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Title: A Workshop on Enhanced National Capability for Neutron Scattering

San Diego II Meeting Report

Author(s): Alan J. Hurd
James J. Rhyne
Paul S. Lewis

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Los Alamos NATIONAL LABORATORY
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A Workshop on Enhanced National Capability for Neutron Scattering

September 5–7, 2007
San Diego, CA

Executive Summary

This report summarizes the findings and recommendations of San Diego II: A Workshop on the Enhanced National Capability for Neutron Scattering. Sixty scientists attended this two-day workshop at the Humphrey's Half Moon Inn and Suites in San Diego, CA, to discuss issues regarding the future of the Lujan Neutron Scattering Center (Lujan Center) at the Los Alamos Neutron Science Center (LANSCE), Los Alamos National Laboratory (LANL), from September 5–7, 2007. More specifically, the workshop was held to further refine, and to act upon, plans developed at several strategic-planning meetings about the future of LANSCE and the Lujan Center held in recent years. The San Diego II workshop was sponsored by the LANL Science Program Office, and hosted by former LANSCE Professor Sunil Sinha of the University of California, San Diego.

San Diego II had the full input from leadership at all the major U.S. neutron facilities: the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR), Oak Ridge National Laboratory; the National Center for Neutron Research (NCNR); and the Intense Pulsed Neutron Source (IPNS). Because attendees represented a broad range of the national—and to a smaller extent, international—neutron scattering community, a national perspective on the neutron scattering landscape was evident at San Diego II.

Alan Hurd, Director of the Lujan Center, gave an overview of LANSCE and the Lujan Center. His overview was followed by a plenary talk given (via video conference) by Pedro Montano, Director of Scientific User Facilities at the Department of Energy's Office of Basic Energy Sciences (BES). Plenary sessions were also provided by Dan Neumann, Associate Director of NCNR, and by Ken Herwig, Director of Neutron Sciences at Oak Ridge National Laboratory. A short, impromptu presentation was given by Ray Teller, Director of IPNS, on plans at Argonne National Laboratory for the Advanced Scattering and Imaging Institute. These plenaries encouraged deliberation and movement toward complementary, yet competitive, instruments to serve the neutron scattering community. Three breakout groups were convened to review broadly defined neutron techniques, diffraction, inelastic scattering, small-angle neutron scattering, and reflectometry. There was discussion in each group about the enabling issues of computing, sample environments, data acquisition, staffing, and beam reliability. A fourth breakout group addressed strategic issues, prerequisites, and barriers to implementing aspects of the emerging vision for the Lujan Center brought about by the LANSCE Refurbishment project (LANSCE-R) and by expected changes at other neutron facilities. There were six major findings and recommendations of this workshop.

1) The Lujan Center has a unique and major role to play in the national strategy for neutron scattering research. For this it is necessary for Lujan to proceed with plans to add capacity to the national neutron scattering capability.
2) To fully capitalize on LANSCE-R and maximize productivity requires the Lujan Center to have a full complement of competitive instruments (13 +) and talented staff. The design, construction, and utilization of these instruments will require a substantial increase in the number of Lujan Center personnel. The details of these recommendations are given in the appropriate sections.
3) It is important for the Lujan Center to exploit the synergies between its strong materials science program and the other materials science capabilities at LANL, including the Center for Integrated Nanotechnologies (CINT) and the National High Magnetic Field Laboratory (NHMFL). The Lujan Center must also develop further strategic alliances and partnerships with the University of California system and other Western universities.
4) The U.S. neutron scattering community should be given the opportunity to utilize the full capability at the Lujan Center. Further, the community is poised to develop and utilize the current and new spectrometers at the Lujan Center that will take advantage of the power and reliability afforded by LANSCE-R.
5) There is a growing willingness in BES to fund expanded operations and to restart instrumentation investment in Lujan Center once LANSCE-R is assured.
6) A window of opportunity exists for Lujan Center's development owing to the imminent closure of IPNS, the turn-on of SNS, and the national commitment to fund physical sciences via the 2007 America Creating Opportunities to Meaningfully Promote Excellence in Technology, Education, and Science Act (America COMPETES) (Figure 1).

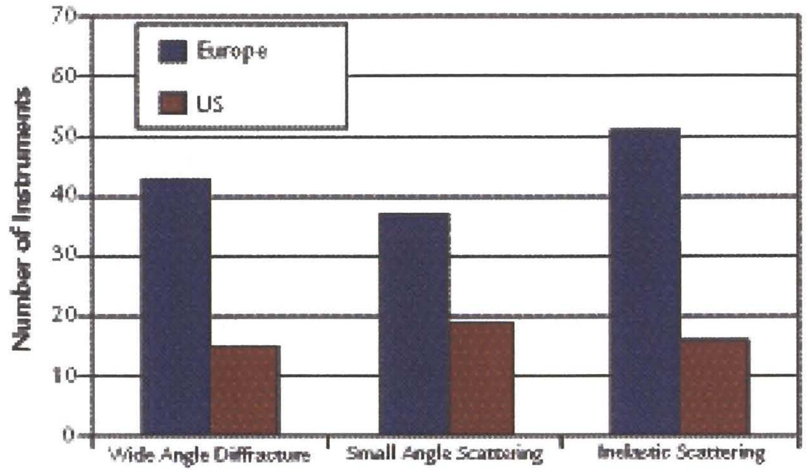


Fig. 1. The U.S. has far fewer instruments than does Europe. China, Japan, Taiwan, Australia, Europe are all moving rapidly to increase their instrumentation.

The Lujan Center today

The Lujan Center, the nation's second most powerful spallation neutron facility, and one of the world's premier spallation neutron facilities, is an integral part of the nation's neutron-based science capabilities. The Lujan Center attracts and serves a wide range of neutron scattering users, providing academic, industrial, and LANL users with an array of world-class instruments and sample environments. For reasons outlined in this report, the Lujan Center has a unique and major role to play in serving the national scientific community's needs in neutron-based science (Figure 2). This report recognizes that completion of LANSCE-R is critical for the future of the facility, because it will enable the Lujan Center to operate reliably at 135 μA for more than 4000 hours per year.

The Lujan Center's signature capabilities include its low 20-Hz repetition rate that favors long wavelength instruments, extreme testing environments, an expertise in hard and soft materials, and national security (and classified) research. For many applications, with appropriate instrumentation, the Lujan Center will be competitive with the SNS within a factor of 2 to 5 in effective flux. The Lujan Center also has the capability of providing the means to innovate, by the inclusion of test bed instruments on experimental beam lines to investigate novel ideas in neutron scattering. For example, new guides, choppers, detectors, polarization, and moderators can be researched by the neutron scattering community.

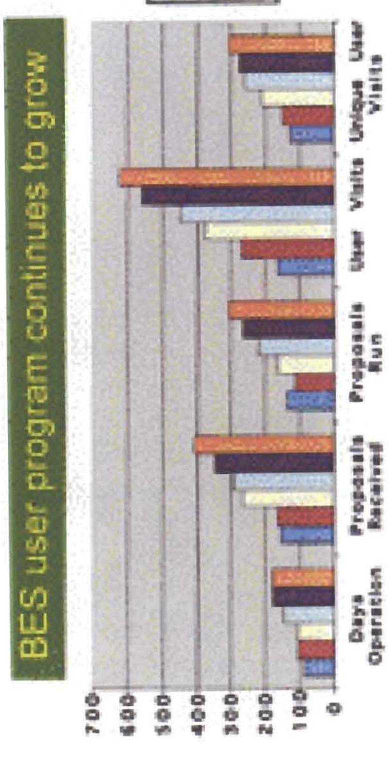
In addition to providing the neutron scattering community with sorely needed spallation neutrons, the Lujan Center provides a powerful partnership with the universities in the University of California system, the universities in New Mexico, and other Western universities.

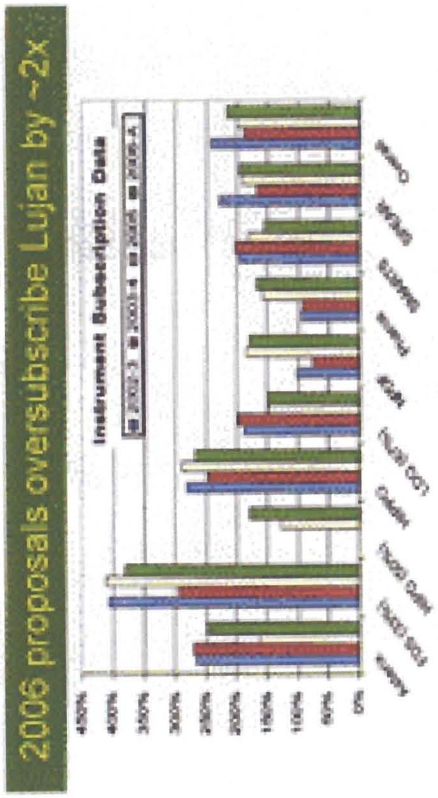
The Lujan Center tomorrow

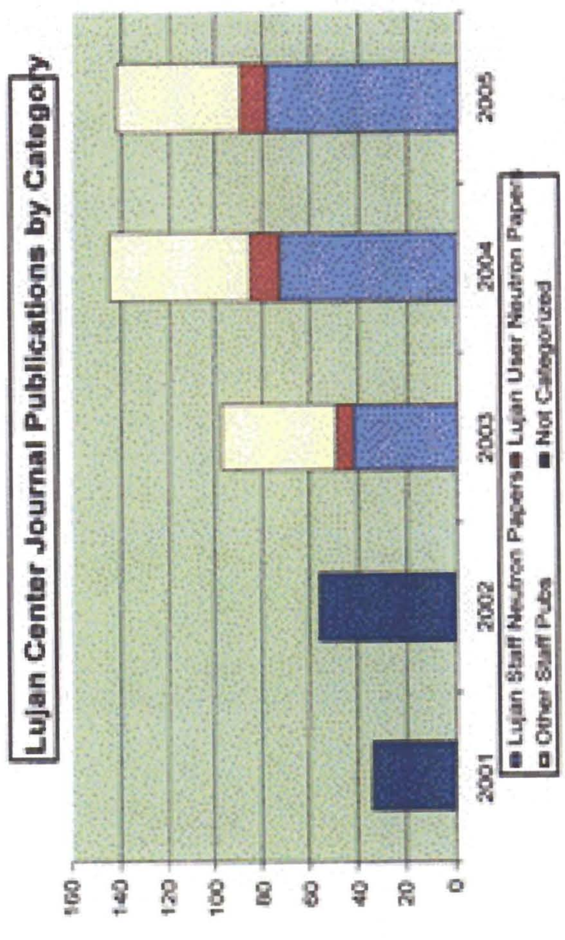
To fully capitalize on LANSCE-R, to maximize productivity, and to operate as an ISIS-class user facility, the Lujan Center should have a full complement of competitive instruments (13 +) and staff. Because users go to facilities with the best capabilities and resources, the suite of instruments should be the best instruments that broadly serve the neutron scattering community and be well staffed. This strategy is strongly supported by the San Diego II participants in this report.

Synergies between the Lujan Center and the materials science capabilities of CINT, NHMFL, the universities in New Mexico, the University of California system, and other Western universities should be enhanced with other alliances, for example, with the University of Texas system. Importantly, funding sources beyond the BES need to be explored. The recommendations from the San Diego II workshop recognize that these are key elements for nurturing the Lujan Center's, and the nation's, future success.

What follows are the specific recommendations from the three San Diego II working groups: Reflectometry and Small Angle Scattering, Instrumentation for Inelastic Scattering, and Instrumentation for Diffraction.







Note: Staff papers generally are collaborative with users, user papers have no Lujan authors. Other publications have data or analysis from non-Lujan facilities

Working Group on Instrumentation for Reflectometry and Small-Angle Neutron Scattering

Working Group on Instrumentation for Reflectometry and Small-Angle Neutron Scattering

Topics: New Instrument Concepts, Upgrades for Reflectivity, and Low-Q Diffraction

Chair: R. Pynn
Planning Group Chair: R. Hjelm
Members: A. Berkowitz, A. Parikh, M. Fitzsimmons, S. Satija, M. Foster, D. Schaefer, E. Fullerton, A. Shreve, J. Majewski, I. Schuller, and T. Mason

Summary of recommendations

1) The Lujan Center has an opportunity to contribute strongly to the national program of structure measurement at long length scales (Figure 3) by providing ISIS-level capability, or better, to its users. Lujan Center's 20-Hz repetition rate and partially-coupled LH2 moderator are ideal for these types of measurements. The installation of a fully coupled moderator could extend Lujan Center capabilities even further.

2) The reflectometers Asterix and SPEAR are world-class, well-understood instruments that could be easily upgraded with minimal investment to provide new experimental capabilities that do not currently exist anywhere in the world.

3) The Low-Q Diffractometer (LQD) will no longer be state-of-the-art when the two instruments planned for the second target station at ISIS are realized. Even though it would continue to provide useful data, LQD should be replaced with a modern instrument that can compete with the two new small-angle neutron scattering (SANS) (Figure 4) instruments at the ISIS second target station.

4) There is an opportunity for scientists at the Lujan Center, in collaboration with facility users, to pioneer novel sample-environment equipment that would enable fundamentally new science at the Lujan Center and at other U.S. neutron centers.

Soft matter studies

Research areas in soft-matter materials science that are likely to be important in the next ten years were discussed by the working group. Working group members were familiar with two lists of important research areas, one of which was recently constructed in an NSF-sponsored workshop on the future of polymer research and another of which was the result of an exercise at the CINT that identified future research directions for soft matter of particular interest to LANL programs. The lists, which have substantial overlap, categorize many exciting opportunities that exist for new science in soft materials using neutrons. For example, work that has already been done on structures found in block copolymers, colloids, surfactants, micelles, and model membranes must be extended to studies of structures that incorporate multiple components or that have characteristic lengths scales larger than the ~100 nm that can be studied at present. Study of the evolution of these structures has generally been lacking and is sorely needed.

Many candidate systems were identified. For example, the time-scales over which polymer brushes grow (tens of hours) mean that the growth could be profitably studied even at a neutron source with modest flux. In the area of biologically relevant membrane structures, past work has focused on simple model membranes and interactions between membrane proteins and simple lipid membranes or detergents. Future work will require studying membranes that more closely mimic biological systems. These systems are necessarily much more sophisticated. Studies of responsive structures that change with environment and studies of interfaces between biological materials and electronic or photonic structures will be key for new sensing technologies.

The elucidation of relationships between properties and architecture (structure-property relationships) is a broad area of inquiry that has opened up future research areas, as advances in synthetic capabilities have made it possible to create polymers and other self-assembled structures with novel molecular architectures for which "shape" is controllable. These architectures are often hierarchical, with one

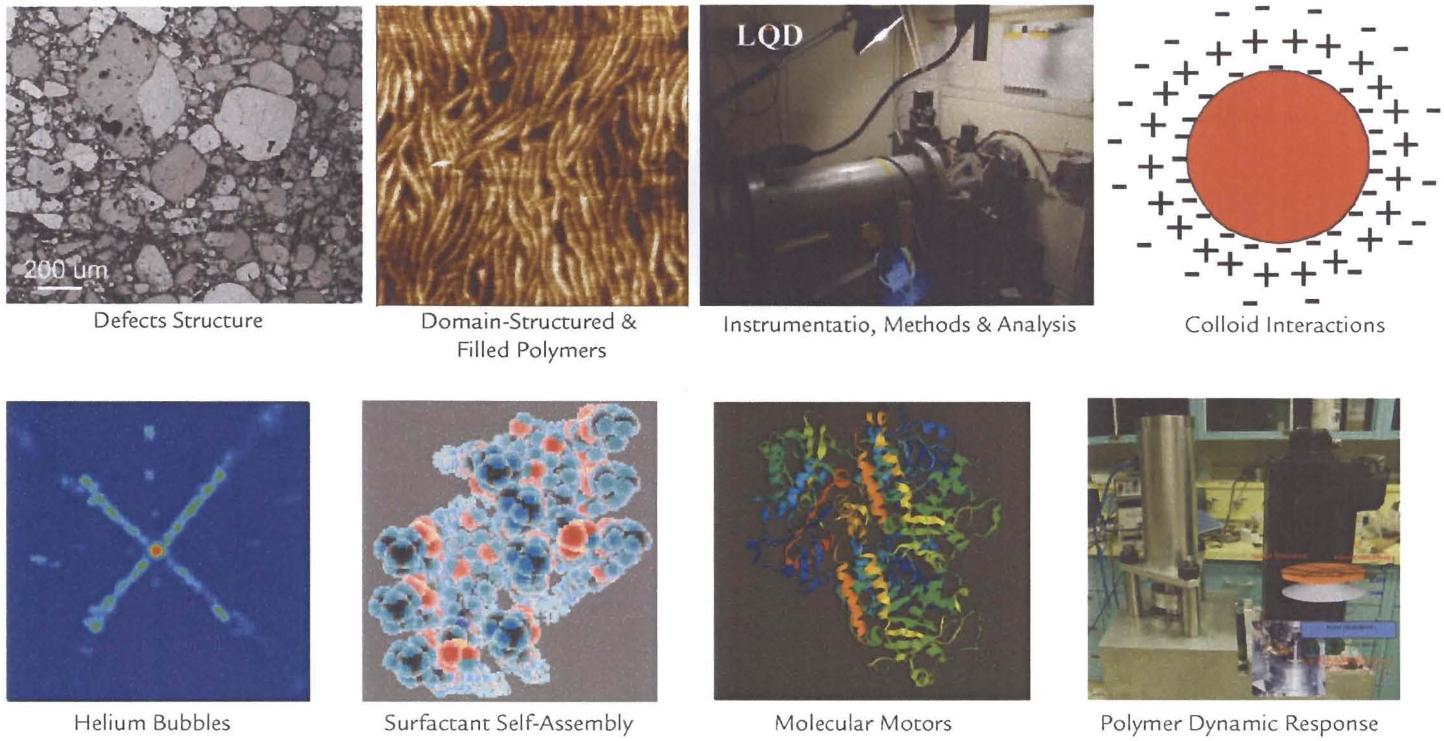


Fig. 3. Long length scales program.

structural element forming the basic unit of a higher-order structure. Complete structural characterization of such systems requires measurements over multiple length scales extending from sub-nanometer to over a micron. Structural biology, where hierarchical structures are common, also requires probes over a similar broad range of length scales.

Neutron scattering has played an important role in soft-condensed matter studies and in structural biology. The method has provided fundamental information that would not have been available otherwise. Most of the work has probed length scales below ~100 nm. Recent improvements to SANS instrumentation have extended the accessible range to ~ 2 μ for isotropic samples. There is a pressing need to extend this domain for SANS to even larger length scales and to measure anisotropic scattering in this domain. Even though other excellent tools exist for probing such large length scales, neutrons can often provide unique or complementary information because of their ability to probe buried structures, or because isotopic enrichment can be used to alter scattering contrast in a manner that perturbs structure less than fluorescent ties or tags. For example, in concentrated systems light scattering suffers from multiple scattering while neutron techniques seldom do.

Often corresponding to the diversity of length-scales, dynamics in soft matter also covers multiple time-scales. Neutron scattering has played an irreplaceable role in understanding polymer diffusion in the bulk and at interfaces, particularly with regard to the reptation postulate. Dynamic neutron scattering has also provided fundamental information on polymer main-chain and pendant-group motion. Future work will deal with confinement effects, dynamics of fractals, and diffusion dynamics of molecules that have complex architectures or are parts of supramolecular structures. Phenomena of this sort can often be studied using either methods that probe dynamics explicitly or those that probe time-dependent structural relaxations following a stimulus. The latter, pump-probe methods, suitable for use with neutron scattering instruments, need to be developed for a variety of stimuli.

