essential for us to be able to establish the boundary conditions over multiple length scales. At interfaces by nature, the dynamics is very different as opposed to the bulk. Establishing the boundary conditions is very important. Interfaces by nature are anisotropic. What you want to look at are structural characteristics and dynamics as well as doing chemistry at interfaces.

The question is why neutrons, as opposed to x-rays. One thing that hasn't been mentioned regarding x-ray is that with soft X-rays, experiments have to be done under high vacuum where the same experiments can be routinely performed in air for neutrons. Neutrons are great in terms of labeling of samples with minimal perturbation. Neutrons have the advantage of being able to look at buried interfaces. In terms of the time and length scales, neutrons are ideally suited for looking at interfacial problems in general.

What sort of impacts does it have? If you look at transport phenomena, structural changes and impurities at interfaces, it will be great. If you can define the interfaces, the boundary conditions may actually tell us how we can design specific interfaces. One goal is, working with theorists, that we can design an interface which has a specific structure and function. For multicomponent, multi-phase systems, interfaces are very important. As mentioned for organic photovoltaics, the interfaces are exceptionally important for the functions of devices. When you got the devices, you can do an experiment using neutrons to probe transport phenomena and dynamics of materials right at the interfaces.

Capability Gaps and Opportunities:

1. New source
    - -Open up q range
    - -Enhance brightness, beam size (x200/CNCS instrument)
2. Enhance BACKSCATTERING resolution

3. We previously mentioned the second target station. One of the advantages of this second target station is that this opens up q range, in another way, opens up spatial resolution that you can decode and define what precise interface it is. That could be important. Increasing the effectiveness about 200 times, if that is true, opens up the ability to be able to look at dynamic phenomena at interfaces relatively straightforward. What generally is going to be necessary would be a brighter source. One has the ability to do the experiments more rapidly and look at the data real time. Processing data in real time during the experiments along with transferring data into information having easy access to the data are very important and this is a critical issue that has been address by the x-ray community.
4. Real time data visualization
5. Data >> information assessment: Data reduction and analysis are very critical. Dedicated high speed computers will be required.
6. Energy filtering
7. Sample environments that can do several functions simultaneously
8. Coupling to other techniques
9. Detector development in terms instrumentation is very important and is going to be the moderator development, basically, being able to enhance long-wavelength running.

E. Instrumental Needs

Presentations

Sunil Sinha, UC San Diego (keynote)

Sunny introduced several grand scientific challenges including chemical functionality at polymer-nanoparticle interfaces; kinetic evolution and non-equilibrium phenomena; studying processes in real time; flow-induced structural phenomena; transport of structure and defects; how to control thermal/electrical/ion structure and transport; controlling glassy, gelled and jammed states in soft matter in bulk and at interfaces (also in frustrated spin/quantum systems); active, anisotropic and multicomponent systems (polymers, suspensions, biological systems); soft matter under extreme environments and confinement; dynamics of biomolecules and relation to their function; super hydrophobicity, and the relation to structure/wetting at surface – developing a more structural understanding of wetting at the nanoscale; diffusion and transport at interfaces; the effect of peptides, proteins, etc. on interfacial structure/curvature and can we extract from scattering something about the membrane properties, e.g. Gaussian curvature (this needs new theories); ionic gels and ionic liquids, particularly in relation to field-driven or charge transport effects; and self-healing and smart materials.

All (or many) of these systems can be characterized by inhomogeneous dynamics, multiple relaxation processes, large number of local free energy minima separated by O(kT), and kinetic processes. For the latter, the x-ray community has a head start on many of these challenges due to better time resolution. The kinds of things we might want to measure with neutrons include velocity-velocity correlations and collective dynamics.

Some of the capabilities challenges include micro (or even nano?)-focused neutron beams; the need for reflectometers with capability for real-time measurements/off-specular measurements (again, hard to compete with x-rays for time – may be some things, especially magnetic phenomena, where neutrons have an advantage); and GIND and GISANS to measure interfacial kinetics using reflectivity and diffraction from membranes. We need time-dependent SANS/USANS and ultra-high resolution (small

beam) SANS. Also, the simultaneous ability to do SANS/diffraction in real time is needed. X-rays already do this with SAXS/WAXS instruments. The community wants all length scales from nm to microns at the same time (without stitching data together). One way to achieve this is for example (Roger Pynn): spin echo scattering angle measurements (SESANS) using polarized neutrons. This technique measures the Abel transform of a correlation function and therefore gives information on the real space correlation function and automatically accounts for multiple scattering. This technique can probe 20 nm – 20 um and is good for strong scatterers.