Neutron reflectometry is playing a role of increasing importance in elucidating interfacial and surface structure in structural biology, biomimetic structures, composites

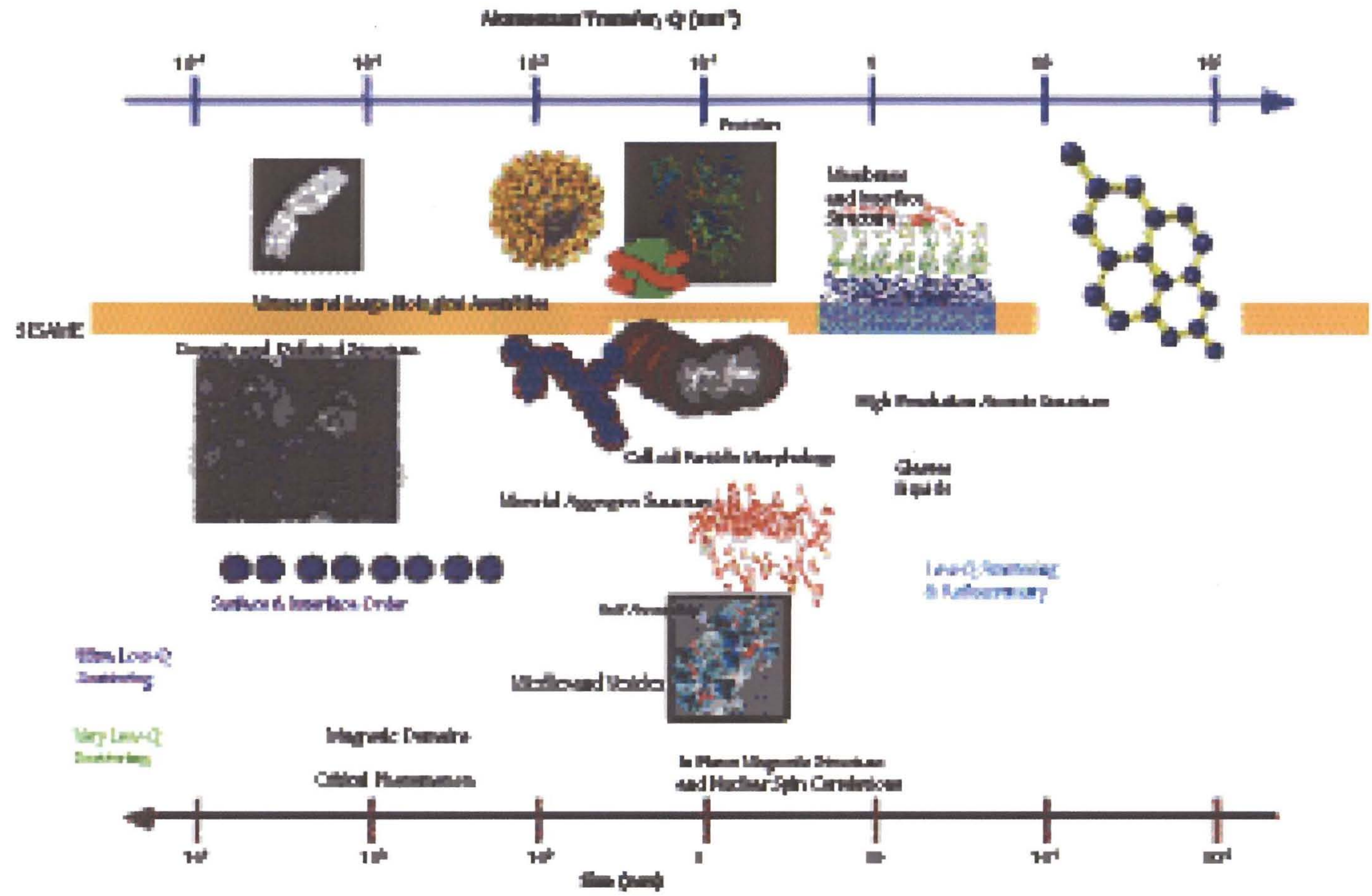


Fig. 4. Small-angle scattering instrument scales.

and hybrids. Currently, the method is used to profile the average depth-dependent structure perpendicular to an interface, with the typical assumption that the interface is laterally uniform, at least on a length scale small enough to disregard curvature. In the future, we will need to study and understand the structures of laterally heterogeneous interfaces that can be probed by neutron off-specular scattering, such as rafts in biomembranes. While rafts can be studied in a coarse way with small-angle scattering, characterization that is more precise should be accessible with off-specular neutron scattering from a structure cast in a planar geometry. The general area of the response of films and membranes to the underlying physical and chemical heterogeneity of the substrate demands careful study.

Nanomagnetism

Future advances in information retrieval and storage technology will depend on our understanding of nanostructured magnetic devices. Detailed information on the structural, magnetic, electronic and dynamics of individual nanocomponents, as well as the interfacial structure between them, is essential to understand artificially layered magnetic structure. Neutron scattering will continue to play a dominant role in experiments that simultaneously probe both physical composition and magnetic structure. Spin-polarized neutron reflectivity (PNR) from layered heterostructures and nanocomposites quantitatively determines the magnetic (vector component and magnitude) and structural profile with sub-nanometer resolution, even in buried interfaces. Information on the lateral magnetic and structural roughness as well as the domain behavior and reversal modes is determined principally from diffuse scattering. Recent advances have allowed the determination of magnetic order in two-dimensional structures, such as arrays, stripes, and dots. The spatial resolution of these measurements is limited by the minimum detectable signal (presently of order 10^{-7} times the intensity of the incident neutron beam). Problems in nanomagnetism that are amenable to study with neutrons are listed in Table 2. Many of these examples are drawn from a published report on neutron opportunities in nanomagnetism that was produced in 2004 by a group that included several of the participants in the current study. (See M. R. Fitzsimmons, S. D. Bader, J. A. Borchers, G. P. Felcher, J. K. Furdyna, A. Hoffmann, J. B. Kortright, I. K. Schuller, T. C. Schulthess, S. K. Sinha, M. F. Toney, D. Weller, S. Wolf. Neutron scattering studies of nanomagnetism and artificially structured materials. Journal of Magnetism and Magnetic Materials 271:103–146.)

Hard materials studies

Although emphasis in current SANS and reflectometry work is largely on soft matter, these techniques have also contributed important information on the structure and phases of hard materials. This includes domain and large defects structures in the solid phases and the physics of nucleation and spinodal decomposition. Measurement over multiple length-scales in hard matter and structure-property relationships is of emerging importance. An example is the effect of strain-induced long-length-scale defects in some nanomaterials that affect mechanical properties. Other recent examples of the importance of SANS and neutron reflectometry include applications to hydrogen storage in films and bulk materials, and the fate of ^3He in metal tritides. The need to study structure over a wide range of length-scales and time-scales is common to studies of both hard and soft matter.

Science opportunities at the Lujan Center in large-length-scale research

Tables 1 and 2 summarize much of the soft- and hard-matter science that is currently studied with SANS and neutron reflectometry, as well as those emerging high-priority topics that are expected to constitute the scientific challenges of the next five to ten years. Based on these challenges, we were able to identify needs for neutron instrumentation and sample environments, to pick out those items where the Lujan Center could provide capabilities that would strengthen the overall national program, and that would complement other neutron centers.

Compelling reasons were identified for continued support and expansion of the Lujan Center:

- In many scientific areas there is a need for more neutron beam lines with particular capabilities simply because the demands by the user community exceed current neutron scattering capacity. This situation is particularly true for both SANS and reflectometry where past increases in capacity at sources worldwide have immediately resulted in increased high-quality scientific output. For this reason, ISIS will soon host two SANS instruments and four reflectometers. Many experiments (perhaps 80%) can be done equally well at an ISIS-class source (such as the Lujan Center) as at a flagship source such as SNS.
- In some cases, the scientific challenges identified in the tables require the development of new instrumentation. A case in point is the study of lateral inhomogeneities of surfaces, interfaces, and buried layers where grazing incidence SANS could, in principle, provide important scientific information. However, for thin layers or single surfaces, such experiments are currently beyond the state-of-the-art because the scattered intensity is low, especially when highly collimated beams are used to provide good Q resolution. SERGIS (spin echo resolved grazing incidence scattering) needs to be explored as a technique to overcome the intensity limitation. The Asterix spectrometer at the Lujan Center provides an ideal test bed because of its flexibility and because the required expertise is already available.
- In many of the scientific areas discussed there is a need to probe length scales that are longer than those currently accessible. There are various ways to reach these length-scales, some of which have been implemented—ultra-small-angle neutron scattering (USANS) at the NCNR at the National Institute of Standards and Technology (NIST), for example—or will soon appear—time-of-flight USANS at SNS, for example. It is not yet clear which methods will provide the best insights in particular types of problems so there is a need to continue to develop alternative methods such as SESAME (spin-echo scattering-angle measurement) and various implementations of focusing SANS. The latter may prove important to provide access to lower-Q anisotropic scatter.

Table 1. Problems in soft matter that lend themselves to neutron scattering and reflectometry. The relevance to Lujan Center current and future capabilities is listed.

Subject	Present	Future	Why Lujan	Enablers
Supramolecular and hierarchical structures	• structures of small and medium size proteins (of order 10 nm or less) • structures of block copolymers (10 to 100 nm) • structures of micelles and vesicles. • model membranes and amphiphilic assemblies	• Probing the kinetic of developing structures	• Established competence with UC colleagues. • For layered structures, requires measurements to the largest Q that are presently limited by background, e.g., from sources like incoherent scattering from the sample, sample environment or delayed neutrons. R&D needed to solve these problems for everyone	• People • Samples (see Physics Today). • Capitalize on synergies with CINT • Event encoding data acquisition systems & extensive computing capabilities (real-time analysis). • Complete "bottoms-up" modeling of neutron scattering data (to correctly include influence of coherence dimension on scattering). • µs-fast two-dimensional position sensitive detectors. • Forming collaborations with those who make complex hierarchical structures
		• Dynamic behavior at short and long time-scales. In particular, those processes that would benefit from measurement at non-zero momentum transfer.	• Requires integrated approach to do reflectometry with inelastic scattering in the sub µs regime (a development activity). • Requires pump-probe neutron scattering experiments (a development activity). A synergy with CINT and NHMFL, which have existing competence and interest in pump-probe techniques.	
		• Structures of more complex biomimetic membranes • Cell/surface interactions • Laterally non-uniform biomimetic membranes • Responsive surfaces, connecting bio/electronic interfaces (sensors)	• Deuteration facility exists • SESAME could be the right tool	• Sample environment designed to minimize sources of background.
		• relation between structure and transport in porous media	• Existing UC competence/synergy • Need to develop specialized sample environment (furnaces, humidity chambers, pump probe, pressure)	
		• confinement effects • dynamics of water • dynamics of complex architectures, side and main chain dynamics	• Electronic chopping and mechanical chopping may be useful	

Table 1. (Continued)

Subject	Present	Future	Why Lujan	Enablers
Biologically relevant structures	• model membranes • protein-protein interactions/complexes, protein/lipid, protein/ nucleic acids, ribosome	• nondestructive analysis of complex systems	• He binders of interest to national defense missions Foams.	• polarized samples • glancing incidence wide angle diffraction • gisans/sergis need to go beyond multilayer stacks • deuterated sample facility • biohazard facility • neutron detection correlated with sample excitation.
Property/architecture relationships	• Rheo-SANS • Fluids/brushes under shear. Current length scales are 2-100 nm)	• Rafts • Influence of substrates on supported membranes • templating	• Lujan-CINT synergy • Lujan-UC collaborations • Develop neutron scattering techniques	• requires ability to take and interpret neutron and optic data simultaneously • software to interpret (asi^2) • flexibility to tailor instrument to problem • collaborating with universities • modeling capability
Dynamics of soft matter	• Reptation • Diffusion dynamics • Glass transition (especially in thin films) • Dynamics of water	• confinement below 2 nm dimensions • Selective absorption	• Existing competence shear cell • Existing Lujan-UC collaboration • Develop sample environment for in situ loading, gas flow, gas into liquids	• reflectometry spin echo to complement XPCS,
Composites and hybrids	• Block copolymers • Polymer reinforcement			• Access to obtain quantifiable statistical view of complex structures in new materials.
Laterally Heterogeneous interfaces	• Interface between phospholipid layer and composite • Nanoparticles at block copolymers	• Reactions • Growth of polymer brush (occurs over several hours)		• Gisans
Physics of confined fluid	• response to shear • fluid behavior in porous media			• requires data at large Q monitor index of refraction with light, incorporate into neutron scattering instrument need to assure stability of neutron experiment over long periods (verify with light scattering) vapor pressure apparatus gas handling contrast matching or not. Simulate data to extract information from many scattering probes (asi^2)
Evolution of structures				Real time data acquisition

Table 2. Problems in nanomagnetism and magnetism that can be addresssed by neutrons, including issues that could be studied at Lujan Center with new capabilities.

Subject	Present	Future	Why Lujan?	Enablers
Nanomagnetism	• Magnetization depth profiles across layers and superlattices— in particular correlated with chemical depth profiles • Exchange coupling across interfaces • Locating pinned spins • Lateral structures, stripes, dots domains	• Lateral structures, dots and domains. Particularly for systems with lateral dimensions less than 20 nm presently below the resolution of scanning probes, including three-dimensional architectures with nanometer-sized structures that are necessarily buried.	• Leverage UC expertise, e.g., sample fabrication; treatment of off-specular reflectometry. • Requires access to upstream collimation. • Benefits from SERGIS/SESAME expertise.	• People. • Samples (see Physics Today). • Conclusion of next generation PNR workshop. • Lasers (to perform DNP). • 2+ and 17+ T high field magnets (to establish known magnetic states, perhaps even to polarize nuclei). • Event encoding data acquisition systems & extensive computing capabilities (real-time analysis). • Microwave cavities • Access to AOT talent. • Solutions to the pinhole problem. • Asterix upgrade. • Complete "bottoms-up" modeling of neutron scattering data (to correctly include influence of coherence dimension on scattering). • MOKE and neutron scattering compatible electrochemical cells. • Access to T-division competencies. • µs-fast two-dimensional position sensitive detectors. • in situ measurement capabilities such as heat capacity and MOKE. • Access to CINT and NHMFL talent. • fast flippers, possibly bootstrap RF flippers • Thought and techniques towards suppression of systematic errors.. • Electronic, mechanical chopping or MIEZE. • Sample environment designed to minimize sources of background.
		• Magnetism of lateral and buried structures in multi-component systems and in variable geometry magnetic and electric fields, complementing resonant soft X-ray scattering. Pump-probe experiments to enhance sensitivity and improve signal-to-noise detection of non-stochastic responses (of the sample to its environment). Needs of enhanced resolution in real space. • Dynamic behavior at short and long time-scales. In particular, those processes that would benefit from measurement at non-zero momentum transfer (origin of anisotropy, magnetic excitations in confined spins, pinning of spin waves at interfaces, damping of spin waves, spin wave bands in confined systems, spin fluctuations as for example fluctuating magnetization of superparamagnetic nanoparticles).	• Leverage UC expertise. • Requires measurements to the largest Q that are presently limited by background, e.g., from sources like incoherent scattering from the sample, sample environment or the W-target. • Some experiments with complex sample environment may benefit from in situ capabilities to measure heat capacity and MOKE. These capabilities help assure that the neutron experiment is being carried out under the proper conditions. In situ heat capacity and MOKE measurement capabilities are existing competencies of the NHMFL. • Requires integrated approach to do reflectometry with inelastic scattering in the sub µs regime (a development activity). • Requires pump-probe neutron scattering experiments (a development activity). A synergy with CINT and NHMFL, which have existing competence and interest in pump-probe techniques	

Table 2. (Continued)

Subject	Present	Future	Why Lujan?	Enablers
		• Polarized nuclei	• Demonstrated competence. Required to further studies of molecular magnets.	
		• Collective spin wave modes at interfaces and in lateral structures.	• Requires development of in situ resonance (microwave) capability. • Requires development of techniques to efficiently measure perpendicular component of magnetization.	
		• Response of magnetism to electric fields, pressure, stress (Heterostructured materials such as multiferroics, exchange biased).	Established expertise with: • electrochemical cells, pressure. • application of stress using ion beam modification. • modeling of complex materials.	
Magnetism in bulk materials	• Extremely limited studies to date. • Emerging interest in 11 T fields. • Flexibility and space of Asterix is attractive.	• Studies of multiferroic single crystals at extremes of field, pressure and temperature. • Nanocomposites	• Leverage established expertise combining: magnetic field, temperature and pressure. • Established expertise in modeling of complex materials.	• Samples (see Physics Today) • Build FP11B • Dilution fridge compatible with high field magnets. • Asterix upgrade: 2D detector.

- The study of dynamics of systems with dynamic correlations over multiple length-scales is in its infancy and more work is needed to work out how to perform such studies effectively with neutrons. Possibilities include the spin echo modulation technique (MEIZE), simple electronic chopping of the beam, neutron spin echo reflectometry, and reflectometry combined with crystal energy analysis. Progress in these areas requires exploratory experiments that can be done only at a source where there is sufficient intensity to be able to measure inelastic scattering, as well as sufficient access to neutron beam time to allow proof of principle experiments, and to explore different design options to make the technique usable.
- Often, new discoveries using neutron scattering require the implementation of new sample environments. The development of new sample environments is better done at a mature facility where "bugs" in the sample environment equipment can be isolated from neutron artifacts. Of course, once equipment of this type has been thoroughly debugged, it can be quickly adapted to any neutron center, so development at Lujan Center would serve the entire community.
- There are several issues that limit current capabilities for studies of large length-scales, such as incoherent scattering background in SANS and reflectometry studies (particularly of liquids), inelastic scattering

from water in SANS measurements, and the presence of delayed neutron backgrounds. These problems are limitations at all spallation sources and require a systematic approach for their solution Advanced polarization and inelastic measurement techniques may be needed to address these issues. It is unlikely that sufficient beam time could be dedicated to solving these problems at a flagship source (like SNS) where user pressure demands forces instrument development to become a lower priority.

- The 20-Hz repetition rate of the Lujan Center is lower than that of other existing spallation sources and comparable to the repetition rates chosen for the ISIS second target station (STS) and the proposed STS2 for the SNS. Low repetition rates are ideally suited for cold neutrons, and thus for studies of large length-scales. In addition, the large wavelength bandwidth that results from low repetition rates is suitable for studying a large range of length scales or momentum transfers in a single measurement. This characteristic makes the Lujan Center source ideal, for example, for studies of the time-dependent evolution of structure by SANS and neutron reflectometry over a large Q-range.
- The Lujan Center was the first pulsed spallation source in the world to install partially coupled cold moderators, and these moderators currently provide greater coupling (and hence greater neutron flux per incident proton) than cold moderators at other neutron sources. The partially coupled LH2 moderator has become a worldwide standard. The development of this moderator is an example of the leadership role that the Lujan Center can provide in the development of spallation targets and moderators. There is an opportunity to install fully coupled LH^2 moderators and to explore new designs (such as beryllium reflector/filters, ortho-para conversion by catalysts, very cold moderators, etc.) that could lead to enhanced performance both at the Lujan Center and at other spallation sources.

There are several opportunities for the Lujan Center to establish partnerships and alliances. For example, in the study of soft matter, the CINT thrust on soft, biological and composite materials provides a natural vehicle for collaboration. This area targets the synthesis and characterization of materials derived from multiscale assemblies, including the integration of such materials with device and on-chip architectures. CINT also hosts capabilities that are inherently complementary to SANS and reflectivity methods. Key opportunities exist regarding complex interfaces, composite organic/inorganic systems, and biomolecular interactions. As an example, coupling state-of-the-art optical and single-molecule spectroscopies with reflectivity could provide a powerful approach to the study of structure and dynamics of complex interfacial systems.

In the study of both soft matter and nanomagnetism, scientists at the Lujan Center have already developed strong collaborative partnerships with University of California Faculties who have similar interests and a need for neutron characterization of samples produced as part of their research programs. This model can (and should) be pursued in other areas.

The final columns in Tables 1 and 2 are the group's assessment of resources and synergistic activities that will enable the success of the Lujan Center in the areas we have described. An extremely important enabler identified during our discussions was the availability of sufficient personnel to exploit the opportunities that the Lujan Center provides for the national neutron scattering program. While there is no doubt that the Lujan Center has the key personnel with expertise in LQD and reflectometry, these individuals are often over committed because they lack necessary technical support.

Sample environments

The recommendations for sample environments from the Large Scale group closely follow those from the other groups. This confluence of recommendations should be noted by the reader.

A particularly effective way to increase the scientific output of the Lujan Center users would be to provide a varied suite of sample environment capabilities. Adequate designs for some equipment already exist but others will need to be developed. NIST's NCNR has started a program in which external users apply for funding to develop equipment for their own research, and leave the equipment at the facility for use by all users. This mode could be applied at the Lujan Center, given the required technical support. The group's ten recommendations are the following:

1) A vacuum furnace with temperature capability from room temperature to 400 °C.
2) A temperature-controlled humidity chamber for reflectometry.

3) A reflectometry sample-cell to expose samples to precise vapor pressure of various organic solvents.

4) A variety of cells for reflectometry experiments with solid/liquid interfaces.

5) A high-pressure cell for reflectometry and SANS experiments.

6) The addition of complementary measurement techniques for both reflectometry and SANS including: Brewster-angle microscopy, ellipsometry, contact-angle measurement and fluorescence microscopy (for reflectometry), magneto-optical Kerr effect (for PNR), and dynamic light scattering (for SANS).

7) Low (~2 T) and high (~17 T) magnetic fields for PNR.

8) Pump-probe capabilities of various sorts.

9) Rheological SANS and reflectometry.

10) Dilution refrigerator adaptable for diffraction, reflectometry, and inelastic machines.

11) Remote user-control of sample changers via the Internet.

Instruments: Asterix

With the Asterix instrument (Figure 5), the Lujan Center is well positioned to answer fundamental questions about magnetic nanostructures, thus enabling the development of new materials. The existing instrument is already world-class and the upgrades described below would extend studies to probe three-dimensional architectures of laterally defined heterostructures and nanocomposites, and to probe magnetic excitations at buried interfaces and in confined geometries.

The Asterix reflectometer was originally a LANL Laboratory Directed Research and Development (LDRD)-funded project to develop neutron-beam-polarization-techniques suitable for pulsed spallation sources. Thus, this spectrometer was not designed as a general neutron scattering instrument and is therefore less than optimal as a user instrument. Nevertheless, the Asterix user program is mature, and its successes have been widely recognized. Critical upgrades are needed that will allow Asterix to solve many of the important problems in nanomagnetism and enhance the opportunities for external users.

Modifications to Asterix's diffractometer, detector, and polarization analysis systems have already been presented to BES as a midscale instrumentation proposal and are awaiting a decision (one of the members of the low-Q working group is the principle investigator on this proposal). Additional improvements before the sample position would increase the neutron flux on the sample by a factor of eight and would be relatively inexpensive. The Asterix polarization cavity is twice the height and half the width of the existing guide on flight path (FP) 11. A two-fold increase of intensity on the sample can be achieved by matching the polarization cavity cross-section to the FP11 guide (by changing the latter). In addition, replacing the regions before and after the sample with vacuum vessels (or by shortening the instrument) and incorporating the polarization cavity into the neutron guide would yield another two-fold increase of intensity. Finally, Asterix uses an antiquated approach—a beryllium filter—to remove the prompt portion of the neutron spectrum. This method attenuates the cold spectrum by almost a factor of two. Removing the beryllium filter and replacing FP 11A with a bent (or kinked) guide (with a cross section matching the polarization cavity) would recover this factor of two. These changes would bring Asterix performance to within a factor of four of a state-of-the-art polarized neutron reflectometer at the SNS. In addition, the changes envisaged to the incident flight path could be made in such a way as to allow for the extraction of another beam of cold neutrons, thus opening up the opportunity for a totally new instrument.

We believe that LANSCE should promote the development of a next-generation polarized neutron reflectometer. Such an instrument should be designed to better manage systematic errors (thus enabling detection of very small spin-dependent neutron signals), to incorporate real-time data analysis, to include novel in situ measurement capabilities, for example, ferromagnetic resonance spectroscopy, magneto-optical Kerr effect , etc., and to allow measurement of dynamic process, for example, spin waves with non-zero momentum transfer. These improvements would lead to new capabilities for polarized neutron reflectometry that could be adopted at neutron sources worldwide.

Moreover, many of the envisaged new techniques might be applicable to neutron scattering beyond PNR. To proceed, we recommend forming an international working group charged with cataloging outstanding issues in PNR and proposing solutions. The Lujan Center is urged to take a leading role in this activity because personnel at the Lujan Center have the expertise

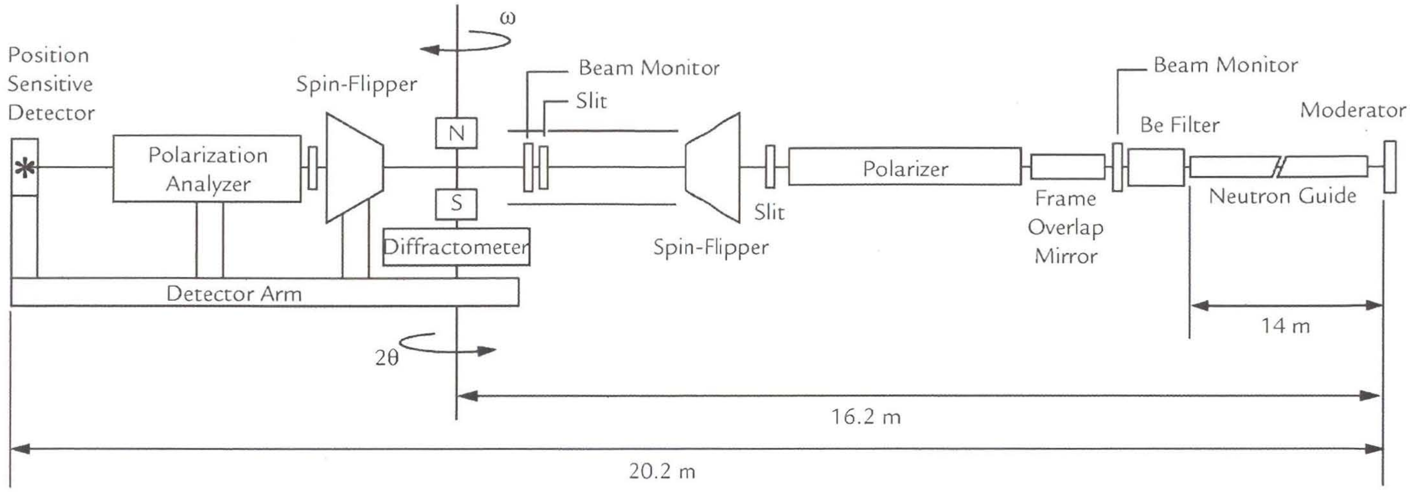


Fig. 5. A diagram of the Asterix instrument.

to take a lead in this area, and because Asterix has the flexibility and stability to allow new concepts to be tested and perfected. This activity will require modifying the Materials Program Advisory Committee to include a sub-committee to review instrumentation proposals, as well as additional support staff including both postdocs and technicians. The proposed upgrades to Asterix will not only grow the user community but will also train a new generation of neutron scattering experts. Among the challenges that should be explored are the following:

- Much better polarized-neutron beams and much better polarization analysis. The challenge will be to measure ever-smaller spin-flip signals. Doing so will require exceptionally well-polarized and analyzed beams with an overall flipping ratio > 100. To achieve very high polarization ratios it is important to use more than one polarizer and to disentangle their phase space. One possibility is to use crossed bender polarizers.
- Improved flux for grazing incidence SANS in polarized (and unpolarized) mode to probe the length scales of interest, particularly in nanomagnetism.
- Dramatic new thinking on how to successfully measure small magnetic signals, perhaps using Larmor precession, to detect small perturbations to the polarization of the neutron beam.
- Combine high magnetic fields with sensitive spin echo.
- Provide true three-dimensional vector polarimetry by reflectometry.
- Study hydrogenous films by polarization analysis. Go beyond asserting that polarization analysis is, in principle, useful for such studies and actually demonstrate that it is far better than unpolarized neutron reflectometry.
- Better magnetic resonance techniques that elucidate how magnetic properties of a nanostructured material differ from the bulk, and where the altered properties are to be found (for example, at the interface, in the center of a dot, etc.).
- Combine magnetic resonance with polarized neutron reflectometry.
- Measure small spin-flip scattering to pinpoint the location of excited spin waves (for example, spin-flip scattering owing to the precession occurring at interfaces), perhaps using pump-probe methods.
- Polarized inelastic scattering from a single interface is still a challenge, but if solved, would have a big scientific payoff.
- Ten times better Q and E resolution for large length- and time-scales, possibly using neutron spin echo to separate both spatial- and time-resolution from collimation and monochromatization.
- Active combination of PNR with other techniques, such as magnetic resonance microscopy, on the same sample for in situ probes, addressing not exactly repeatable effects.

- Exploit symmetries that cancel systematic effects.
- Use nuclear magnetic resonance to manipulate spins and setting up pulse trains.
- Enable studies of much smaller samples (say ten-times smaller volume) while doing high-quality pump-probe experiments on surfaces and interfaces.
- Eliminate the factor-of-two loss of intensity currently suffered whenever a neutron beam is polarized.
- Resolve in-plane length scales up to 1 µm using diffuse scattering.
- Inelastic neutron signal from a thin film in reflectometry mode.
- Upgrade the software for data analysis and visualization at Asterix to make it more user-friendly.
- Develop software to analyze off-specular scattering by collaborating with SNS.

Instruments: LQD

LQD (Figure 6) is another instrument that was originally built using LDRD funds in the late 1980s. Although the instrument provides good data, especially on moderate to strongly scattering samples, the technology on which it is based is being superseded and it should be replaced. Perhaps the most fundamental change that is needed is a curved or kinked guide to eliminate line of sight, and the backgrounds (both neutron and gamma) that are caused by the current direct viewing of the neutron moderator. The instrument should be upgraded to include a moveable small-angle detector and a fixed large-angle detector to allow a large range of momentum coverage in a single measurement.

One could imagine several ways in which LQD could be replaced. The most obvious is to strip out the current instrument and install a new SANS machine. However, if the incident flight path of Asterix is upgraded and a new cold beam becomes available on FP 11B, one could imagine building a new SANS machine on this beam

LQD Specifications	
Wavelength Range	2 - 15 Å
Angular Range	4 - 60 mrad
Q-Range	0.0023 - 0.5 $Å^{-1}$
Typical Sample Size	10 x 13 mm
Detector	Two dimensional proportional counter
Moderator	Partially-coupled liquid H_2 at 20 K
Sample Environments	Air, vacuum, closed cycle temperature control, pressure to 3 KB, shear cell
Typical Measurement Times	2 min - 6 hours

- Brightest pulsed spallation cold moderator.
- Advanced background suppression.
- Advanced optics and count rate control.

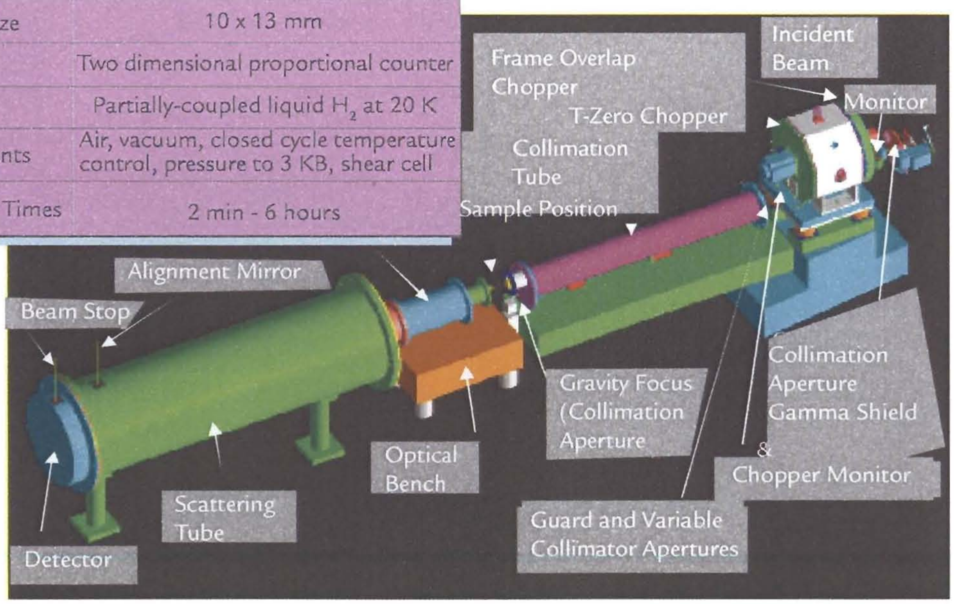


Fig. 6. LQD: a state-of-the-art time-of-flight SANS.

line to help satisfy the large national demand for SANS. Preserving LQD as a test bed for new SANS methods, such as polarized neutron SANS, converging pin-hole focusing, mirror testing, etc., should be considered. A strategy that enables the Lujan Center to contribute optimally to the national SANS program is needed and should be developed in collaboration with other U.S. neutron centers.

An attractive new capability for the Lujan Center would be USANS. Flight path 10 could be explored as the test bed for new USANS ideas. The development of SESAME into a full instrument is one such possibility.

Instruments: SPEAR

SPEAR (Figure 7) is a modern neutron reflectometer with a vertical scattering plane designed to enable the study of liquids. Its only limitation in this regard is the available angle of incidence for these studies (1°). Over the past years, various upgrades to the spectrometer have been implemented making SPEAR a reliable, internationally competitive reflectometer. Nevertheless, there are a few further improvements that could be made to the instrument to enhance its output. In the late 1990s, when the most recent round of new instrumentation was built at the Lujan Center, a proposal for an upgrade to SPEAR was submitted by G. Smith and C. Durning. Unfortunately, this proposal was not funded. The proposal included the installation of a neutron guide and more flexible incident beam collimation. The working group believes that this proposal should be pursued.

It is important to upgrade SPEAR's software for data analysis and visualization to make it more user friendly. Users will appreciate the development of software to analyze off-specular scattering, in collaboration with SNS, as mentioned in the Asterix section.

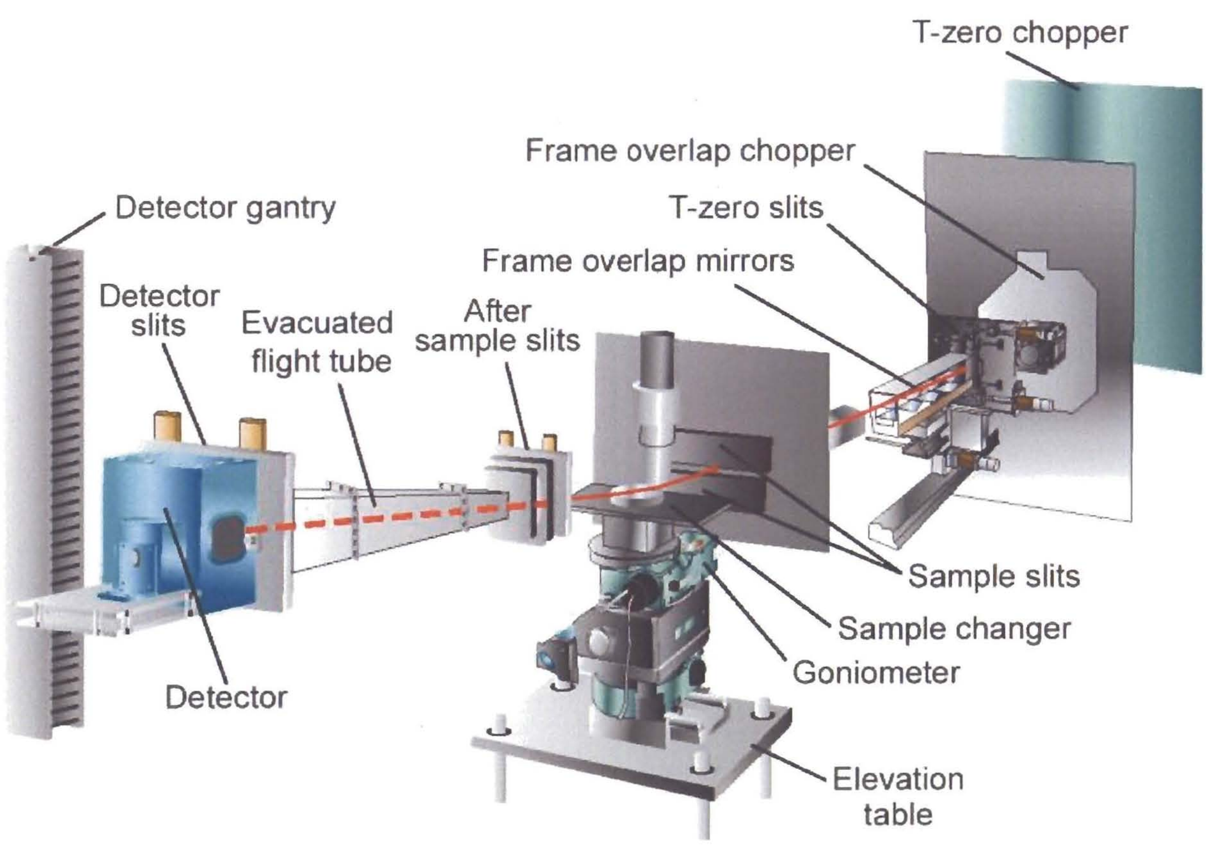


Fig. 7. SPEAR: State of the art time-of flight neutron reflectometer.

Working Group on Instrumentation for Inelastic Scattering

Working Group on Instrumentation for Inelastic Scattering

Topics: New Instrument Concepts, Upgrades for Inelastic Scattering

Chair: F. Mezei
Lujan Planning Group Chair: F. Trouw
Members: C. Batista, H. Glyde, C. Broholm, R. McQueeney, P. Dai, R. Osborn, J. Eckert, S. Shapiro, B. Fultz, and A. Sokolov

Summary of recommendations

The Working Group on Instrumentation for Inelastic Scattering offers seven recommendations.

1) Lujan Center should have a balanced suite of neutron scattering instruments about one-third of which should be inelastic spectrometers.
2) Lujan Center's source advantages (low repetition rate, 5-kJ per proton pulse power) should enable competitive science in the hottest challenges in neutron scattering.
3) For FDS, improved filters and embedded collimators should be implemented.
4) For Pharos, a supermirror guide is a high priority, with which beam intensity on-sample can be enhanced by an order-of-magnitude. Repetition rate multiplication (RRM) could provide an additional tripling in the data collection rate. Upgrades of background-reducing collimation—begun in 2006—at low scattering angles should be implemented to enhance Brillouin scattering, and an optional statistical chopper would help to single out the elastic signal in studies of structural disorder.
5) There is community support for an instrument optimized for hydrogen in materials to support national initiatives in the hydrogen economy and energy storage. A follow-on to quasi-elastic neutron scattering (QENS) is needed.
6) A community-driven workshop should be convened to consider the technical merits of a graphite-analyzer backscattering instrument and a time-of-flight (TOF) machine with RRM.

Discussion

Historically, inelastic scattering instrumentation has been relatively underrepresented at the Lujan Center. The capability to explore microscopic and nanoscale dynamics in space and time is one of the key contributions of neutron scattering in the exploration of condensed matter, achieved with the help of a variety of inelastic neutron scattering techniques. These methods cover a wide range of the space-time domain from a fraction of the nanometer to some 100 nm, and from femtosecond to microsecond, respectively, with parts of this domain only accessible to neutrons. Experience shows that in a complete and balanced suite of neutron scattering instruments about one-third needs to be devoted to the study of dynamics. Thus, in a strategy aimed at full utilization of the Lujan Center, four to five inelastic scattering instruments are envisaged. By building on the strengths of LANL's scientific environment, innovative instrument design, and the particular features of the Lujan Center's neutron source (low repetition rate, 5-kJ/pulse proton-beam power matching that of ISIS, and amounting to 22% of that of SNS when SNS achieves full designed power), these instruments will be fully competitive nationally, and internationally, to address the vast majority of the hottest challenges in neutron scattering.

Two venerable inelastic scattering instruments are currently operational at the Lujan Center, each more than a decade old. The Filter Difference Spectrometer (FDS), built in 1976, and the thermal neutron TOF spectrometer, Pharos, designed in 1989, continue to deliver state-of-the-art performance focused on the hot and thermal neutron energy range. Upgrade options have been identified for both to keep them competitive for the future, in the rapidly changing environment marked by the advent of SNS.

Compared to competitor spectrometers, FDS offers the advantage of larger-detector solid-angle coverage and variable resolution by the unique filter-edge method.

The FDS is on par with the TOSCA spectrometer at ISIS dedicated to chemical spectroscopy. Substantial gains in the data-collection rate, in the range of a factor of three, are envisaged for FDS by improving the filters and introducing embedded collimators to reduce background; this will secure an important role for FDS in the SNS era.

Since the conception of Pharos, decisive progress has been made in the technique of TOF spectroscopy at pulsed spallation sources. With advanced supermirror-based neutron-guide beam delivery (already used at SNS), the beam intensity on the sample can be enhanced by up to an order-of-magnitude, and repetition rate multiplication (RRM), which is part of the design concept of the new instruments under construction at ISIS and J-PARC, will provide an additional gain in the data collection rate by a factor of three, on average, by extracting several monochromatic neutron pulses from each source pulse. The upgrade of Pharos will also allow Lujan Center users to explore unique, innovative opportunities by developing an interchangeable, reduced-background collimation system for inelastic experiments at low scattering angles (such as Brillouin-scattering study of sound wave phenomena), and using an optional statistical chopper to single out the elastic signal in the study of structural disorder.

The Lujan Center currently lacks inelastic neutron scattering capabilities in the crucial cold-neutron energy range, which is most important for the study of soft and nanostructured matter. Direct geometry TOF spectrometers are the centerpieces of instrument suites for cold neutron spectroscopy, and the Cold Neutron Chopper Spectrometer (CNCS) will become the best in this class once SNS reaches full power. The lower source-repetition-rate of the Lujan Center and the use of the RRM method (particularly effective for cold neutron spectrometers using extended incoming flight path), open up the opportunity to build a first-rate cold-neutron spectrometer at Los Alamos, which will approach the power of CNCS. A longer flight path optimized for RRM use will also offer exceptional resolution capabilities, in particular for the study of optical-type excitations in the energy range 5–50 meV. The competitive power of an upgraded Pharos at the Lujan Center's FP 16, and the new cold neutron TOF spectrometers installed on the 63-m-long existing guide on FP 13, are illustrated in Figure 8.

The innovative implementation of an inverted geometry spectrometer specifically designed for the investigation of correlated electron systems will open new opportunities at the Lujan Center. There is also community support for an instrument optimized for hydrogen in materials to

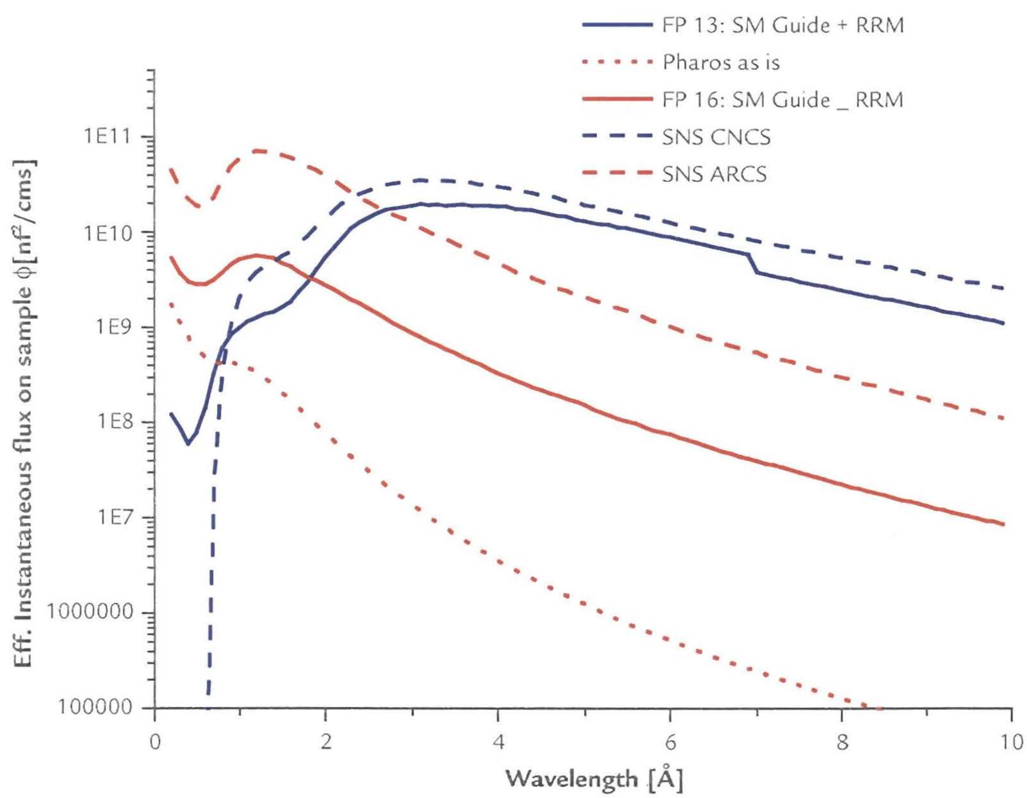


Fig. 8. A comparison of incoming beam intensities of direct geometry TOF spectrometer options at the Lujan Center and SNS. The SNS instruments utilize state-of-the-art neutron guides but do not have RRM capability. The moderator to sample distances for FP 16 and FP 13 are 20 m and 63 m, respectively, which leads to inherent incoming beam energy resolutions better than those for SNS's ARCS and CNCS (13.6 m and 36.2 m, respectively).

support national initiatives in the hydrogen economy and energy storage. The QENS at IPNS (Figure 9) has served an important role and a follow-on is needed.