For inelastic instruments, we need to extend NSE to longer time scales. We also need faster experiments: can we do real time measurements on NSE? This would allow new measurements of diffusion/jump-diffusion in ionic/electronic systems. Ultra-cold neutrons using Doppler-shifted Bragg scattering could be used to shift the spectral peak very long wavelengths. Single-neutron coherence lengths would allow for speckle pattern measurements, e.g. angular autocorrelation functions. This would allow for direct measurements of rotational symmetry in samples that are macroscopically isotropic on average.

New data analysis methods to treat complex/multi-component systems are critical. Right now there is very little user-friendly software to analyze data. We need convenient, widely-spread software that is accessible to users at all skill levels. Sample environments and ancillary equipment available at the facility are also crucial. Langmuir troughs, humidity/temperature cells, Brewster angle microscopy, electric and magnetic fields, flow cells, and more are needed. When researchers perform experiments, people focus on the "big hit" studies and projects. They go to the facilities that have what they need in terms of experimental support, not necessarily the facility with the highest flux.

Questions/comments:

- How do we focus a beam so small? What is the theoretical limit? Series of neutron lenses can allow for focusing down to sub-mm. Can use Fresnel zone plates to do further focusing (as is done in x-rays). Could also make the beam ultra-cold.
- Is this relevant/could be achieved at a second target? Yes. Purpose of second target station planned to be for low-energy, long-wavelength neutrons and instruments.
- Comment: comparison between HFIR and SNS, shocking that fluxes are higher at the steady state reactor.
- What is not clear is what the advantages of neutrons are to scientific grand challenges for the non-experts. What can we do with neutrons that we can't do with anything else, especially x-rays? Not clear whether all of these problems *should* be addressed using neutrons. Biggest problem with x-rays is damage to sample, big advantage for neutrons particularly with poorly scattering/dilute systems. Contrast variation/selectivity is still an advantage. Penetration of neutrons through materials that x-rays can't. Neutrons are particularly good for quasi-ordered/disordered systems. Tonya: neutron scattering provides an extremely important complimentary data set to microscopy, x-ray, etc.
- On ancillary equipment – do x-ray/other facilities do this better? Europeans equip their facilities with much better equipment. More funding is needed for ancillary equipment.

- Also, there is a big need for support for preparing/modifying surfaces.

Tom Russell, University of Massachusetts, Amherst

Tom started by discussing glasses and jamming – and the need for mapping out relaxation spectra. Kinetically trapped interfacial systems, and coarsening of interfacial structures (bi-gels) … very difficult to look at with x-rays in bulk sample, but easy with neutrons. To look at polymer chain topology effects on dynamics/rheology is problematic using soft x-rays. Soft particle assemblies and effects of particle deformability on connectivity and assembly is another question. What is happening with surface ligands that drive assembly? One should look at surface instabilities at polymer interfaces. In shape-changing materials, we need information on morphological changes in large objects due to differential swelling at the nanoscale and neutrons are good for solvated systems vs. electron microscopy.

Instrumental needs: Beam focusing for SANS/inelastic/neutron microscopy. Low energies/frequencies to look at slow modes. Inelastic reflectivity. High-q dynamics w/ high resolution. How fast can we do a measurement? Really need sub-second resolution. Can we get it all in one pulse? Can the pulse structure be used by analysis of wavelengths? Can we do something analogous to speckle scattering?

Wei Chen, Argonne National Laboratory

Wei presented interfacial profiling of buried interfaces in polymer thin films using soft resonant x-rays. RSoXS gives similar info to SAXS and soft x-ray spectroscopy, i.e. small angle scattering with chemical specificity. It uses the x-ray absorption edge to isolate signals from individual types of atoms. Results on PS spheres (40 nm) dispersed in PAA thin film (~250 nm thickness) were presented where scattering close to absorption edge shows shift in particle size due to compositional heterogeneity at particle/polymer interface. Results on block copolymer thin films, lamellar microdomain structure (PS-PMMA, 90 nm film thickness). Enhancement/dispersion of higher order diffraction peaks at absorption edge allows access to interfacial profile between lamellae. The technique can be performed in reflection geometry to obtain depth sensitivity to interfacial profiles. Challenges: complex hierarchical systems with interfaces at multiple length scales.
Questions/comments:

- Without resonance, looks like the structural information is still there for polymer-particle films. What does resonance provide? Intensity is enhanced by 3 orders of magnitude.

Chinedum Osuji, Yale University

Chinedum posed the question of how can we fabricate perfect single crystals of soft matter with arbitrary orientation? How do we better characterize perfectness/defect density? This would enable lots of new technology. Magnetic field-driven assembly was discussed where high-field magnet environments have been constructed for simultaneous SAXS/WAXS – yielding structure up to 60 nm. This allows one to break degeneracy problem by rotating sample. Need field compensation at source to prevent interactions with magnet. Applications include nanoporous membranes by selective degradation of blocks and polymerization of lyotropic surfactant mesophase. Use TEM as complementary technique to look at low density of defects.

Grand challenges: Characterizing defect density and relating to transport. Need ability to impose multiple/complex structured (spatial/temporal variation) fields on soft matter while doing scattering. Can neutrons really help?

Questions/comments:

- What type of defects? Domain ends, grain boundaries, line defects.
- How quick are the kinetics? Ten minutes.

Tom Witten, U. Chicago

Tom discussed the question of how do we measure spatial distribution of stresses in soft matter, even when spatial distribution of matter is unimportant/irrelevant? Many hypotheses in rheology gels/emulsions/lyotropic systems depend on spatial distribution of stresses within the material. Posit: nuclear spins are sensitive to stresses in inorganic materials. Does the same hold for soft matter, and can we measure it? Possible to do from neutron spin flips. Coarsening colloidal gel – decay of dynamics with 3/2 power law. Hypothesis: collapse of force dipole explains exponent. Can we see this with neutrons? Some results from NMR indicate anisotropic stress/strain from dipole splitting in d-PDMS. One idea for measuring this would be to scatter a beam of magnetically polarized neutrons. In this case the modulation of spins would be due to stress (similar to NSE, but tracking stress instead of dynamics). Questions/comments:

- In scattering, we would measure stress-stress correlations, correct? Yes.
- Sample neutron polarization is possible at ORNL: is it sufficient? Would need ~30 tesla. Could be possible by optical pumping. Can this be done for "real" samples? Alan: long-term, plans for 40 tesla magnets.
- Trying to look at correlations of stress orientation, not direction/magnitude. Are the two analogous? This assumes that all stress due to tension.
- Could a similar principle be used to look at diffusion, similar to diffusion NMR? Possibly, but practically not soon.
- Could this have implications on jamming, where there is no connectivity? Yes.

Post Presentations Discussions

A large amount of work in biological areas on stress in fibers/chains has been done by fluorescence microscopy with ultra-resolution imaging. Neutrons would have much higher resolution. The group talked about the need to have ancillary facilities. Implication is that certain facilities should focus on certain capabilities to avoid redundancy. How do we prioritize? In the U.S. we are down to 2 facilities, run by different agencies. In this case perhaps we need redundancy? Equipment can be prioritized between different sources at Oak Ridge. There are tradeoffs in making a higher-quality beam. Spallation makes hot neutrons, gives dispersion but higher flux … cooling down significantly decreases flux. How do you optimize the tradeoff? If you could make moderators at 4 K, then could go up by factor of 25 in flux for cold neutrons. Heat transfer is a challenge from radiation heating. This is a challenge for instrumentation. Will the second target station give any capabilities for neutron spectroscopy? Yes, pulses of cold neutrons could provide distinct advantages. Huge gains in backscattering.