A graphite-analyzer backscattering instrument (such as IRIS at ISIS) has been proposed for the Lujan Center.

A community-driven workshop should be convened to consider the technical alternatives, such as a graphite-analyzer backscattering instrument versus a TOF machine with RRM (see Backscattering and TOF-RRM).

Backscattering and TOF-RRM

As the community converges on the science directions for instrumentation upgrades at the Lujan Center, design comparisons are useful. The calculation below (Figure 10) compares energy-loss scattering on a 10-meV sharp excitation on a 34-m-long IRIS-type backscattering machine on the Lujan Center's coupled cold moderator (top), with two of the RRM frames measured simultaneously by a proposed 63-m-long FP 13 TOF instrument on the same moderator. In the rapid Monte Carlo simulation calculation (the noise on the data is due to statistics), equal scattered-beam solid-angles were assumed and the time bins set equal. The $E_{incoming}$ = 12.5-meV RRM frame shows an advantage in resolution and intensity. Backscattering provides much higher intensity at the lower resolution E_i = 15.5 meV. Arguably, the RRM frame provides about the same quality of information. Background and Q resolution must be similarly compared.

Backscattering is optimal for resolutions that cannot be achieved at the same wavelength by TOF, for example, using silicon analyzers, like QENS. Simultaneous diffraction data and access to a broad range in energy loss scattering are generally considered benefits of backscattering. However, a TOF instrument, with the series of RRM frames with different incoming neutron wavelengths starting below 1 Å, will cover both the Q range needed to have a full diffraction pattern and the energy transfer domain up to 100 meV.

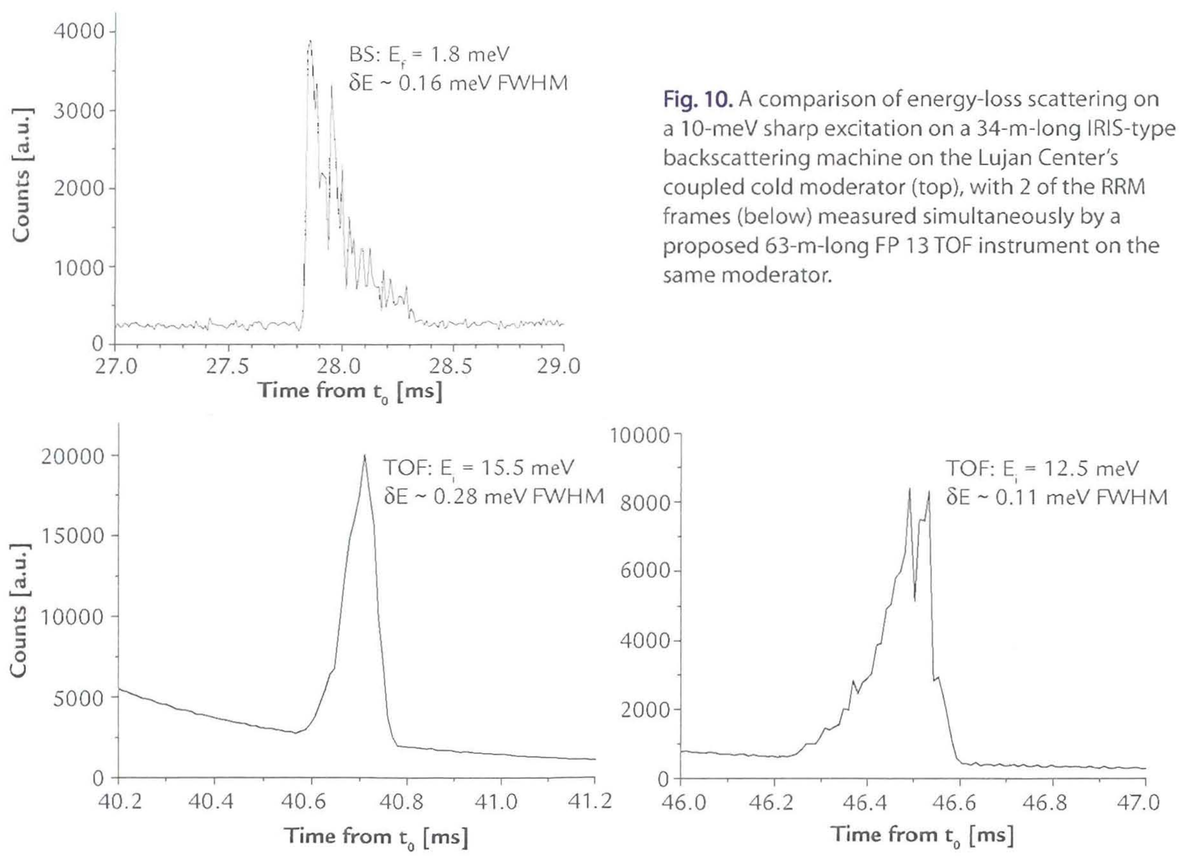
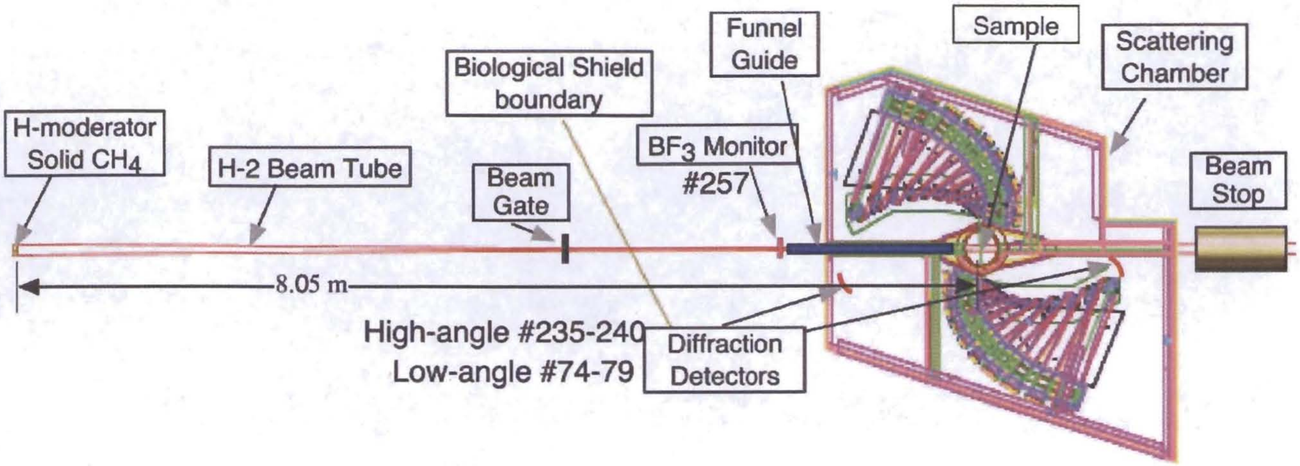


Fig. 10. A comparison of energy-loss scattering on a 10-meV sharp excitation on a 34-m-long IRIS-type backscattering machine on the Lujan Center's coupled cold moderator (top), with 2 of the RRM frames (below) measured simultaneously by a proposed 63-m-long FP 13 TOF instrument on the same moderator.



Funnel Guide
Sample
Scattering Chamber
Biological Shield boundary
H-moderator Solid CH4
H-2 Beam Tube
Beam Gate
BF3 Monitor #257
Beam Stop
8.05 m
High-angle #235-240
Low-angle #74-79
Diffraction Detectors

Working Group on New Instrument Concepts and Upgrades for Diffraction

Working Group on New Instrument Concepts and Upgrades for Diffraction

Topics: Future Directions, Priority Needs, Science Niche and Strengths, General Instrument Upgrades, Future Instruments, Specific Instrument Upgrades, Conclusions

Chair: D. Louca
Members: W. Beyermann, D. Brown, B. Clemens, R. Hemley, A. Llobet, H. Nakotte, Th. Proffen, J. Urquidi, S. Vogel, and H. Xu

Summary of Recommendations

The members discussed the scientific needs, priorities, mainstream and new science-focus areas, general and future instrument developments, and current instrument upgrades at the Lujan Center. Lujan Center's diffraction capabilities can be enhanced to create a world-renowned diffraction center with capabilities that can address soft and hard condensed-matter materials issues and be in a position to compete with other facilities in the world. Our seven conclusions are the following:

1) The Lujan Center is in a position to play a vital role in enhancing the national capabilities for neutron scattering. The Lujan Center, having been in the forefront in introducing neutron diffraction to biology users, has a growing user program that could expand by several proposed changes. As the neutron-scattering community continues to grow, the need for multiple sources remains strong. To fulfill its mission, however, more investment is clearly needed in the following areas at Lujan Center.
2) The need to increase the number of personnel for the diffractometers to operate successfully is a priority. This includes both the instrument scientists and the staff for sample environments and software.
3) The Lujan Center should strengthen, and provide support to, established strong connections within the Laboratory, and with academic facilities in New Mexico and California.
4) Improved diffraction capabilities could play a major role in national security issues, such as the hydrogen economy and nuclear proliferation.
5) Specific areas to address include the following:
   - Expand extreme sample environments
     - Mbar, mK, 10's Tesla magnetic fields, hot (radiologically) cell, controlled atmospheres
     - In situ capabilities
   - Expand mail-in samples program
   - Allocate additional fast-access beam time
6) Desired instrument upgrades include advances in neutron optics, neutron focusing, neutron polarizers, and correlation choppers that allow separation of dynamics from static.
   - HIPD: modify existing configuration
   - NPDF: small-angle detectors, neutron guide and focusing
   - SMARTS: in situ sample environments capabilities
   - HIPPO: upgrade to reduce background and improved focusing
7) Proposed new instruments.
   - Long-wavelength single-crystal diffractometer
   - LAPTRON (Los Alamos Pressure-Temperature Researches Online Neutron Diffractometer)
   - HIPDF (liquids, glasses, nanomaterials)
   - Fourier diffractometer/spectrometer
   - Hot cell diffractometer

Future Directions

The expected growth of the neutron community in the U.S. presents major opportunities for growth of neutron diffraction at the Lujan Center in the coming years.

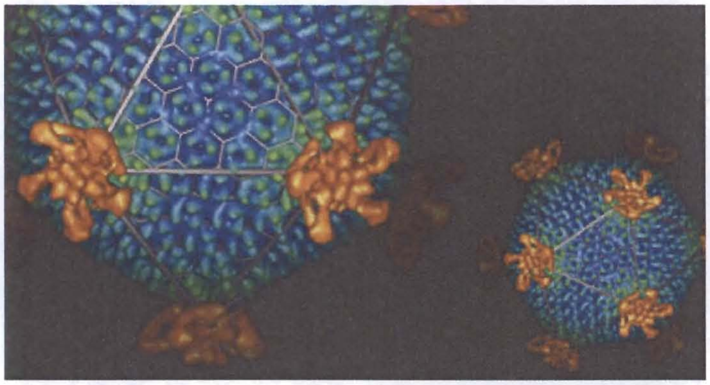


Fig. 11. Protien encapsulated nanocrystals for hydrogen production. Neutron diffraction has unique advantages for studying these systems.

Diffraction is not only the standard workhorse technique essential for a broad range of materials problems, it is crucial for fundamental structural studies at frontiers of many fields. Thus, there are great new opportunities for the integration of new techniques in unique world-class facilities, while at the same time recognizing continuing needs for conventional experiments. The Lujan Center will, therefore, have important niches in specific areas of neutron diffraction and will complement both the SNS and the portfolio of synchrotron x-ray facilities supported by BES.

We envisage two classes of beamlines: 1) those dedicated to specific experiments that include instruments that integrate multiple analytical probes, and 2) sample environments and general instruments that can accommodate a broad range of experiments. Extreme conditions studies will take advantage of developments in large volume, high-pressure devices, and variable temperature capability from mK to eV (~105 K) temperatures, combined with magnetic fields. Advances in neutronics, such as those in focusing optics, for example, Kirkpatrick-Baez mirrors that can focus beams to 100-micron spot sizes, are desirable. This development is enabling a new generation of experiments ranging from imaging measurements of texture to studies of small samples at megabar pressures unprecedented for neutron scattering. Important developments in producing polarized neutrons will enable new classes of magnetic studies.

Many emerging areas of research are undergoing accelerating growth, where neutron scattering is essential, as it provides unique information on structure and dynamics (Figure 11). These include many areas in energy science, such as hydrogen storage, fuel cells, and bioenergy, the search for new materials under the auspices of the COMPETES Act, and multidisciplinary studies of materials under extreme conditions. All of these will leverage and enhance new and existing programs within LANL.

Next-generation diffraction capability at the Lujan Center is an essential national need when SNS instruments come on line. As mentioned above, the Lujan Center has an important niche in the materials studies associated with national defense (for example, in stockpile stewardship) and for homeland security. Specifically, there is a need for fundamental studies of materials aging and new materials for weapons systems, detectors, and sensors. In several key scientific areas, the SNS will be unable to support demand. For example, the dedicated high-pressure instrument (SNAP) at SNS is essentially a single crystal instrument that can accommodate small to medium size presses and no magnetic fields. The Lujan Center can also have an advantage in providing a strong, local support laboratory for complementary off-line measurements, such as sample synthesis and preparation, x-ray diffraction, optical spectroscopy, thermochemistry, and mechanical testing. A strong sample environment program is needed with a full range of devices for variable pressure, temperature, and magnetic fields over the full range of conditions achievable in the laboratory. There should be close integration of this program for diffraction with the inelastic scattering measurements in variable sample environments.

Three Priority Needs

Increased staffing

The diffractometers at the Lujan Center are the backbone of the user program accounting for roughly two-thirds of the publications in the 2003-2005 BES report. Staffing of these instruments, at present, does not allow for progress beyond simply running the instrument. Without the development of instruments and techniques, as well as outreach, the future of the Lujan Center looks very grim. In addition, data are backlogged and the present capacity and capabilities are not fully utilized. As a result, the highest priority is to increase full-time personnel on the current instruments, as well as in the support groups, such as data acquisition, ancillary equipment, and the mechanical team. Staff levels should be comparable to facilities such as ISIS. Note that the BES refers to the Lujan Center as an ISIS-class facility.

Outreach and collaborations

Increased staffing levels will enable the Lujan Center to embark on the second priority for a successful future: outreach and collaborations with the University of California, the universities in New Mexico, other universities, and within LANL. The collaborations grow the neutron user base, educate future neutron scatterers, and broaden the science scope and expertise of the facility.

Ancillary equipment

The third area in need is ancillary equipment. Following the NIST model, a promising approach to develop novel ancillary equipment is collaboration with universities and other LANL groups. The concept of funding this new equipment through the Lujan Center will attract many competing proposals and enhance the capabilities of the Lujan Center.

It is important to ensure the continuity of the current user program and scientific productivity and, initially, to focus on operations, with small- investment and high-payoff improvements ("Just get it done," said Steve Shapiro). Upgrades and the development of new instruments are vital to ensuring the future. Planning for upgrades and new instruments needs to start in parallel with the ramping of the operations budget.

Science Niche and Strengths

Our vision for the Lujan Center's future builds on its traditional and emerging strengths in materials science and engineering, highly-correlated systems, geosciences, nanoscience, and soft matter (including biological matter, polymeric materials, and complex fluids). These focus areas take advantage of the characteristics of the neutron source, which is well-suited to long-wavelength applications, and address critical national priorities in engineering science, energy technology, and defense. Our vision also builds on connections within LANL, as well as with CINT, Sandia and Lawrence Livermore National Laboratories, the University of California, and New Mexico universities.

Moving forward, the Lujan Center proposes to dramatically increase its ability to impact these areas, focusing on improving neutron optics and sample environment capabilities in its diffractometer beamlines, as well as by developing new diffraction experimental stations. These include a station with high-pressure, low-temperature and high-magnetic-field capabilities, as well as high-temperature and high-pressure chemical and environmental cells. These new capabilities would ensure that the Lujan Center continues to be a center of excellence in neutron diffraction.

General Instrument Upgrades

Several upgrade paths are common and necessary to the powder diffraction machines. Below is an outline of general proposed upgrades that could be beneficial to all instruments.

1) **Sample environments:** Low temperature (mK) and magnetic fields of tens of Tesla will open the path to new science on all diffraction machines. Due to the complexity of such devices, a dedicated staff member is required in addition to the hardware; otherwise the investment will be lost. A low-temperature sample-changer could be used on HIPPO and NPDF. The potential of a hot cell to investigate lethally radioactive materials, shared between the powder diffraction machines, to utilize their specific strengths (PDF, texture, high resolution versus time resolution), should be evaluated. This would align the Lujan Center with programs such as GNEP, AFCI, or MaRIE, the proposed new signature facility at LANL. Dedicated personnel for the current sample environments (furnaces, displexes, sample changers, load frames) will relieve the instrument scientist from maintenance duties and avoid disappointing users due to non-functioning hardware during their visit. Some sample environments, such as a dilution refrigerator, are complex instruments requiring expert staff for operation and maintenance.

2) **Beam focusing:** By using focusing techniques, for example, Kirkpatrick-Baez mirrors, smaller sample volumes will be possible. This, in turn, will allow more extreme environments (pressure, fields). All diffraction machines would benefit from such devices, which potentially could be transportable and shared between beamlines. Besides the focusing hardware, modifications to incident beam paths will be required. Design, commissioning, and installation of such devices require a dedicated staff member.

3) **Neutron polarizers:** Recent developments in neutron polarizers make it conceivable to install them as interchangeable components into various beam lines. Such devices will greatly improve the Lujan Center's capabilities for magnetic studies. The unique Lujan Center capabilities, for instance, in texture on HIPPO and PDF studies on NPDF, will open the way to new science, such as magnetic textures and magnetic PDFs.

4) **Data acquisition and detector development:** The next version of the data acquisition system is close to release and, in an intermediate version, is running already on HIPPO (September 2007). It will improve stability and allow event mode (continuous data acquisition without saving individual runs), which will improve capabilities, for example, for studies of phase transformations and other parametric time-resolved studies. However, the current staffing level is inadequate to support this important activity. The same is true for desirable development of the next generation of detector hardware.

Future Instruments

Long-wavelength single-crystal diffractometer

The extant single-crystal diffractometer, SCD, at the Lujan Center is no longer competitive with the best single-crystal diffractometer designs, in particular with the SNS diffractometer, TOPAZ, which has large coverage of the reciprocal space with a spherical detector. However, geometrical constraints of magnets and other special sample environments negate much of the advantage in coverage. Furthermore, the effects of magnetic stray fields on close-by detectors in TOPAZ severely limit the maximum magnetic field (5 Tesla or so).

Because there is already a strategic alliance with other LANL groups in the field of correlated electron systems that exhibit interesting magnetic phenomena at low temperatures, there is an obvious need for a magnetic single-crystal diffractometer capable of extreme sample environments, such as low temperature, high-magnetic fields, and high pressures. Moreover, recent developments of broad-band polarizers will allow magnetic studies that traditionally could be done only at reactor sources (for example, magnetic form-factor studies).

The Lujan Center has a large opportunity to establish a niche area in the area of polarized single-crystal diffraction for the magnetism community.

It is proposed to form an IDT that explores the possibilities for a new single-crystal diffractometer dedicated for magnetic studies. The machine could be placed on a cold liquid hydrogen moderator that takes advantage of long wavelengths for magnetic studies, and for such studies it would be more than competitive with TOPAZ that uses a water moderator. Additional requirements for such an instrument are to accommodate large sample environments (superconducting magnets, dilution fridge, pressure cells and so on).

HIPDF: Total-scattering high-intensity powder diffractometer

Local structure studies have been a key in resolving the interplay of the different length scales in many areas of materials science, such in the domain of functional materials, ferroelectrics, and nanoscience.

The high-resolution diffractometer, NPDF, at the Lujan Center is oversubscribed with experiments that require high resolution and PDF analysis. Currently, there is no high-intensity powder-diffractometer capable of studying small quantities of a sample, which can reach low temperatures (< 10 K), or accommodate a magnetic field or high pressure (15 kbar), and allow pair distribution function (PDF) studies.

A new diffractometer optimized for high intensity that would have detector coverage from 10° to 160° in the scattering plane and ± 15° above and below the plane, and be optimized for total scattering studies (very low background). The instrument would be able to accommodate large magnets and very low- and high-temperature capabilities (for example, dilution fridge, ILL furnace, and orange cryostat). Ideally, this instrument should also have the capability of focusing optics for nanoscience, as well as collimators to reduce the background.

This type of instrument would exploit the in-house expertise and success of total scattering techniques in the areas of nanoscience, condensed matter, multiscale science, polymers, disordered materials, glasses, liquids, and allow PDF studies on systems that do not require the high resolution of NPDF, and that are currently overloading NPDF.

LAPTRON

The design of LAPTRON aims at the important field of pressure study. Since SNAPS at SNS mainly serves the earth science community, in spite of its very high-pressure capability, its sample volume is relatively small and the stress can include shear components, not purely hydrostatic pressure. LAPTRON has a large sample volume and provides more homogeneous hydrostatic pressure.

We can routinely perform high-pressure high-temperature experiments at pressures up to 10 GPa and temperatures up to 1500 K using the toroidal anvil press (TAP-98) at HIPPO. We can also conduct high-pressure low-temperature measurements at hydrostatic pressures up to 10 kbar and temperatures down to 5 K with various fluid-driven cells. Construction of a stand-alone beamline, LAPTRON, will allow significant extension of the accessible pressure-temperature ranges, to 20 GPa and 2000 K, using the innovative multi-anvil and internal heating techniques. More importantly, we will integrate thermal analysis, ultrasonic interferometry, and neutron radiography and tomography with neutron diffraction at LAPTRON, so that all these measurements can be performed simultaneously at variable pressure-temperature conditions. This combination of multiple techniques is a powerful way of enhancing and broadening instrument capabilities for more complete and accurate characterization of material properties, and will benefit the broad scientific community in materials science, condensed matter physics, and geosciences.

The heart of LAPTRON will be a large-volume 2000-ton press with a multi-anvil high-pressure deformation module. We have constructed/purchased the press, TAPLUS-2000, high pressure-temperature controller, and other associated accessories with support from the LANL Weapon Physics programs, and have finished all conceptual designs of the multi-technique modules. LAPTRON is expected to greatly contribute to the defense programs, such as by measuring the equations-of-state and deformation behavior of plutonium and uranium at extreme conditions. Moreover, it will well serve other LANL missions, such as climate change and carbon dioxide sequestration. For example, the new tomography/radiography capabilities will allow in situ examination of rock-water interaction, a critical geochemical process with important implications of sequestration of carbon dioxide in depleted oil reservoirs.

Other instruments and needs

More detailed instrument simulations will be needed for LAPTRON and other new instrument concepts. For example, ideas were discussed for a novel diffractometer with a Fourier chopper to be able to separate elastic (static disorder) from inelastic (dynamic) scattering contributions. This instrument could be important, for example, for the study of multiferroic materials. One might also investigate the possibility of using an RRM spectrometer. This concept is further developed by T. Proffen and F. Trouw (inelastic working group).

It was also clear that there was a need for an instrument designed to handle very hot (active) samples and provide diffraction, texture, and possibly inelastic-scattering data. This idea also needs research and further development, but the payoff in relation to the LANL mission is obvious.

Specific instrument upgrades

HIPPO

The HIPPO diffractometer is optimized for high-throughput measurement of texture and measurement of small samples, for example, samples under high pressure, and upgrades should be focused accordingly. A prioritized list of upgrades is as follows:

- The highest priority upgrade to HIPPO is toward background mitigation by secondary beam path collimation. This enables PDF studies.
- Focusing optics, for example, Kirkpatrick-Baez mirrors or focusing funnels, to increase neutron flux on small samples, in particular, on samples under high pressure.
- Ultrahigh-temperature furnace, approaching or exceeding 3000 °C, with quenching capability, environmental capabilities (for example, oxidizing or reducing atmospheres), and simultaneous DSC capability (what's this?).
- Neutron-resonance-spectroscopy detector to enable sensorless temperature measurement at very high temperatures.

SMARTS

SMARTS was the first diffractometer in the world built specifically for the study of engineering materials under conditions approximating their processing and/or operating conditions. SMARTS has remained unique in the world by the inclusion of unique sample environments, such as the ability to apply load at high temperature. As evidenced by the similarities SMARTS has with the design of VULCAN (the next generation engineering diffractometer), from a neutronics point of view, SMARTS is well designed for its task. The one exception is that SMARTS needs an upgrade to double-ended position-sensitive detectors that would enable future studies of single crystals, studies that are currently very difficult to do.

Other upgrades to SMARTS are focused on continued development of unique sample environments. The future of engineering neutron diffraction lies in sample environments that push ever closer to realistic conditions.

- The first and highest priority of these is an in situ casting stage.
- Complementary to this would be a versatile press/furnace that could approximate rolling, swaging, forging, etc., conditions.

Both of these upgrades would enable studies of the crystallographic response (such as recrystallization), with time resolution, during and shortly after processing steps.

NPDF

NPDF is designed for the measurement of atom correlations in disordered solids. It requires high resolution and a large Q-range to complete the Fourier transformation of the diffraction data from reciprocal space to the real space correlation function. Prioritized upgrades are as follows:

- A neutron guide (or supermirror) to increase flux on the sample enabling kinetic studies of reactions and transformations, for example, crystallization of bulk metallic glasses, and studies of small quantities of sample.
- Low-angle detector banks that will increase the assessable Q-range of the measurement (toward smaller Q). This will enable studies on glasses, magnetism, and liquids.
- A dilution refrigerator (mK capability) with moderate magnetic field is needed. This will open the field of multiferroics to PDF analysis.
- Low-background pressure cell to allow PDF analysis of materials under pressure.

HIPD

HIPD is one of the oldest instruments at the Lujan Center and has recently been removed from the general user program. While we recommend a major upgrade to HIPD to a total scattering instrument, HIPDF, small-scale upgrades will allow HIPD to continue to do science and support the remaining instruments.

- A new door and sample-well to allow use of the general Lujan Center sample environment, for example, orange cryostat.
- Robotic sample-changer to allow mounting and manipulating of several samples in series.

PCS

Currently, there is only one protein crystallography instrument in the world at a spallation neutron source, the PCS, and the Lujan Center is the only facility of its kind for macromolecules in North America. The PCS is used for studying the structure of macromolecules and fibrous polymers. Based on the success of the PCS, an instrument called MANDI has been proposed for SNS. MANDI will have a comparable flux, at equal divergence as the PCS, but with a very different wavelength range due to the different source frequencies and moderator types. The PCS and MANDI will be complementary due to their different beam characteristics. PCS and MANDI will not be able to support a proposed new biology-neutron user community, which will lead to the establishment of a biology-neutron user community for the second target at the SNS.

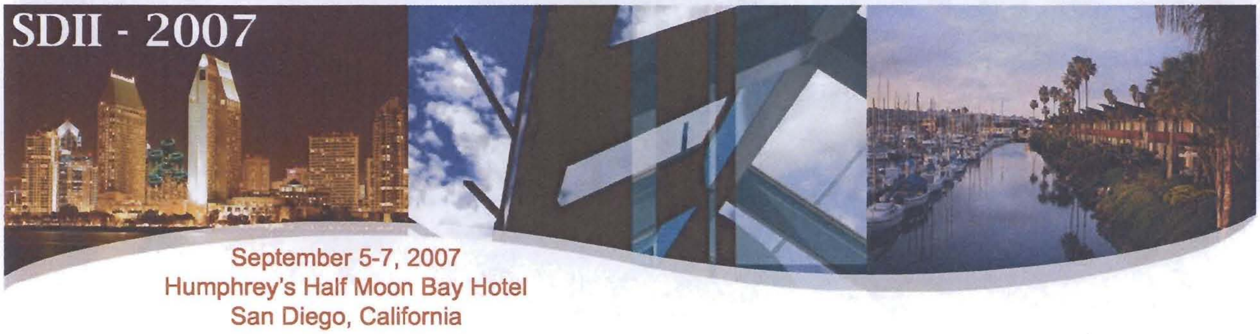
Conclusions

The Lujan Center's strengths lie in materials-based diffraction techniques. Enhancing the existing and proposed new instruments will make the Lujan Center both competitive and complementary with SNS. For this to happen, we should invest in sample environments and instrument upgrades. We believe this is the best strategy for the Lujan Center to remain strong and productive, and continue to play a vital role in enhancing the national capabilities for neutron scattering. The proposed upgrades/developments will enable the Lujan Center to open new fields of science and attract new talents with strong motivations for science.

Appendices

Appendices

Appendix A. Final Agenda and Participants List



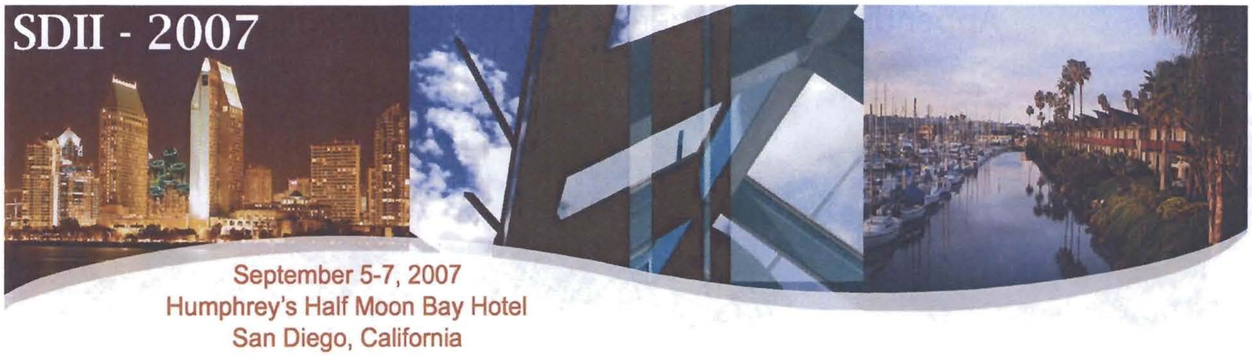
AGENDA
Lujan Neutron Scattering Center Workshop
Enhanced National Capability for Neutron Scattering
A Strategy for LANSCE Neutron Scattering

Wednesday, September 5, 2007 - Humphrey's Hotel

6:00pm - 7:00pm	Hotel Lobby	Registration
7:00pm - 9:00pm	Harborview Room	Reception

Thursday, September 6, 2007 - Humphrey's Hotel

7:30am - 8:00am	Marina Ballroom	Continental Breakfast
8:00am – 8:30am	Marina Ballroom	Welcome and Overview of LANSCE Plans, Kurt Schoenberg
8:30am – 9:10am	Marina Ballroom	BES Plans for Neutron Scattering, Pedro Montano (video)
9:10am – 9:40am	Marina Ballroom	Potential for growth of Lujan/LANSCE , Alan Hurd
9:40am –10:10am	Break	
10:10am – 10:50am	Marina Ballroom	Complementarity to SNS, HFIR, Ken Herwig
10:50am – 11:30am	Marina Ballroom	Complementarity to NIST NCNR, Dan Neumann
11:30am – 12:00pm	Marina Ballroom	Summary and charge to break-out groups, Jim Rhyne
12:00pm – 1:00pm	Upperdeck	Lunch
1:00pm – 4:00pm	Breakout Session Meetings	
	Pt. Loma Room	*New Instrument Concepts and Upgrades for Inelastic Scattering
	Pacific Room	*New Instrument Concepts and Upgrades for Diffraction
	Sunset Room	*New Instrument Concepts, Upgrades of Reflectivity, and Low-Q Diffraction
	Dockside Room	*National Perspectives and Vision for the Lujan Center
4:00pm – 5:30pm	Harborview Room	Preliminary reports (15 – 20 minutes each) by breakout chairs
6:30pm – 7:00pm	Harborview Room	Reception
7:00pm – 9:00pm	Harborview Room	Dinner



AGENDA
Lujan Neutron Scattering Center Workshop
Enhanced National Capability for Neutron Scattering
A Strategy for LANSCE Neutron Scattering

Friday, September 7, 2006 - Humphrey's Hotel

7:30am - 8:30am	Marina Ballroom	Continental Breakfast
8:30am – 11:00am	Breakout Sessions (report writing)	
	Pt. Loma Room	*New Instrument Concepts and Upgrades for Inelastic Scattering
	Pacific Room	*New Instrument Concepts and Upgrades for Diffraction
	Sunset Room	*New Instrument Concepts, Upgrades of Reflectivity, and Low-Q Diffraction
	Dockside Room	*Future Vision of the Lujan Center
11:00am – 1:00pm	Working lunch	
1:00pm– 2:00pm	Wrap-up Reports (by chairs)	
	Pt. Loma Room	*New Instrument Concepts and Upgrades for Inelastic Scattering
	Pacific Room	*New Instrument Concepts and Upgrades for Diffraction
	Sunset Room	*New Instrument Concepts, Upgrades of Reflectivity, and Low-Q Diffraction
	Dockside Room	*National Perspectives and Vision for the Lujan Center
2:00pm – 6:00pm	Dockside Room	Report Writing (by writing team)
8:15pm – 9:00pm	Hotel Restaurant	Dinner for Writing Team (Dinner Reservations)

Saturday, September 8, 2006 - Humphrey's Hotel

7:30am – 8:30am	Dockside Room	Continental Breakfast
8:30am – 11:00am	Dockside Room	Report writing
11:00am – 1:00pm	Dockside Room	Wrap-up (by writing team)
11:30am	Dockside Room	Box Lunch available

September 5-7, 2007
Humphrey's Half Moon Bay Hotel
San Diego, California

Breakout Session Members

1. **New Instrument Concepts and Upgrades for Inelastic Scattering**
   Point Loma Room: *Feri Mezei, chair - Frans Trouw (Lujan planning group chair)*
   Christian Batista
   Colin Broholm
   Pengcheng Dai
   Juergen Eckert
   Brent Fultz
   Henry Glyde
   Robert McQueeney
   Ray Osborn
   Steve Shapiro
   Alexei Sokolo

2. **New Instrument Concepts and Upgrades for Diffraction**
   Pacific Room: *Despina Louca, chair - Thomas Proffen (Lujan planning group chair)*
   Ward Beyerman
   Don Brown
   Bruce Clemens
   Rus Hemley
   Anna Llobet
   Heinz Nakotte
   R. Ramesh
   John Sarrao
   Doug Tobias
   Jacob Urquidi
   Sven Vogel
   Hongwu Xu

3. **New Instrument Concepts, Upgrades for Reflectivity, and Low-Q Diffraction**
   Sunset Room: *Roger Pynn, chair - Rex Hjelm (Lujan planning group chair)*
   Ami Berkowitz
   Mike Fitzsimmons
   Mark Foster
   Eric Fullerton
   Jarek Majewski
   Tom Mason
   Atul Parikh
   Sushil Satija
   Dale Schaefer
   Andrew Shreve
   Ivan Schuller

4. **National Perspectives and Vision for the Lujan Center**
   Dockside Room: *Tonya Kuhl, chair*
   Moe Boussoufi
   Cory Coll
   Phil Goldstone
   Ken Herwig
   Barry Klein
   Alex Lacerda
   Christian Mailhiot
   Gunther Muhrer
   Dan Neumann
   Don Rej
   Kurt Schoenberg
   Ray Teller
   Guebre Tessema

September 5-7, 2007
Humphrey's Half-Moon Bay Hotel
San Diego, California

Breakout Sessions

1. New Instrument Concepts and Upgrades for Inelastic Scattering
   Feri Mezei, chair – Frans Trouw (Lujan planning group chair)

2. New Instrument Concepts and Upgrades for Diffraction
   Despina Louca, chair -Thomas Proffen, (Lujan planning group chair)

3. New Instrument Concepts and Upgrades for Reflectivity and Low-Q diffraction
   Roger Pynn, chair - Rex Hjelm (Lujan planning group chair)

4. National Perspectives and Vision for the Lujan Center
   Tonya Kuhl, chair
   –National and International horizon scan
   –MaRIE and LANSCE-R
   –Barriers to success

Charge to Breakout Sessions

Issues to be addressed in discussions and in report

–Review and evaluation of current Lujan capabilities
–Where should Lujan go in the future?
  •New instrument capabilities (either new instruments or rebuild present instruments)
  •Upgrade path for present instrumentation
  •Future desired sample environment capabilities
–Complementarity of Lujan capabilities with the SNS, HFIR, NIST, and other neutron centers

Does the Lujan Center Strategic Plan 2007-2013...

•Adequately set the stage for MaRIE or similar signature facility at LANL?
•Optimally utilize, from the general user science perspective, the Lujan spallation sourced for neutron scattering and nuclear physics?
•Meet the expectations for mission science at the Laboratory?
•Incorporate relevant recommendations from prior planning workshops, such as San Diego I (2005) and Santa Fe I (2006)?
•Define the best instrumentation suite in view of SNS and other national neutron centers?
•Determine a proper strategy for future spallation targets to serve the instrument suite and user science?
•Address implementation and ownership?

September 5-7, 2007
Humphrey's Half Moon Bay Hotel
San Diego, California

Participant List

Christian Batista
Los Alamos National Laboratory
cdb@lanl.gov

Ami Berkowitz
University of California, San Diego
aberk@ucsd.edu

Ward Beyerman
University of California, Riverside
byerman@citrus.ucr.edu

Moe Boussoufi
University of California, Davis
mboussoufi@ucdavis.edu

Colin Broholm
John Hopkins University
broholm@jhu.edu

Don Brown
Los Alamos National Laboratory
dbrown@lanl.gov

Bruce Clemens
Stanford University
clemens@sierra.stanford.edu

Cory Coll
University of California,
Office of the President
cory.coll@ucop.edu

Leilani Conradson
Los Alamos National Laboratory
leilani@lanl.gov

Pengcheng Dai
University of Tennessee
pdai@utk.edu

Juergen Eckert
University of California, Santa Babara
juergen@mrl.ucsb.edu

Mike Fitzsimmons
Los Alamos National Laboratory
fitz@lanl.gov

Mark Foster
University Akron
mfoster@uakron.edu

Eric Fullerton
University of California, San Diego
efullerton@ece.ucsd.edu

Brent Fultz
California Insitute of Technology
btf@caltech.edu

Henry Glyde
University of Delaware
glyde@physics.udel.edu

Phil Goldstone
Los Alamos National Laboratory
pgoldstone@lanl.gov

Rus Hemley
Carnegie Insitute of Washington
chemley@gl.ciw.edu

Tanya Herrara
Los Alamos National Laboratory
tanyah@lanl.gov

Ken Herwig
Oak Ridge National Laboratory
herwigkw@ornl.gov

Rex Hjelm
Los Alamos National Laboratory
hjelm@lanl.gov

David Holtkamp
Los Alamos National Laboratory
dholtkamp@lanl.gov

Alan Hurd
Los Alamos National Laboratory
ajhurd@lanl.gov

Barry Klein
University of California, Davis
bmklein@ucdavis.edu

Tanya Kuhl
University of California, Davis
tlkuhl@ucdavis.edu

Alex Lacerda
Los Alamos National Laboratory
lacerda@lanl.gov

Paul Lewis
Los Alamos National Laboratory
lewis@lanl.gov

Anna Llobet
Los Alamos National Laboratory
allobet@lanl.gov

Despina Louca
University of Virginia
louca@virginia.edu

Christian Mailhiot
Lawrence Livermore
National Laboratory
Mailhiotl@llnl.gov

September 5-7, 2007
Humphrey's Half Moon Bay Hotel
San Diego, California

Participant List

Jarek Majewski
Los Alamos National Laboratory
jarek@lanl.gov

Tom Mason
University of California, Los Angeles
mason@chem.ucla.edu

Robert McQueeney
Ames Laboratory
mcqueeney@ameslab.gov

Feri Mezei
Los Alamos National Laboratory
mezei@lanl.gov

Gunther Muhrer
Los Alamos National Laboratory
muhrer@lanl.gov

Heinz Nakotte
New Mexico State University
hnakotte@nmsu.edu

Dan Neumann
National Institute of
Standards and Technology
dan@nist.gov

Ray Osborn
Argonne National Laboratory
rosborne@anl.gov

Atul Parikh
University of California, Davis
anparikh@ucdavis.edu

Thomas Proffen
Los Alamos National Laboratory
tproffen@lanl.gov

Roger Pynn
University of Indiana
pynn@mrl.ucsb.edu

R. Ramesh
University of California, Berkeley
rramesh@berkeley.edu

Don Rej
Los Alamos National Laboratory
drej@lanl.gov

Jim Rhyne
Los Alamos National Laboratory
rhyne@lanl.gov

John Sarrao
Los Alamos National Laboratory
sarrao@lanl.gov

Sushil Satija
National Institute of
Standards and Technology
sushil.satija@nist.gov

Kurt Schoenberg
Los Alamos National Laboratory
kurts@lanl.gov

Ivan Schuller
University of California, San Diego
ischuller@ucsd.edu

Dale Schaefer
University of Cincinnati
schaefdw@email.uc.edu

Steve Shapiro
Brookhaven National Laboratory
shapiro@bnl.gov

Andrew Shreve
Los Alamos National Laboratory
shreve@lanl.gov

Sunil Sinha
University of California, San Diego
ssinha@physics.ucsd.edu

Alexei Sokolov
University of Akron
alexei@uakron.edu

Ray Teller
Argonne National Laboratory
rteller@anl.gov

Guebre Tessema
National Science Foundation
gtessema@nsf.gov

Doug Tobias
University of California, Irvine
dtobias@uci.edu

Frans Trouw
Los Alamos National Laboratory
trouw@lanl.gov

Jacob Urquidi
New Mexico State University
jurquidi@nmsu.edu

Sven Vogel
Los Alamos National Laboratory
sven@lanl.gov

Hongwu Xu
Los Alamos National Laboratory
hxu@lanl.gov

Appendix B: Expected Outcomes
San Diego II
A Workshop on the
Enhanced national capability for neutron scattering
September 5-9, 2007

This two-day workshop will engage the international neutron scattering community to vet and improve the Lujan Center Strategic Plan 2007–2013 (SP07). Sponsored by the LANL SC Program Office and the University of California, the workshop will be hosted by LANSCE Professor Sunny Sinha (UCSD). Endorsement by the Spallation Neutron Source will be requested. The discussion will focus on the role that the Lujan Center will play in the national neutron scattering landscape assuming full utilization of beamlines, a refurbished LANSCE, and a 1.4-MW SNS. Because the Lujan Strategic Plan is intended to set the stage for the "L-PARC Era" at LANSCE, there will be some discussion of the long-pulse spallation source at Los Alamos. Breakout groups will cover several new instrument concepts, upgrades to present instruments, expanded sample environment capabilities, and a look to the future. The workshop is in keeping with a request by BES to update the Lujan strategic plan in coordination with the SNS and the broader neutron community. Workshop invitees will be drawn from a broad cross section of the US neutron scattering research communities.