Breakout Session Report

Grand Challenges:

- Data analysis. ALS has team of people and the neutron source should have something similar
- Kinetic measurements with (sub-)second time resolution.
- Achieving spatial profiling at the micron-scale.
- Developing experimental environments for imposing fields (electric, magnet, flow) and extreme conditions on soft matter of arbitrary duration and spatial configuration.
- Developing facilities for sample preparation and characterization on site, particularly for biological or interfacial samples.
- Expanded capabilities for isotopic labeling of molecular components.
- Developing tools for more detailed computation/simulation methods where complex data can be modeled in real time for data where "traditional" analysis fails.
- Extending the range of dynamic measurements to the microsecond scale.
- New methods to measure local distributions of stress or anisotropy in materials.
- Making the case for neutrons as opposed to x-rays, other measurements. Neutron community operates in a closed-loop fashion.
- Phase contrast neutron imaging

Capability Gaps and Opportunities:

- For highest flux instruments and strong scattering, currently limited to minutes. Second target could achieve 100-fold increase in flux, could get down to 1 second for single-shot.
- Developing neutron optics for focusing small, sharp beams down to 1 micron. Advances in lens and mirror technology.
- Need better infrastructure at facilities for sample environment development that researchers can interface with. Europe has this, US doesn't. Need flexibility with beam time for iterative experimental design process, and funding mechanisms to move it forward.
- Limited resources and institutional barriers. For very high-value materials, expanding bandwidth.
- Need simulation methods that can be constrained using data, supplementary information. Expanding capabilities for computationally-involved data analysis, streamlining data analysis with simulation tools and supercomputing resources.
- Currently, Oak Ridge can achieve 100 ns with NSE. ILL can do 800-1000. Can we push further? Development of spin echo at HFIR would allow order of magnitude faster measurements with higher dynamic and q-range.
- Need ways to homogeneously polarize spins in the sample (stress). Need very long wavelength neutrons (speckle). Better magnets. Labeling materials with nuclear spin probes?
- More broadly highlight advantages of neutrons:
    - Penetration into solids, buried interfaces
    - Isotopic sensitivity
    - Measurements utilizing magnetic spin (NSE, SESANS, etc.)

- Low-energy dynamics
- Many x-ray techniques require special conditions (high vacuum, etc.)

F. Industrial Needs

Presentations

Eric Amis, United Technologies (keynote)

In his talk Eric discussed that in his industry, manufacturing issues are the challenge. Industry has increasing pressures in manufacturing. The old techniques were well understood (like machining) but as new techniques (e.g. additive manufacturing) come along there is an associated cost with understanding the properties of these new manufacturing techniques. He presented a new paradigm for an integrated model where manufacturing, performance and materials are connected by manufacturability, process and new materials properties. An example of a physics-based manufacturing process is in the machining of turbine blades where the machining time was reduced by a factor of two by optimizing the machining code based on materials physics properties. Another example of new materials technologies is in composites of soft and hard materials. More than 50% of the weight of modern commercial aircraft is made from composites. These materials were well known twenty years ago, but the qualification process and learning how to incorporate these materials into the manufacturing process takes time. Modeling of composite materials traverses science from matrix chemistry to surfaces and interfaces to manufacturing based on characterization, modeling and reinforcement strategy. Another example where advanced technology could be used is in wing deicing. Currently nichrome wires or expensive chemical deicing are used to deice wing, but using a composite carbon nanotube film would be lighter and more efficient yet, the lag in knowledge of the technology has prevented it's commercial use to date.

In aerospace composites, the materials have to have a high reliability, and in application, there has to be a low probability of failure. New materials must "buy their way in." The challenge is to reduce uncertainties in the materials manufacturing and processing using a process of Integrated Computational Materials Engineering. Another example of a new materials technology is o the various Direct Write Technologies (additive manufacturing). Soft materials play a large role in these new manufacturing processes, and there is still a lot to be learned about the materials properties. The grand challenges were summarized as: Science and Technology to Manufacturing, Process Validation and Optimization, Understand Defects and Uncertainty (structure), Understand Failure, Reliability, and Durability (time).