Expected Outcome

The primary deliverable will be a workshop report defining questions and recommendations for the future of the Lujan Center. Among the questions to be addressed, does SP07

1. Adequately set the stage for L-PARC or similar signature facility at LANL?
2. Optimally utilize, from the general user science perspective, the Lujan spallation sourced for neutron scattering and nuclear physics?
3. Meet the expectations for mission science at the Laboratory?
4. Incorporate relevant recommendations from prior planning workshops, such as San Diego I (2005) and Santa Fe I (2006)?
5. Define the best instrumentation suite in view of SNS and other national neutron centers?
6. Determine a proper strategy for future spallation targets to serve the instrument suite?
7. Address implementation and ownership?
8. Provide reasonable resource requirement estimates?
9. Cover contingencies?

Selected participants will draft a workshop report on-site following an out-brief from breakout groups on the second day. A final report and CD should be ready for circulation by October 15, 2007.

Invited Speakers

Because the workshop focuses on LANSCE plans, many of the speakers will be drawn from Lujan Center and LANSCE staff who are directly involved in the planning and execution of SP07. In addition, especially for new instruments and major upgrades, champions and partners within the user community will be invited to speak. Speakers will be asked to make the science case for an investment or identify a need for addressing new science. Speakers will address breakout groups or plenary sessions.

Among the expected invited speakers and panelists are the following (non-LANL attendees noted):

Alan Hurd
Benno Schoenborn
Don Brown
Feri Mezei
Frans Trouw
Greg Smith (HFIR)
Guenter Muher
Ian Anderson (SNS)
Jarek Majewski
Jim Rhyne

Juergen Eckert
Ken Herwig (SNS)
Kurt Schoenberg
Kurt Schoenberg
Mike Fitzsimmons
Mike Rowe (NIST)
Pedro Montano (BES)
Rex Hjelm
Scott Wilburn
Steve Wender
Sunny Sinha (UCSD)
Sven Vogel
Tonya Kuhl (UCD)
Yusheng Zhao

Additional names are listed below.

Venue

The importance of University of California (UC) involvement cannot be overstated for this critical workshop. Former LANSCE Professor Sunny Sinha has graciously offered to host San Diego II. Nearby UC San Diego has very active condensed matter physics and bioscience communities with neutron experience who will lend credibility and insight to the proceedings.

The venue will help to draw well from the University of California campuses, California State and Pomona systems, Stanford, USC, and other private universities. Livermore, Berkeley and Sandia labs are a short flight away. Southern California and the Bay Area are major centers for high tech industry. California and Tennessee are the largest user states of the Lujan Center through 2006. As SNS and HFIR come into full operation, Tennessee users may decrease, leaving California as the most important base of users for the Lujan Center. Outreach to California users is important for Lujan visibility and to replace potential losses in Tennessee.

The site of the first San Diego workshop, Humphey's Half Moon Inn and Suites is a small, excellent conference facility with competitively priced meeting rooms and sleeping units. The entertainment diversions in the San Diego area are a draw for attendees during the summer, and it is hoped that UC faculty will be particularly enticed by the scientific possibilities. Humphrey's is well served by the San Diego International Airport. Attendees from Japan, China, and Australia (if any) will have easy access to the workshop.

Funding

Based on San Diego I (SD-I), approximately 50 attendees will be adequately served by a budget of \$45–\$55K for travel, hotel, food, meetings rooms, and publication costs. As with SD-I, external funding will be sought from UCOP and BES.

Attendees	Travel	Hotel	Food Total	Grand Total	
50	31000	9700	6500	47200	
Estimates					
Breakfast	Lunch	Dinner	Daily Food Total	Daily Hotel	Typical Airfare + Car
$10	$15	$25	$40	$125	$1000

Roadmap

Reports and pictures are or will be available for the following events in bold.

October 1995	Defense and Basic Research, Los Alamos (NNSA-I)
March 1997	Defense and Basic Research, Los Alamos (NNSA-II)
January 1999	LPSS Workshop, Berkeley (LPSS-I)
August 2001	20Hz Workshop, Los Alamos (LUG6)
January 2003	Defense and Basic Research, Los Alamos (NNSA-III)
July 2003	Cold Neutron Spectroscopy, Bethesda (DC-I)
June 2005	LPSS Workshop, San Diego (SD-I)
June 2005	NNSA-BES Workshop II (DC-II)
September 17-19, 2006	Lujan Center in the SNS Era (SF-I)
September 25	Draft Report SF-I
November 15-16	LANL NNSA Workshop (NNSA-IV)
December 15	Draft Report NNSA-IV
January 8	Draft Lujan Strategic Plan 2007-13
February 15	Final Report SF-I, mailing
March 19	Final Lujan Strategic Plan 2007-13, mailing
June 15	Final Report NNSA-IV, mailing
September 5-9	Strategy for Neutron Scattering, San Diego (SD-II)

Appendix C:

Summary of San Diego Workshop Planning Meetings June–August 2007

These notes summarize outlines from Lujan staff planning leading up to three conference call discussions by the Organizing Committee.

Members
Alan Hurd, LANL, Chair
Jim Rhyne, LANL
Roger Pynn, University of Indiana
Sunil Sinha, UCSD
Kurt Schoenberg, LANL
Feri Mezei, LANL and HMI
Ward Beyermann, UC Riverside
Ian Anderson, ORNL
Mike Rowe, NIST (ret)

The discussion centered on what the Lujan Center can do to excel and distinguish itself from the SNS in the area of SANS and NR (Somewhat on the model of HMI), leveraging from Lujan facility and staff capabilities.

- Scientific motivation leveraging from Lujan Staff interests and expertise:
  - ➢ Measurement of off specular reflections to probe lateral structure such as dot, lines and other surface and interfacial features.
  - ➢ Measurements of diffusion.
  - ➢ Probes of long length scales down to 2 μ.
  - ➢ Probes of smaller length scales between 10 and 1 Å.
  - ➢ Neutron spectroscopy at low-Q.
  - ➢ Simultaneous and in situ sample probes independent and complementary to NR or SANS measurements.
  - ➢ Pulse-probe (stroboscopic) measurements.
- Support of proposed core missions for Lujan (From Fitzsimmons' diagram):
  - ➢ Classified measurements.
  - ➢ Development of novel neutron scattering techniques requiring extensive R & D and beam time:
    - New neutron instrument techniques.
    - Sample environments.
    - Novel hardware and software.
  - ➢ Hands-on education in neutron scattering techniques.
  - ➢ Experiments exploring evolving hypotheses.
- Lujan facility advantages, planned and potential upgrades:
  - ➢ Cold neutrons using the current frequency of 20 Hz, access to larger simultaneous dynamic range than 60 Hz SNS.
  - ➢ More efficient TMRS design for cold neutron production:
    - More cold neutrons
    - Less higher energy neutron contamination
    - Lower gamma flux
  - ➢ Partially coupled cold moderators with Be filter (Mark III design): anticipated factors relative to present Lujan cold moderator
    - 2x cold neutron production above ca 4 Å.
    - Decreased neutron production below ca 4 Å.
    - Softer gamma output: attenuated by one-third using 1 cm aluminum.
  - ➢ Blue sky:
    - Fully coupled cold moderators: anticipated factors relative to present Lujan cold moderator: 1.5 to 2x.
    - Accelerator upgrade: 2x proton current.
    - Blue sky totals 5-6x relative to present Lujan cold moderator. Note comparison of 3-5x cold neutrons per pulse at SNS compared to present Lujan cold source.
- New instrument/experimental capabilities:
  - ➢ Polarized neutrons:
    - Incoherent background measurements.
    - Discrimination of magnetic from nuclear scattering.
    - Spin echo techniques for decoding Q values at long coherence lengths.

  - Pulsed-probe (stroboscopic) experiments of materials dynamic response:
    - Mechanical
    - Electric fields
    - Light
    - Pressure
    - Temperature
    - Magnetic fields
    - Etc.
  - Novel instrumentation:
    - Mirror VLQ
    - SESAME ULQ
    - MESANS LQS (Low-Q spectroscopy)
    - Double crystal
    - Dual purpose instruments: e.g. SANS or NR + neutron spectroscopy (add frequency domain).
    - Double mirror polarization NR or SANS.
    - Grazing incidence SANS
- Enhancement of current capabilities:
  - In situ and/or simultaneous measurements independent measurement techniques with SANS and NR, eg optical spectroscopy,
  - Advanced, real-time data reduction, assessment and analysis.
  - Professional staff to cover chemical inventories, sample environments, maintenance, etc.
- Upgrades to current instruments:
  - Asterix:
    - Replace shutter on 11A to enable separate 11A/B operations.
    - Install bent guide with dimensions matching polarization cavity: gamma background reduction 2x increase neutrons on sample.
    - Primary and secondary flight path evacuation: 4x increase in neutrons t detector)
    - Moveable sample position for reflectometry: more efficient use of neutron footprint.
  - SPEAR:
    - Evacuated guide in bulk shield.
    - Area detector.
  - LDQ
    - Large area detector (pencilated?).
    - Bulk shield guides with optics matched to collimator apertures and acceptance angles.
    - Extended flight path beamline with variable detector positions and third (frame definition) chopper.
  - General:
    - New data acquisition systems with multichannel inputs and TOF encoding for multidimensional pulse-probe experiments.
    - New cold beam lines, will require considerable study:
  - Issues:
    - Fps 3-8, with the possible exception of fp-5 are not very useful for new cold instruments unless ER-1 and be reconfigured.
    - Current viable instruments on H_2O moderators would have to be moved.
    - Likely a total reconfiguration of the Lujan facility would have to be considered.
  - New cold moderator types:
    - Premoderated-moderators.
    - CH_4
    - NH_3

Appendix D: Presentations

Plenary (Hurd, Neumann, Teller, Rhyne)

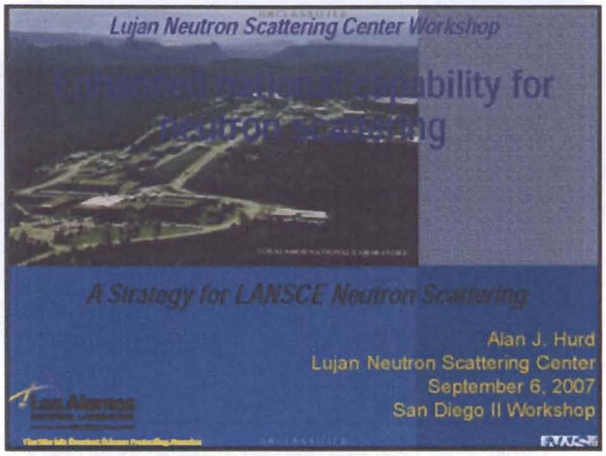
Vision (Bousoufi, Vision Summary)

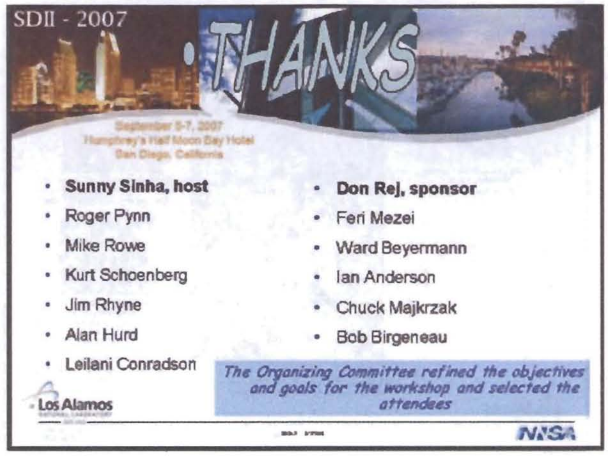
Diffraction (Clemens, Nakotte, Hemley)

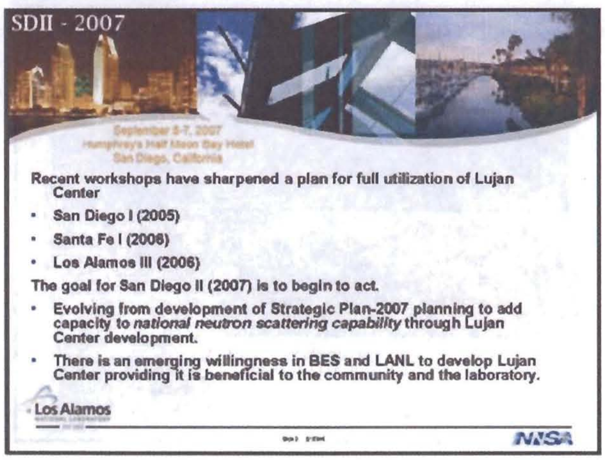
Inelastic (Eckert, Mezei, Sokolov, Teller, Shapiro, Fultz, Summary)

Low Q and Reflectivity (Hjelm, Foster, Mason, Fitzsimmons)

Writing Team Summary


Lujan Neutron Scattering Center Workshop
A Strategy for LANSCE Neutron Scattering
Alan J. Hurd
Lujan Neutron Scattering Center
September 6, 2007
San Diego II Workshop


SDII - 2007
THANKS
Sunny Sinha, host
Roger Pynn
Mike Rowe
Kurt Schoenberg
Jim Rhyne
Alan Hurd
Leilani Conradson
Don Rej, sponsor
Feri Mezei
Ward Beyermann
Ian Anderson
Chuck Majkrzak
Bob Birgeneau
The Organizing Committee refined the objectives and goals for the workshop and selected the attendees
Los Alamos
NNSA


SDII - 2007
Recent workshops have sharpened a plan for full utilization of Lujan Center
San Diego I (2005)
Santa Fe I (2006)
Los Alamos III (2006)
The goal for San Diego II (2007) is to begin to act.
Evolving from development of Strategic Plan-2007 planning to add capacity to national neutron scattering capability through Lujan Center development.
There is an emerging willingness in BES and LANL to develop Lujan Center providing it is beneficial to the community and the laboratory.
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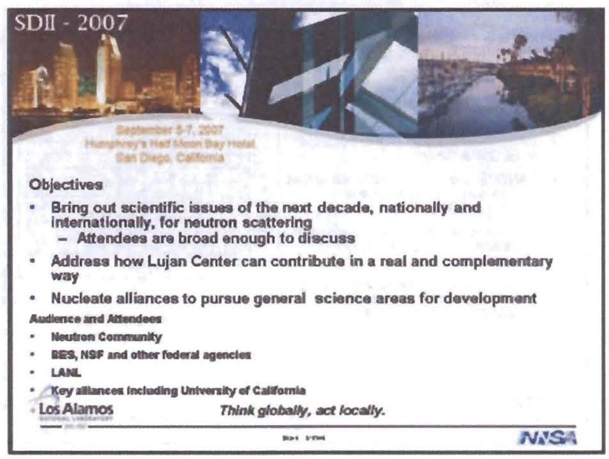
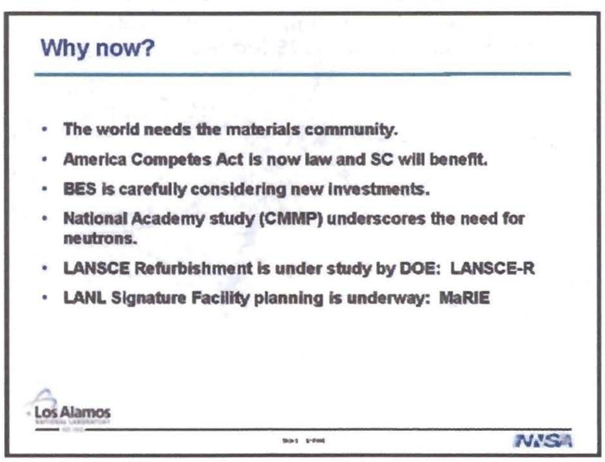
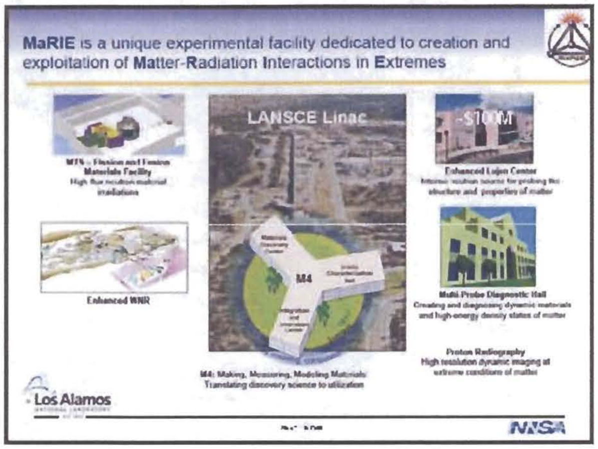
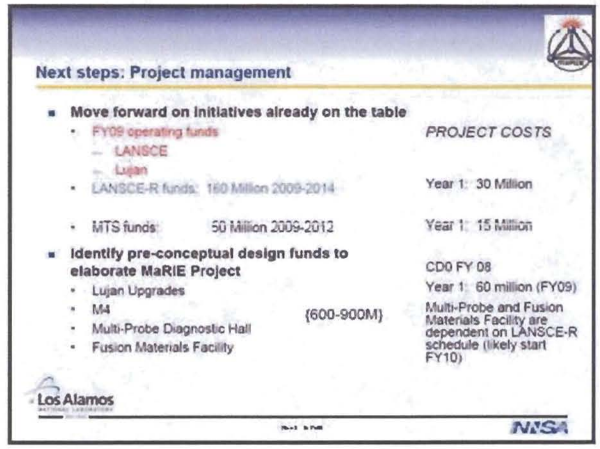
NNSA


SDII - 2007
Objectives
Bring out scientific issues of the next decade, nationally and internationally, for neutron scattering
– Attendees are broad enough to discuss
Address how Lujan Center can contribute in a real and complementary way
Nucleate alliances to pursue general science areas for development
Audience and Attendees
Neutron Community
BES, NSF and other federal agencies
LANL
Key alliances including University of California
Los Alamos
Think globally, act locally.
NNSA


Why now?
The world needs the materials community.
America Competes Act is now law and SC will benefit.
BES is carefully considering new investments.
National Academy study (CMMP) underscores the need for neutrons.
LANSCE Refurbishment is under study by DOE: LANSCE-R
LANL Signature Facility planning is underway: MaRIE
Los Alamos
NNSA


Things are happening at LANSCE
Lujan Neutron Scattering Center
Weapons Neutron Research
Isotope Production
800-MeV Proton Linear Accelerator
Proton Radiography
Future UCN Area
NNSA


MaRIE is a unique experimental facility dedicated to creation and exploitation of Matter-Radiation Interactions in Extremes
LANSCE Linac
~$100M
Enhanced Lujan Center
Enhanced WNR
M4
Multi-Probe Diagnostic Hall
Proton Radiography
M4: Making, Measuring, Modeling Materials
Translating discovery science to utilization
Los Alamos
NNSA


Next steps: Project management
Move forward on initiatives already on the table
FY09 operating funds
LANSCE
Lujan
LANSCE-R funds: 160 Million 2009-2014
MTS funds: 50 Million 2009-2012
Identify pre-conceptual design funds to elaborate MaRIE Project
Lujan Upgrades
M4
Multi-Probe Diagnostic Hall
Fusion Materials Facility
(600-900M)
PROJECT COSTS
Year 1: 30 Million
Year 1: 15 Million
CD0 FY 08
Year 1: 60 million (FY09)
Multi-Probe and Fusion Materials Facility are dependent on LANSCE-R schedule (likely start FY10)
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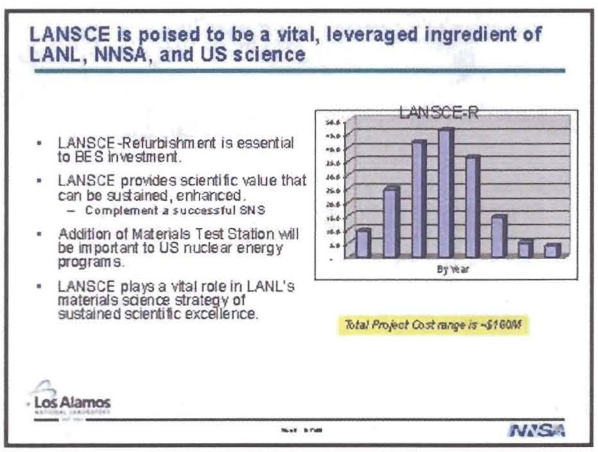
NNSA