In the post presentation discussions it was asked how much information on these materials is open information? There is a lot of information available on these new composite materials. However, finding out what is known is often a challenge. Are Intellectual Property issues a problem? Since industry funding for research is on the rise, it is easier to get involved with industrial research, also the present innovative programs sponsored by the present White House such as the Advanced Manufacturing Initiative help in sharing information. What kind of experiments would you envision at ORNL? These might be composite to composite binding, materials repair, and cost reduction studies for aerospace grade materials. In the past, there used to be bridges from industry to universities through the large industrial labs such as Exxon, Bell Labs, etc. what is the state of the connection today? It's intriguing that the Europeans seem to have more investment in industrial science with a plan. Maybe in the US there could more ways to tie industry more closely to the national labs and those labs could fulfill that role. As

of today, it is much easier to work with some universities in terms of IP and those are the ones that industry will seek out.

Larry Hough, Solvay Corporation

Larry gave a presentation on ways industry could use neutron scattering. In the past places like Exxon had neutron scattering experts on their staff, but those resources are gone. Now, the expertise needs to be developed at the facilities for data interpretation. Also, the issue of turnaround time for experiments needs to be addressed. The time scales are often much too long for industrial problems.

Ryan Murphy, Solvay Corporation

Ryan gave the second presentation from Solvay Corporation. Industrially relevant problems that are fundamentally interesting can mutually coexist. The grand challenge is shared by academia and the national labs, but also by industries. Information form neutron scattering can add to the material portfolio with new materials (to "fill the innovation pipeline") and to reduce the barrier-to-market problems (pre-commercial to commercial). For this to happen we need to make neutrons "less mysterious" for the industrial user. Since neutron scattering expertise isn't widely available in industry, the facilities need to educate more in what can and can't be done using neutron scattering. For neutron scattering to become more useful for industry they need timely, predictable access to the facilities including an understandable IP agreement, dedicated technical resources for industrial users, help the industrial users develop knowledge of how to perform experiments, and tools and expertise for analyzing and understanding the data. Also, sample environments instrumentation and data analysis need to be developed specifically for problems in manufacturing. Some of the scientific problems that Solvay is currently exploring with universities and laboratory partners is to understand the equilibrium phases, non-equilibrium phase dynamics and high shear properties, evolution of the phases, and effects of processing in PEDOT:PSS based transparent conducting electrodes. Other examples of problems to be explored included several problems from seed germination to polymer composite structure all involving soft matter.

Bobby Sumpter, Oak Ridge National Laboratory

Bobby presented a talk on large scale simulations of soft materials. Organic materials are diverse and earth abundant, are flexible for processing, can be adapted to various substrates and are multifunctional. On the other hand soft materials age and don't yet have the performance of hard materials. There is a need for shortening the time from discovery to application through development of in-situ, real time data analysis and validation over many lengths and time scales. The challenges are to bring modeling and simulation into the experiment chain using reliable, validated models which can in turn be used to guide experiments towards new discoveries. By then combining theory/modeling/simulation with synthesis and physical characterization, behavior can be controlled and predicted. The challenges for simulations of soft materials include no universal force fields, time scales spanning ten orders of magnitude, length scales over five orders of magnitude, rough energy landscapes, non-equilibrium complexity with aging and processing, and integration with experiment. These can be mediated through use of Polymer Field Theory and hybrid approaches, automated generation of accurate potentials, efficient electrostatic models and incorporation of specialized models to run on coprocessors and accelerators. A study of the self-assembly of P3HT/PCBM blends using large scale MD simulations was presented. The size scale is consistent with thin films and the simulations covered microseconds. The simulations took five days on 10% of the Titan supercomputer. The focus of these studies was to model the domain size as a function polymer molecular weight or of additive concentration. The result of the calculations can be directly related to neutron scattering studies through the calculated intermediate scattering function S(q,t). This example highlights the needs for the

challenge of integrating synthesis, modeling/simulation/theory, in situ probes of transport (or other properties) and simultaneous probes of the structure and dynamics (neutrons).

Mike Weaver, Procter and Gamble

Mike gave the final presentation of the session. He discussed microstructural aspects and dynamics of aging in colloidal systems. Shampoo products are formulated and tested for stability. These tests over long periods of time are costly and if the system fails the test and phase separates, for example, the tests don't reveal why. More tools are needed to predict failure in these and other products. Medicated shampoos have a complicated structure containing colloidal structuring agents, active ingredients, conditioners, and surfactants. The length scales of these systems are from ~ 0.1 – 10 microns. There are models for the physical aging of these materials, but more information is needed to validate and understand these systems. Using tomographic x-ray radiography at the Swiss Light Source, they can image the materials with good resolution, however, tools with better contrast for organic materials are needed and structural information is required where the thermal fluctuations are suppressed. Ideally a method is needed in this case to study length scales form .1 – 10 microns with a sampling rate of ~ 100Hz.