LANSCE is poised to be a vital, leveraged ingredient of LANL, NNSA, and US science
LANSCE-Refurbishment is essential to BES investment.
LANSCE provides scientific value that can be sustained, enhanced.
– Complement a successful SNS
Addition of Materials Test Station will be important to US nuclear energy programs.
LANSCE plays a vital role in LANL's materials science strategy of sustained scientific excellence.
LANSCE-R
By Year
Total Project Cost range is ~$160M
Los Alamos
NNSA


Capability has been built by various programs to support basic research
PCS (biology, built by BER)
NPDF (pdf, built by NSF)
HIPPO (texture, built
100 μA to Lujan
SMARTS (strain, built by BES)
LANSCE and Lujan Center development since 1997 has borne fruit.
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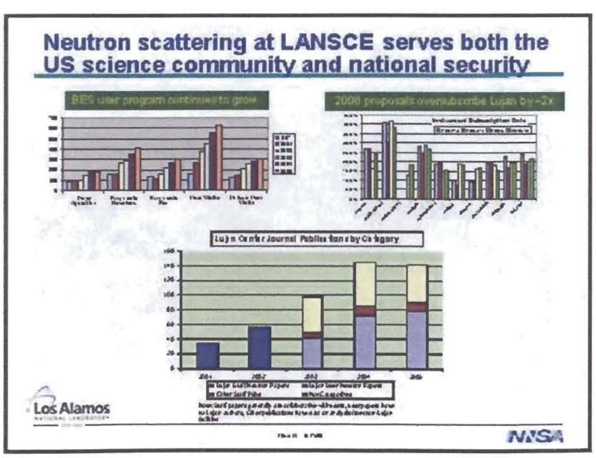
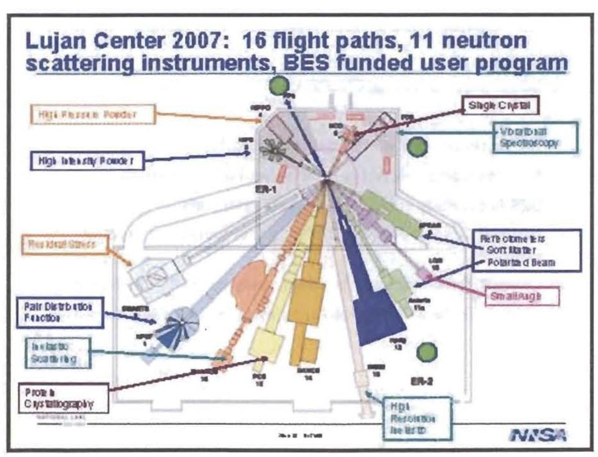
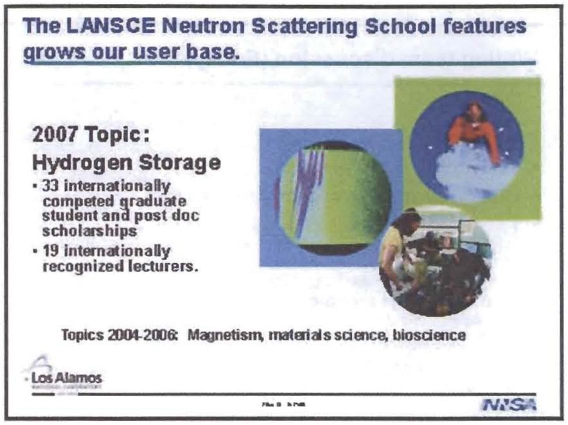

Neutron scattering at LANSCE serves both the US science community and national security
BES user program continues to grow
2008 proposals oversubscribe Lujan by ~2x
Lujan Center Journal Publications by Category
Los Alamos
NNSA


Lujan Center 2007: 16 flight paths, 11 neutron scattering instruments, BES funded user program
High Pressure Powder
High Intensity Powder
Single Crystal
Vibrational Spectroscopy
ER-1
Reflectometers
Soft Matter
Polarized Beam
Small Angle
Pair Distribution Function
Inelastic Scattering
Protein Crystallography
ER-2
High Resolution
NNSA


The LANSCE Neutron Scattering School features grows our user base.
2007 Topic:
Hydrogen Storage
• 33 internationally competed graduate student and post doc scholarships
• 19 internationally recognized lecturers.
Topics 2004-2006: Magnetism, materials science, bioscience
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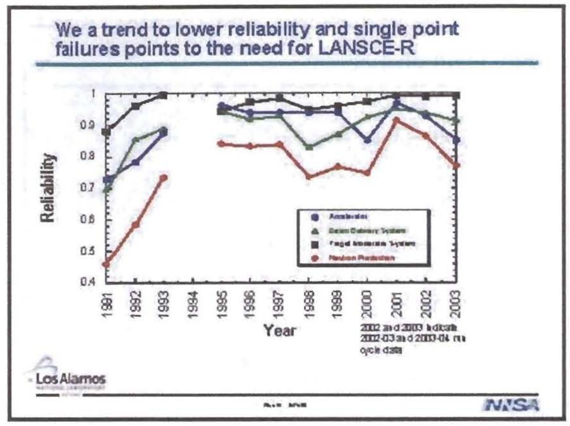
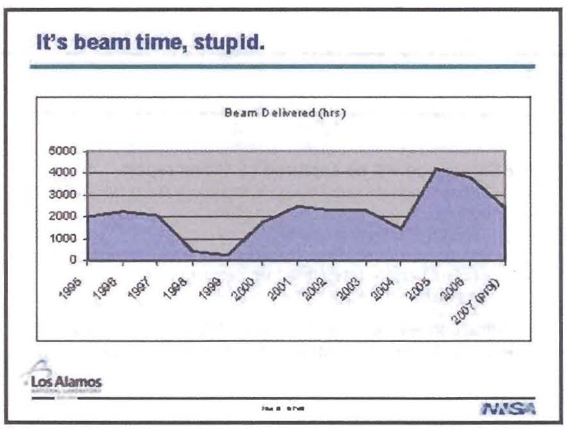
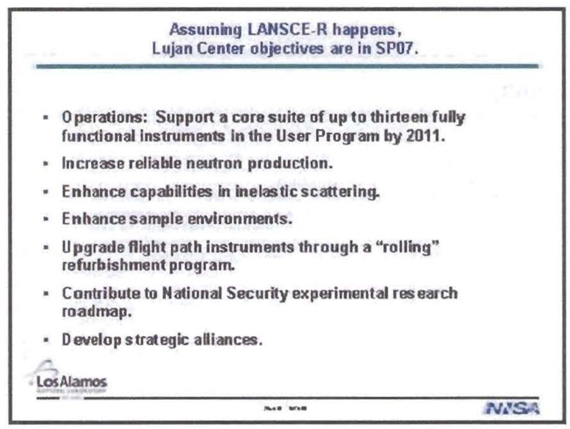
NNSA


We a trend to lower reliability and single point failures points to the need for LANSCE-R
Reliability
1
0.9
0.8
0.7
0.6
0.5
0.4
1991
1992
1993
1994
1995
1996
1997
1998
1999
2000
2001
2002
2003
Year
Los Alamos
NNSA


It's beam time, stupid.
Beam Delivered (hrs)
5000
4000
3000
2000
1000
0
1995
1996
1997
1998
1999
2000
2001
2002
2003
2004
2005
2006
2007 (proj)
Los Alamos
NNSA


Assuming LANSCE-R happens,
Lujan Center objectives are in SP07.
• Operations: Support a core suite of up to thirteen fully functional instruments in the User Program by 2011.
• Increase reliable neutron production.
• Enhance capabilities in inelastic scattering.
• Enhance sample environments.
• Upgrade flight path instruments through a "rolling" refurbishment program.
• Contribute to National Security experimental research roadmap.
• Develop strategic alliances.
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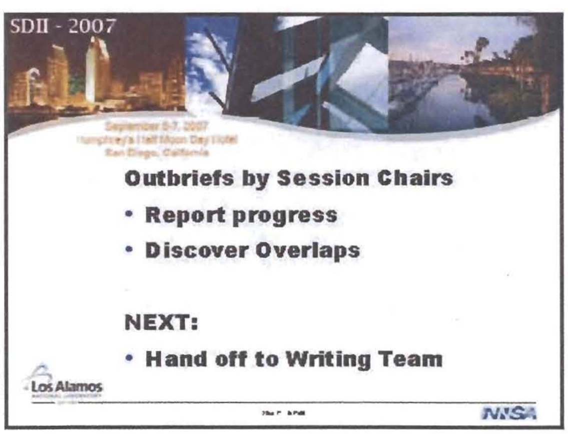
SDII - 2007
Outbriefs by Session Chairs
• Report progress
• Discover Overlaps
NEXT:
• Hand off to Writing Team
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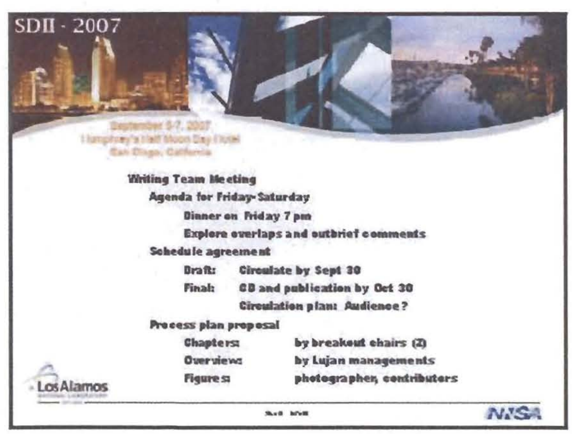
SDII - 2007
Writing Team Meeting
Agenda for Friday-Saturday
Dinner on Friday 7 pm
Explore overlaps and outbrief comments
Schedule agreement
Draft: Circulate by Sept 30
Final: CD and publication by Oct 30
Circulation plan: Audience?
Process plan proposal
Chapters: by breakout chairs (2)
Overviews: by Lujan managements
Figures: photographer, contributers
Los Alamos
NNSA

Writing team discussion

- Audience includes LANL management. Shall there be recommendations to them?
  - Synergies within the lab
  - Policy issues--ammo
- NNSA as the audience?
  - Put in community needs and BES needs
  - National security needs is less of a priority
  - Lujan has moved beyond demonstrating need and value to LANL and NNSA management
- Roll this workshop up to a business plan built on the strategic plan
- Cater to certain groups in LANL (e.g. condensed matter community)
  - Work on synergies, e.g. biothreat, CINT, Shreve,...
  - CINT: Need to refresh that relationship

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Writing team discussion (Friday)

- Add executive summary to chapters
- Aim for 5 page text single spaced
- Each chapter should address sample environments
- Provide a prioritized list.
  - Indicate interest in community if possible and have group address the sketch
  - Roll up the investment list up front including staffing
  - Suggestion: immediate and mid-term lists.
  - Indicate basis of priority (scientific interest, time sequence, etc)
  - IDT push is important
- Discuss real estate, moderator, staffing, user, and other global implications

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Staffing

- Opportunity:
  - Define the staffing plan without whining
  - Strategy drives staffing—even for proposal writing
  - Will be captured in all chapters: flow from vision chapter down to science area chapters including sample environment team
  - Invoke the OSTP IWG report that cites number of unique users per scientific staff member including all direct technical support.
  - Look at ISIS and ILL metrics
  - Maxed out such that we are limited in users by staffing
- Team formation check
- INS reflectometry and USANS
  - Lo Q will address
  - Teams to coordinate
  - Techniques for Asterix—crystals, NSE,... be careful with being complementary to the exclusion of success
  - Pulse probe and other synergies

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- **BES session will be captured by Vision report**
  - Travel, Programmatic Proposals, Mail-ins, training students, fast access,
  - LANSCE-R down time aspects
  - Synchrotron issue: Take this up within the neutron community exp facilities directors' meeting in February
  - Emphasize complementarity.
- **Diffraction with energy analysis: INS will take this up in Pharos discussion; Diffraction will include where valued.**

Los Alamos NNSA

The NIST Center for Neutron Research

Recent Developments, the NCNR Expansion, and the Future

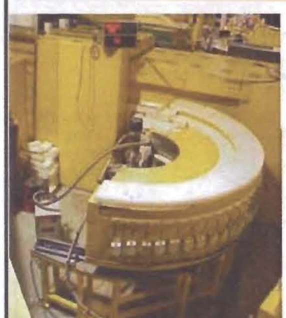
Dan Neumann
dan@nist.gov
www.ncnr.nist.gov

NIST

NIST Center for Neutron Research

NIST

"Mail-in" Service for Diffraction



BT-1 Powder Diffractometer

$\frac{1}{4}$ of the time for mail-in samples

sample environment limited to cryofurnaces (4K to 600K)

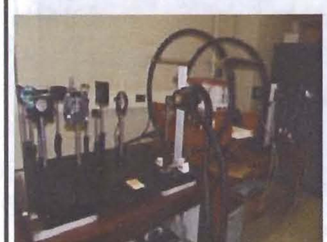
data treatment is performed, but not analysis

NIST

^{3}He Polarization Program

^{3}He program for scattering applications

SEOP lab with two stations

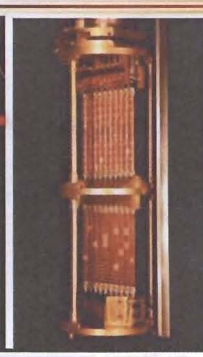


Currently available for 3-axis, reflectometry, and SANS

NIST

BT7 Thermal 3-Axis Spectrometer

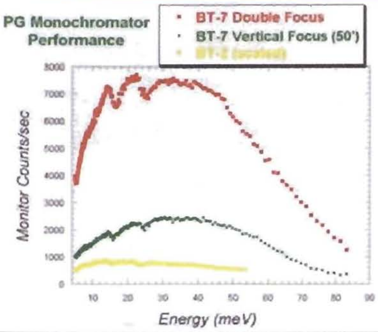
Double focusing monochromators



PG(002) d = 3.35 Å
Cu(220) d = 1.27 Å

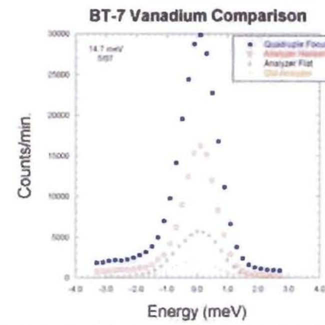
NIST

Double focusing monochromators



NIST

BT-7 Analyzer Performance



Overall gain from previous 3-axis instrument at BT-2

6 to 60

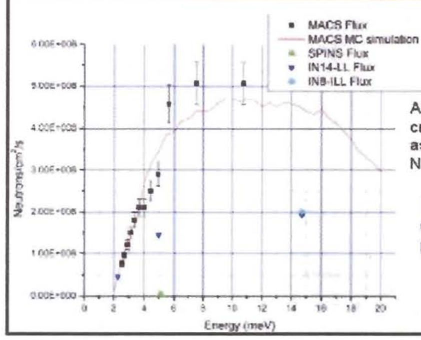
Joined the user program in the most recent call.

2/3 of the time will be offered in the next call (deadline in the spring).

NIST

MACS Primary Spectrometer

MACS Performance



Analyzer system is currently being assembled in the NCNR high-bay area.

Expect initial experiments next year.

NIST

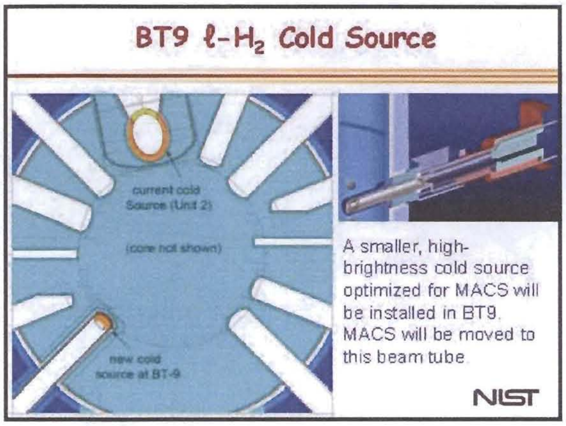
Expansion Activities

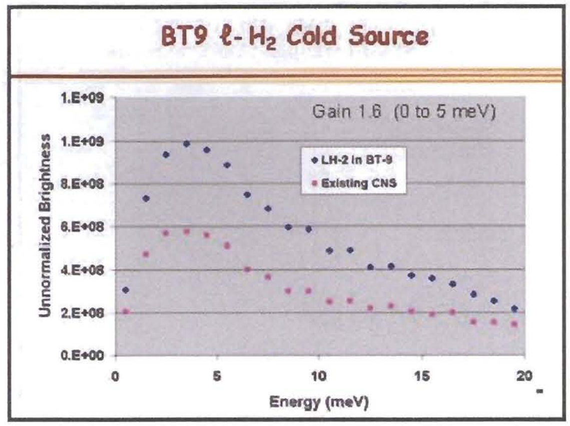
- New Cold Source
- Construction
- Instrument development
- Beam delivery
- Reactor reliability enhancements

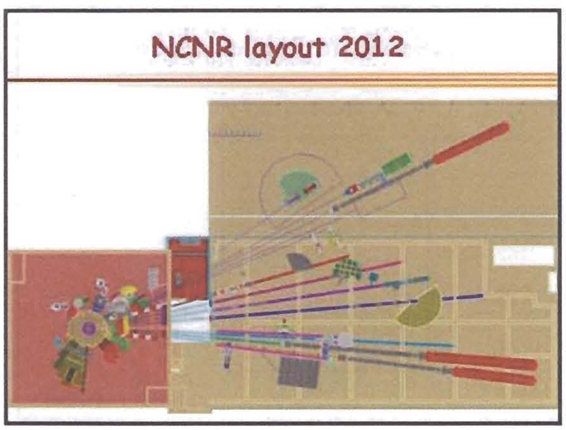
NIST

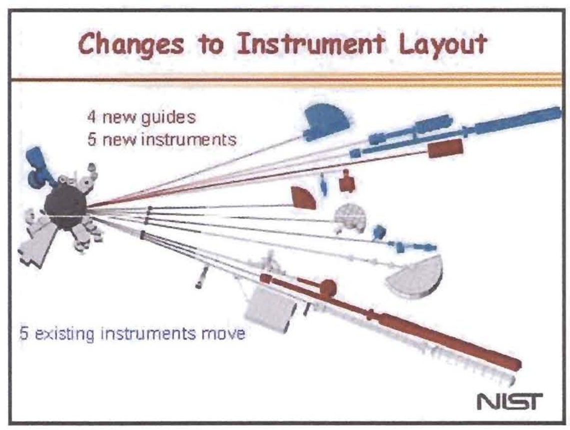
NIST Center for Neutron Research

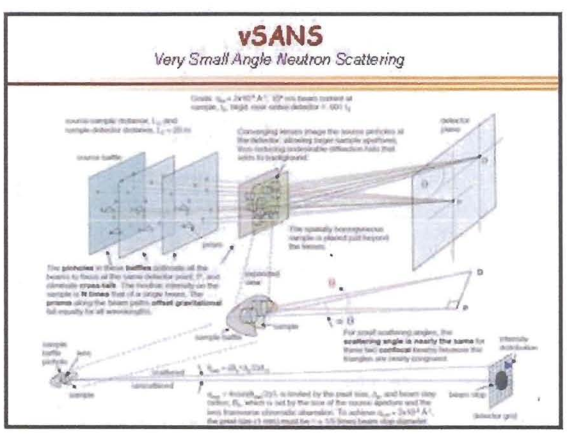
NIST

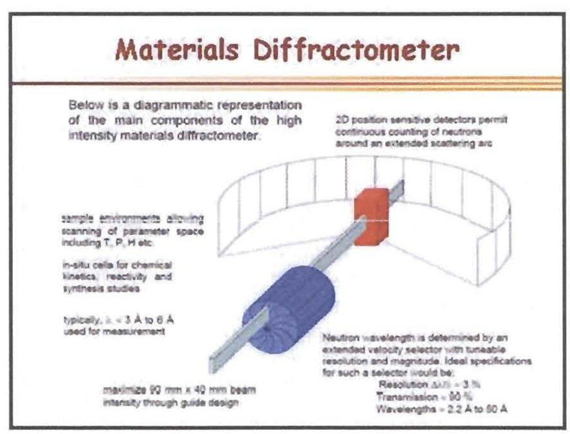

BT9 ℓ-H_2 Cold Source
current cold Source (Unit 2)
(core not shown)
new cold source at BT-9
A smaller, high-brightness cold source optimized for MACS will be installed in BT9. MACS will be moved to this beam tube.
NIST


BT9 ℓ- H_2 Cold Source
Gain 1.6 (0 to 5 meV)
LH-2 in BT-9
Existing CNS
Unnormalized Brightness
1.E+09
1.E+09
8.E+08
6.E+08
4.E+08
2.E+08
0.E+00
0
5
10
15
20
Energy (meV)