Appendix I.

Workshop Agenda

OAK RIDGE NATIONAL LABORATORY

MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

Grand Challenges in Soft Matter Workshop
University of California, Santa Barbara
Elings Hall, Room 1601
May 17 - 18, 2014

Saturday, May 17th

UCSB hotel shuttle pick-up times: 7:40 a.m., 8:00 a.m., 8:20 a.m.

8:00 - 8:30 a.m. **Continental Breakfast**

8:30 - 9:00 a.m. **Welcome and charge**

- Fyl Pincus, University of California, Santa Barbara
- Matthew Tirrell, University of Chicago
- Greg Smith, Oak Ridge National Laboratory

9:00 - 10:30 a.m. **Polymers**
Chair: Fyl Pincus
Keynote Speaker: Brett Helms
Scribe: Ryan Murphy

- Brett Helms, Lawrence Berkeley National Laboratory
- Michael Chabinyc, University of California, Santa Barbara
- Gary Grest, Sandia National Laboratory
- Julie Kornfield, California Institute of Technology
- Lynn Walker, Carnegie Mellon University
- Yang Zhang, University of Illinois, Urbana-Champaign

10:30 - 11:00 a.m. **Break**

11:00 a.m. - 12:30 p.m. **Lipids/ Membranes/ Assemblies**
Keynote Speaker: Oleg Gang
Chair: Tonya Kuhl
Scribe: Cecilia Leal

- Oleg Gang, Brookhaven National Laboratory
- Monica Olvera de la Cruz, Northwestern University
- Chris Santangelo, University of Massachusetts
- Ting Xu, University of California, Berkeley
- Margie Longo, University of California, Davis

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OAK RIDGE NATIONAL LABORATORY

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12:30 - 1:30 p.m.	**Assemble for group photos** **Continued discussions from previous sessions on Polymers and Assemblies / Working lunch** **Chair: Greg Smith, Fyl Pincus, Matthew Tirrell**
1:30 - 3:00 p.m.	**Biomaterials/ Charged Systems/ Colloids** **Chair: Matthew Tirrell** **Keynote Speaker: Juan de Pablo** **Scribe: Margie Longo** • Juan de Pablo, University of Chicago • Matt Helgeson, University of California, Santa Barbara • Tonya Kuhl, University of California, Davis • Michael Rubinstein, University of North Carolina, Chapel Hill • Cecilia Leal, University of Illinois, Urbana-Champaign
3:00 - 3:30 p.m.	**Break (Refreshments provided)**
3:30 - 5:00 p.m.	**Surfaces/ Interfaces** **Chair: Thomas Russell** **Keynote Speaker: Dvora Perahia** **Scribe: Wei Chen** • Dvora Perahia, Clemson University • Paul Nealey, University of Chicago • Christopher Soles, National Institutes of Health • Igal Szleifer, Northwestern University
5:00 - 5:30 p.m.	**Daily wrap-up/discussion**
5:30 - 6:00 p.m.	**Break and walk to Mosher Alumni Building**
6:00 - 9:00 p.m.	**Dinner and Discussions** **Neutron Sciences: Present and Future** Alan Tennant, Oak Ridge National Laboratory

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OAK RIDGE NATIONAL LABORATORY

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Sunday, May 18th

UCSB shuttle hotel pick-up times: 7:40 a.m., 8:00 a.m., 8:20 a.m.

8:00 - 8:30 a.m.	**Continental Breakfast**
8:30 - 10:00 a.m.	**Instrumental Needs** **Chair: Greg Smith** **Keynote Speaker: Sunil Sinha** **Scribe: Matt Helgeson** • Sunil Sinha, University of California, San Diego • Thomas Russell, University of Massachusetts • Wei Chen, Argonne National Laboratory • Chinedum Osuji, Yale University • Thomas Witten, University of Chicago
10:00 - 10:30 a.m.	**Break**
10:30 a.m. - 12:00 p.m.	**Discussion and preliminary report writing, collecting presentations** **Chair: Greg Smith**
12:00 - 1:00 p.m.	**Continued discussions on instrumental needs and workshop preliminary report: Working lunch** **Chair: Greg Smith, Fyl Pincus, Matthew Tirrell**
1:00 - 2:30 p.m.	**General/ Industrial Needs** **Chair: Fyl Pincus, Matthew Tirrell** **Keynote Speaker: Eric Amis** • Eric Amis, United Technologies • Larry Hough, Solvay COMPASS Lab • Ryan Murphy, Solvay COMPASS Lab • Bobby Sumpter, Oak Ridge National Laboratory • Mike Weaver, Procter & Gamble
2:30 - 3:00 p.m.	**Wrap-up**

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Appendix II.

List of Attendees

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

Participants	Affiliation
Eric Amis	United Technologies
Phil Brit	Oak Ridge National Laboratory
Michael Chabinyc	University of California, Santa Barbara
Wei Chen	Argonne National Laboratory
Hans Christen	Oak Ridge National Laboratory
Juan de Pablo	University of Chicago
Oleg Gang	Brookhaven National Laboratory
Gary Grest	Sandia National Laboratory
Craig Hawker	University of California, Santa Barbara
Matt Helgeson	University of California, Santa Barbara
Bret Helms	Lawrence Berkeley National Laboratory
Larry Hough	Solvay COMPASS Lab
Julie Kornfield	California Institute of Technology
Edward Kramer	University of California, Santa Barbara
Tonya Kuhl	University of California, Davis
Cecilia Leal	University of Illinois, Urbana-Champaign
Marjorie Longo	University of California, Davis
Ryan Murphy	Solvay COMPASS Lab
Paul Nealey	University of Chicago
Monica Olvera de la Cruz	Northwestern University
Chinedum Osuji	Yale University
Dvora Perahia	Clemson University
Philip Pincus	University of California, Santa Barbara
Roger Pynn	Indiana University
Michael Rubenstein	University of North Carolina at Chapel Hill
Thomas Russell	University of Massachusetts
Chris Santangelo	University of Massachusetts
Sunil Sinha	University of California, San Diego
Greg Smith	Oak Ridge National Laboratory
Christopher Soles	National Institute of Standards and Technology
Bobby Sumpter	Oak Ridge National Laboratory
Igal Szleifer	Northwestern University
Alan Tennant	Oak Ridge National Laboratory
Matthew Tirrell	University of Chicago
Lynn Walker	Carnegie Mellon University
Mike Weaver	Procter & Gamble
Thomas Witten	University of Chicago
Ting Xu	University of California, Berkeley
Yang Zhang	University of Illinois, Urbana-Champaign

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Appendix III.

List of Invited and Contributed talks

Polymers		
Pincus, Fyl	**N/A**	**Chair**
Murphy, Ryan	**N/A**	**Scribe**
Helms, Brett	**Understanding Interfacial Structure-Transport Relationships in Hybrid Mesostructured Composites**	**Keynote Speaker**
Chabinyc, Michael	Moving electrons in polymers	
Grest, Gary	Accessing Long Times in Polymers/Soft Matter	
Kornfield, Julie	Transient Conformation and Structure	
Walker, Lynn	Structural Changes in Block Copolymer Solutions	
Zhang, Yang	Liquids, Supercooled Liquids, and Glasses -- Challenges in Understanding Slow Dynamics	
Lipids/Membranes/ Assemblies		
Kuhl, Tonya	N/A	**Chair**
Leal, Ceclia	N/A	**Scribe**
Gang, Oleg	**Programmable Matter and Its Transformations**	**Keynote Speaker**
Olvera de la Cruz, Monica	Electrostatic Driven Assembly	
Santangelo, Chris	Responsive gels for designer materials	
Xu, Ting	Toward Hybrid Biomaterials Based on Peptide, Protein and Synthetic Polymer	
Longo, Margie	Engineered membranes: too small, too dynamic, too buried for standard fluorescence microscopy.	
Biomaterials/ Charged Systems/Colloids		
Tirrell, Matt	N/A	**Chair**
Longo, Margie	N/A	**Scribe**
de Pablo, Juan	**Emerging opportunities and challenges for biomaterials research**	**Keynote Speaker**
Helgeson, Matt	Beyond fractals: probing structure and evolution of colloidal and macromolecular gels	
Kuhl, Tonya	Structural characterization of integral membrane proteins	
Rubinstein, Michael	Staying Active - a Way Towards Soft Life	
Leal, Ceclia	Dynamics of Lipids, Membranes, and Assemblies Self-organization	
Surfaces/ Interfaces		
Russell, Thomas	N/A	**Chair**
Chen, Wei	N/A	**Scribe**
Perahia, Dvora	**Structured Soft Matter: a Key to Controlled Interfacial Structure and Dynamics**	**Keynote Speaker**
Nealey, Paul	Quantitative four-dimensional characterization of nanostructured soft materials	
Soles, Christopher	Data analysis 2.0: The need for modeling when interpreting scattering data from functional polymers	
Szleifer, Igal	Coupling between molecular organization, physical interactions and chemical state in layers of soft materials	
Dinner Lecture		
Tennant, Alan	**Neutron Sciences: Present and Future**	**Keynote Speaker**

Instrumental Needs		
Smith, Greg	N/A	**Chair**
Helgeson, Matt	N/A	**Scribe**
Sinha, Sunil	**Instrumental Needs for a Stellar Soft Matter Research Program**	**Keynote Speaker**
Russell, Thomas	Soft Matter	
Chen, Wei	Sketch interfacial profiles using resonant soft x-ray scattering	
Osuji, Chinedum	Scattering Studies in Soft Matter Under High Magnetic Fields and Complex Geometries	
Witten, Thomas	Scattering off T-2 relaxation	
General/Industrial Needs		
Pincus/Tirrell	N/A	**Chairs**
Amis, Eric	**Advanced Manufacturing: The 21st Century Materials Challenge**	**Keynote Speaker**
Hough, Larry	Soft Matter in Harsh Media	
Murphy, Ryan	Organic/Inorganic Hybrid Materials for Industrial Applications	
Sumpter, Bobby	Large-Scale Simulations of Nanostructured Soft Matter and Multicomponent Materials for Energy Science Applications	
Weaver, Mike	Microstructure and dynamics of aging in colloidal systems	

Appendix IV.

Invitation Letter

Gregory Smith
Biology and Soft Matter Division
P.O. Box 2008
Oak Ridge, TN 37831-6473
(865) 241-1742

March 7, 2014

Dear Colleague:

As part of a process to identify the needs of the scientific community in Neutron Scattering, we are organizing workshops to identify Scientific Grand Challenges for the next decade. Workshops are being convened in four complementary topics: Soft Matter (@ UCSB), Quantum Condensed Matter (@ LBNL), Energy Science and Technology (@Chicago) and Biological Systems (@UCSD).

In particular, we would like to identify problems where neutron scattering may be used alone or in combination with complimentary techniques. The key outcomes of all these workshops will be presented to DOE in order to assist them in defining the future course of Neutron User Facilities. The workshops are limited to approximately 40 participants and are by invitation only. Each participant will get an opportunity to contribute a short presentation as they wish.

With this letter, we are inviting you to join us in defining the needs in Neutron Science as relevant to Soft Condensed Matter. We are planning to hold the workshop on May 17-18 at University of California Santa Barbara. There will be no registration fee for the workshop and local arrangements (food and lodging) will be covered. Blocks of rooms at a local hotel will be reserved for the workshop. Limited travel funds may be available. In order to facilitate the logistics of organizing the workshop, we would appreciate it if you could let us know by return email if you are able to join us, by March 12. Please direct your responses to Ava Ianni (ianniav@ornl.gov).

We look forward to a vigorous and thought-provoking workshop.

Best wishes,

Fyl Pincus
Workshop Convener

Matt Tirrell
Workshop Convener

Greg Smith
Workshop Facilitator

Appendix V.

Acknowledgments

Workshop logistics were managed by Ava Ianni (ORNL) and Joanne McNie (UCSB). The organizers would also like to thank Peter Chung for providing transportation and to Ram Sheshadri for taking the workshop photograph. The organizers are grateful to ORNL, UCSB Physics and Engineering, and UC IME for providing financial support and to UCSB for hosting us Elings Hall.