NCNR layout 2012

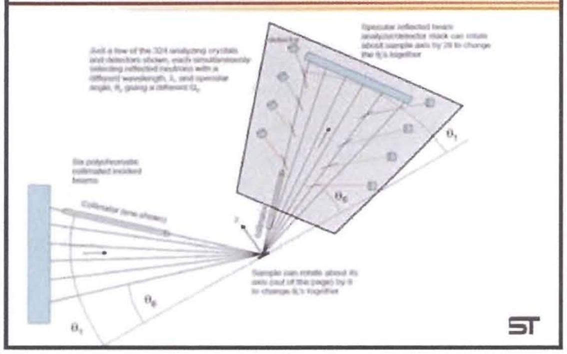

Changes to Instrument Layout
4 new guides
5 new instruments
5 existing instruments move
NIST


vSANS
Very Small Angle Neutron Scattering


Materials Diffractometer
Below is a diagrammatic representation of the main components of the high intensity materials diffractometer.
2D position sensitive detectors permit continuous counting of neutrons around an extended scattering arc
sample environments allowing scanning of parameter space including T, P, H etc.
in-situ cells for chemical kinetics, reactivity and synthesis studies
maximize 90 mm x 40 mm beam intensity through guide design

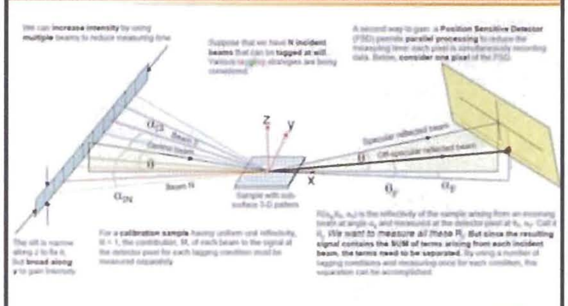
CANDoR

Chromatic Analysis Neutron Diffractometer or Reflectometer



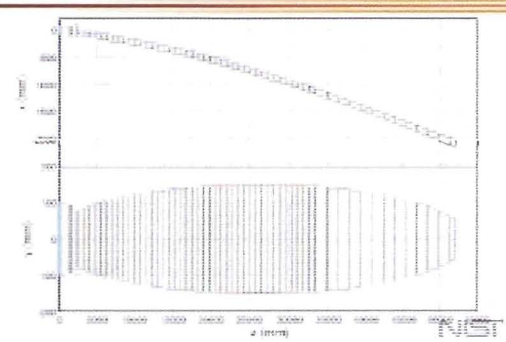
MAGIk

Multiple Angle Grazing Incidence k (vector)

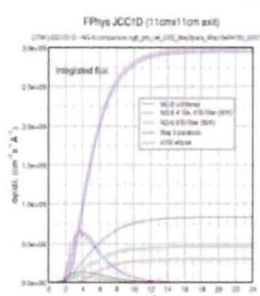


NIST

NGc Guide



NGc Guide Performance



NIST

Expansion Instruments

vSANS - min Q about 5 times smaller than current 30 m SANS with choice of beam geometries (pin holes, slits, lenses, and/or mirrors) – *John Barker*

MD - very fast, low-resolution diffractometer using wavelengths of 3 to 8 Å

CANDOR - multi-wavelength, multibeam reflectometer ~60x faster than current NCNR instruments – *Frank Heinrich*

MAGIk - reflectometer optimized for off-specular scattering using modulation techniques (spin precession *etc.*) - *Brian Maranville*

Neutron Physics - guide NGc - 6x neutron flux on NG6

The NSE spectrometer will be upgraded and placed on NGa

The 10 m SANS will be installed on NGb1 & a 30 m SANS will be installed on NGb2

MACS will be relocated to its own cold source in a "thermal" beam port

NIST

Construction Milestones

- 15 Feb 07 – President signs FY 07 Bill for NIST
- 16 Apr 07 – NCNR transmitted Requirements Documents for NIKA/HDR
- 15 May 07 – Review of floor plans: NCNR/Plant/NIKA/HDR
- 21 Jun 07 – Acquisition Plan briefed to DOC
- 20 Aug 07 – 100% Review of "Bridging Design" Documents, Drawings & Specs

UPCOMING SCHEDULE

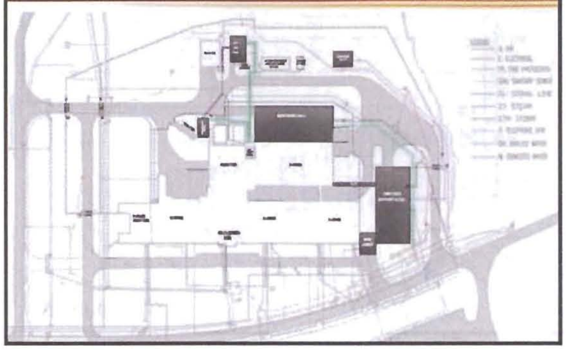
Sep 07 – Award D/B Task Orders for:
Utilities/Site Prep – work to start in Fall
Secondary Cooling Pump Building – work to start Jan/Feb

When 08 Funds are available – Award D/B Task Orders for:
Guide Hall
Technical Support Building
Remaining Utilities/Site Work

Occupancy – Late 2009

NIST

Construction



NCNR Expansion

NIST

Going forward

Continue to Develop New Capabilities

- Continue to expand polarized beam capabilities
- Program for joint development of sample environments
- New thermal 3-axis (many components procured)
- Funding in place for one major upgrade or new instrument per year
- Emphasize spin echo methods
- D_2 cold source plus modernize guide system
- Extend neutron measurement core competence at NIST
- Expand external partnerships

NIST

Instrumentation

The 2002 OSTP report emphasized that the expense of building and operating neutron sources requires that they be "fully-instrumented" and that the instruments be well-staffed.

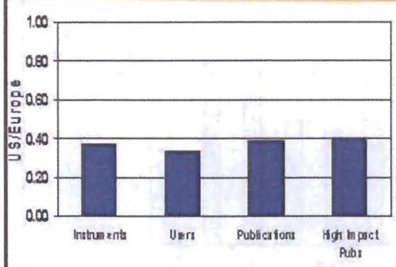
It also pointed out that the SNS alone cannot meet US needs for neutron scattering capability.

So would there be high quality science to fill the additional beam time if Lujan were fully instrumented with high quality instruments?

We needn't speculate as Europe has already done this.

NIST

Current Status – US and Europe



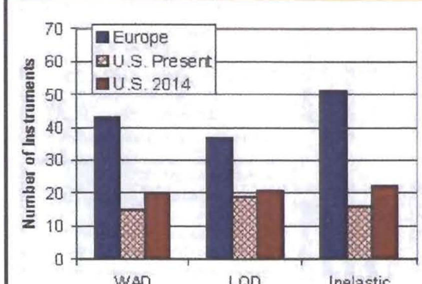
By basically any measure, the US neutron scattering community is ~35% of that in Europe.

This includes publications in high-impact journals (as defined by C. Vettier).

The US neutron community would almost certainly grow and produce more great science if it had more good neutron scattering instruments.

NIST

Number of Instruments



Even with the NCNR expansion and the continuing development of instrumentation at SNS and HFIR, in 2014 the US capacity in neutron scattering will still only be about 50% of that in Europe.

NIST

Build it and they will come!

Nearly 40 PhD's are awarded each year that contain neutron data from NIST.

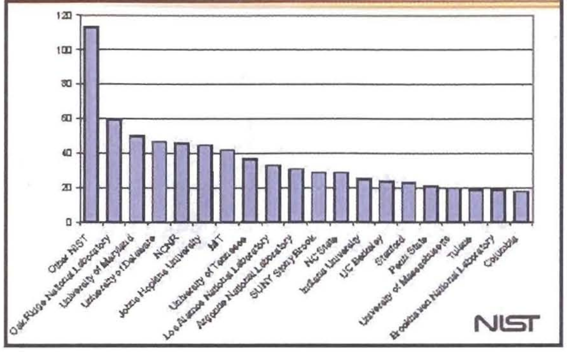
7 new neutron scattering junior faculty were hired last year (that I know of).

I know of 3 this year:
- Wendy Mao – Stanford
- Michel Kenzelmann – University of Minnesota
- Danilo Pozzo – University of Washington

We need to do better, but...

NIST

NCNR Participants FY2005



NIST

Instrumentation

Play to one's strengths:

NCNR Expansion emphasizes instrumentation that appeals to our current user community (more heavily soft matter than any other neutron source in the world) and/or makes good use of a continuous source

It's important that the US neutron community optimize instrumentation overall.

This does NOT mean that there shouldn't be significant overlap in the instrument suites of the various sources.

High Demand, High Impact Science

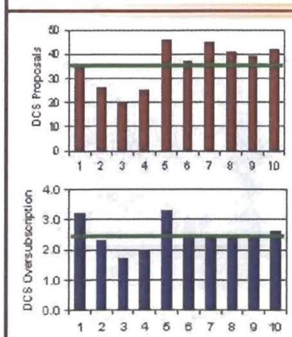
NIST

Disk Chopper Spectrometer

CHRNS

DCS

CHRNS



Our last 10 "Calls for Proposals"

Ave. Proposals: **36**
Ave. Oversubscription: **2.5**

71 Publications since 2004
13 PRL
4 Nature, Science, PNAS

About ½ of proposals receive beam time.

Experience teaches that ~20% of proposals are not "well thought out".

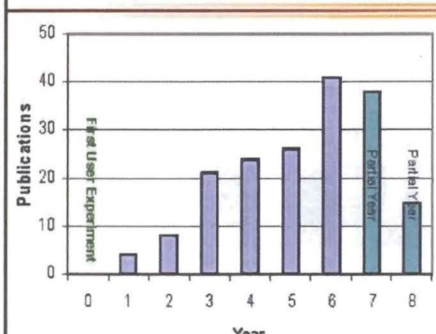
So roughly 10 worthy proposals per call don't get time.

These would have led to at least 20 publications over the same time frame..

With more capacity, these numbers would undoubtedly increase.

NIST

Backscattering and DCS



It takes time for publications to achieve steady state.

NIST

Argonne Scattering and Imaging Institute (ASI^2)

Argonne NATIONAL LABORATORY

... for a brighter future

Principal Investigators:

Raymond Osborn (MSD-ANL)

James W. Richardson, Jr. (IPNS-ANL)

Gabrielle Long (XSD-ANL)

UChicago ▸ Argonne

Office of Science

ASI^2 executive summary

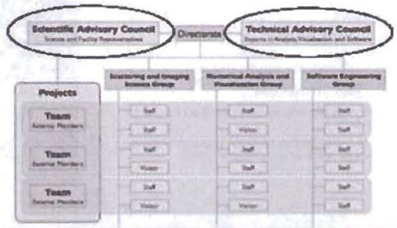
- **An institute situated at Argonne for the benefit of the US scattering community**
- **Intended to address the "new" generation of users**
  - focused on analysis results and not instrumentation details
- **Focus on grand challenges (e.g: CMMP2010 report, B**
- **Develop professional software for the general com**
  - Project orientation (6-8 projects, 2-3 new/yr)
  - Projects originate from the general community
- **Holistic approach to scientific problems**
  - Linking theory/simulation more closely with scattering
  - New algorithms that incorporate constraints from x-ray, neutron and electron scattering measurements
  - New algorithms for new science with new instrumentation
  - Ubiquitous visualization

from Opportunities for Discovery: Theory and Computation in Basic Energy Sciences, January, 2005

Argonne

ASI^2 organizational structure

- **Matrix structure, with ASI^2 staff being members of groups and projects**
- **Visitor program to supplement expertise and facilitate close collaborations**
- **Formal process for evaluating proposals (SAC) and assigning personnel to projects**
- **Outside technical support (TAC) to maintain professional computational standards**



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ASI^2 project focus

- **ASI^2 will support 6-8 projects at any given time**
  - 3-4 year duration, i.e., 2-3 new projects each year
  - ASI^2 staff members will be active participants in one or more projects
  - Goal: gain critical mass of expertise to tackle well-defined scientific challenges
- **Project proposals solicited from general community**
  - Scope of projects determined by consultation among PI's or as result of workshop(s)
  - Project teams composed of multiple partners from outside ASI^2 and staff members from all ASI^2 groups
- **Typical features of successful proposals**
  - Address grand scientific challenges (beyond reach of individual PI's)
  - Requiring multiple scattering and imaging probes
  - Recognize pressing needs and scientific interests at facilities (software tools)

Argonne

Near-term plans for ASI² (if proposal is successful)

- **Start-up funds have been requested for FY08**
- **Projects for FY08**
  - 1-2 projects chosen after consultation with facility representatives
  - Focus on projects with broad reach and requiring ASI²s unique mix of talent
- **Workshops**
  - Science-focus - Self-assembled groups of scientists identifying future challenges for ASI²
  - Among national facilities to settle on computing platforms and approach to community software development
- **Staff hiring**
  - Extensive searches would be initiated for key personnel, such as Director, Deputy Director, and Group Leaders
  - Software engineers

Argonne

Perspective from US neutron facilities

- **Very strong (professional and personal) relationships between facilities**
  - SNS, HFIR, LANSCE, IPNS, NCNR - Strong letters of support
- **Computing groups at facilities should flourish**
  - The needs are greatly beyond the scope and anticipated funding of ASI²
- **But ASI² will have some unique features**
  - Largest collection of scattering-science computing experts
  - Broad scientific focus - x-ray, neutron, electron, etc.
  - Strong links to theory, simulation, large-scale computing

- **ASI² can therefore:**
  - Serve immediate needs linked to high-impact science
  - Precipitate computing standards decision-making for the long-term
- **Upshot:**
  - SNS, HFIR - Limited resources in the near-term, so welcome strong collaborations
  - LANSCE - See new developments at ASI² as advantageous to their science
  - IPNS - Limited lifetime, but new developments would have immediate impact
  - NCNR - Has active computing effort, but welcomes collaboration

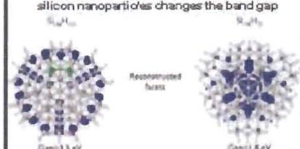
Argonne

Example 3: The Nano problem

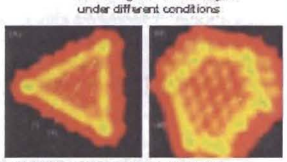
Simon Billinge

- **Currently, structures of nano-materials can not be routinely solved - the crystallographic paradigm (infinite repeating unit cell) is not applicable**
- **Multiple techniques must be combined**
  - (e-, x-, n-diffraction, EXAFS, direct imaging, Raman, *etc.*)
- **A scientific program that explores how to successfully combine these approaches is needed if this hurdle is to be overcome**

Surface reconstruction of hydrogenated silicon nanoparticles changes the band gap



AFM images of HDS catalysts under different conditions



From "Nanoscience Research for Energy Needs", DOE workshop report,, Mar 16-18, 2004

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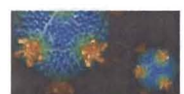
Example 4: Mechanisms of catalysis

- **We don't currently have the tools to leverage facility resources in the pursuit of more efficient catalysts for hydrogen production.**
- **Probe nano-catalysts changes and chemical transformations simultaneously with dual (or more) probes *in-situ***
  - *Techniques: EXAFS, Raman, diffraction....*
  - On-line analysis of data sets
  - Simultaneous MD simulations of catalyst structure changes
  - Leading to identification of solid state transformations that correlate to conversion and selectivity differences
- **This transforms the experimental operation into the "discovery mode"**
  - Enables the researcher to tailor experiments to identify "active" sites and configurations



Protein encapsulated nano-catalysts for hydrogen production

Yttria nano-rod supports for photo-catalytic hydrogen production

Argonne

Lujan of the Future
Where should we go in the national context?

Jim Rhyne
Deputy Director, Lujan Neutron Scattering Center
Los Alamos

Los Alamos NNSA

National support for neutron science

- **The SNS will be the nation's flagship neutron source**
  - Experiments requiring the highest flux
  - Full complement of inelastic and elastic machines for widest spectrum of current applications
  - Will have the largest user program and address the widest range of scientific disciplines
- **HFIR and NIST (reactors)**
  - Triple axis neutron spectrometers
  - SANS
  - Other complementary elastic and inelastic instruments
  - Major broad-based user programs
- **Lujan – The second BES Pulse source – An ISIS-class facility (>100 μa reliable operation > peak intensity)**

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Where does Lujan fit in?

- **Provide for experiments not requiring ultimate flux**
- **Provide instruments appropriate for Lujan user community**
- **Address areas where Lujan has a special niche to fill**
- **Provide flexibility for trying new instrument/sample environment concepts**

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This workshop – recommendations for new/upgraded instruments – please consider (at least) the following classes:

- **"Must have" elastic and inelastic instruments for any comprehensive national user facility (Lujan user community, including defense science)**
- **Instruments tailor-made for specific areas of science**
  - Requiring unique instrument characteristics
  - Requiring dedicated specialized sample environments
  - Examples (from many)
    - » Correlated-electron materials spectrometer (later slide)
    - » High pressure instrument
    - » Engineering strain-scanning diffractometer
    - » Hydrogen in materials
    - » Neutron/nuclear polarization effects
- **Lujan has a special niche**
  - Advantage of 20 Hz repetition rate (cold neutrons, long wave-length)
  - Specialized moderators (e.g., coupled L-H_2)
  - Flexibility in instrument configuration (i.e., test-bed for new concepts)
  - Flexibility in sample environments (e.g., pressure, magnetic field)

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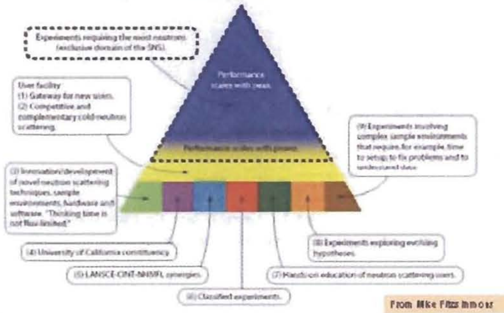
Rhyne

1 of

Pyramid of neutron scattering experiments and Lujan missions in the SNS-era.



From Mike Fitzsimmons

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Example of science-specialized instrument (admittedly biased example)

- **Correlated-electron inelastic spectrometer (specialized sample environment capabilities**
  - Cold moderator emphasizing long wave-lengths, energy transfers (e.g., < 30 meV in neutron energy loss), and moderately high resolution (0.1 – 1 meV).
  - Single crystal capability
  - Magnetic fields up to 15T (split superconducting solenoid geometry) upgradable to 25 – 30T series connected hybrid
  - Temperatrures down to 40 mK available in magnetic field environment
  - Hydrostatic (fluid driven) pressures to 15 kbar again in field and temperature environment
  - Neutron polarization capability

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Summary - Charge to break-out groups

- **Plot the course for future instrument development at Lujan**
  - Propose new instruments
  - Propose modifications to existing instruments
  - Recommend new neutron moderator/source characteristics
  - Recommend new sample environment capabilities (either general or integral with specialized instruments)
  - Evaluate feasibility of instruments tailored to specific area of science
- **If appropriate, identify spectrometer advisory teams to lead proposal development for specific instruments**
- **Identify new areas of science (or user groups) Lujan should address**
- **Evaluate present and proposed instrumentation and source characteristics in light of research needs of present and future users**
- **Lead Lujan in a mutually supportive role for the SNS and the national neutron landscape**
- ***Lujan Center Strategic Planning and Institutional Vision* breakout may wish to consider other issues as outlined in hand-out**
- **References: Lujan Strategic Plan, *Lujan in the SNS Era*, Workshop Report**

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Breakout Groups

- **New Instrument Concepts and Upgrades for Inelastic Scattering**
  Feri Mezei, chair – Frans Trouw (Lujan planning group chair) – Room A
- **New Instrument Concepts and Upgrades for Diffraction**
  Despino Luca, chair -- Thomas Proffen, (Lujan planning group chair) – Room B
- **New Instrument Concepts and Upgrades for Reflectivity and Low-Q diffraction**
  Roger Pynn, chair – Rex Hjelm (Lujan planning group chair) – Room C
- **Lujan Center Strategic Planning and Institutional Vision**
  Tonya Kuhl, chair – Dockside Room
- **The breakout group assignments sent to you earlier can be considered "notional." Feel free to participate in any (or more than one) breakout group.**

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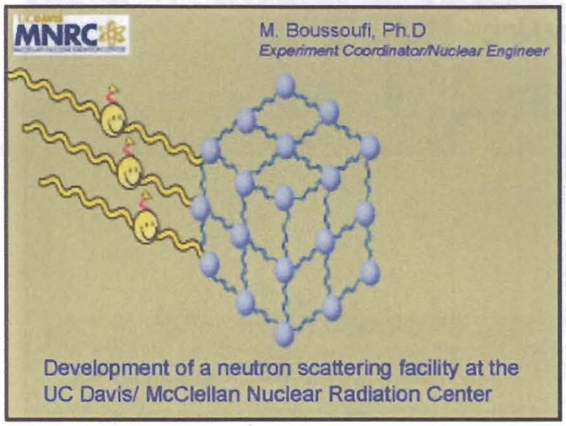
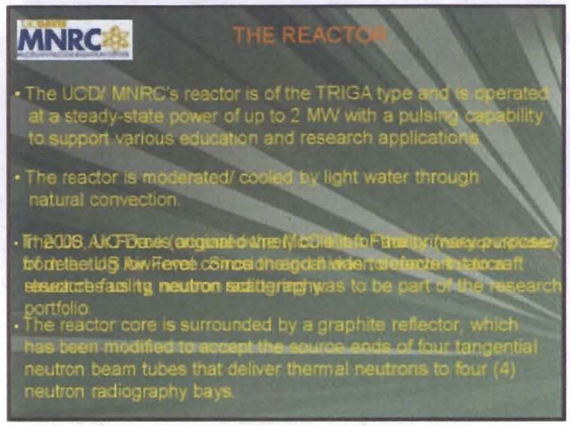
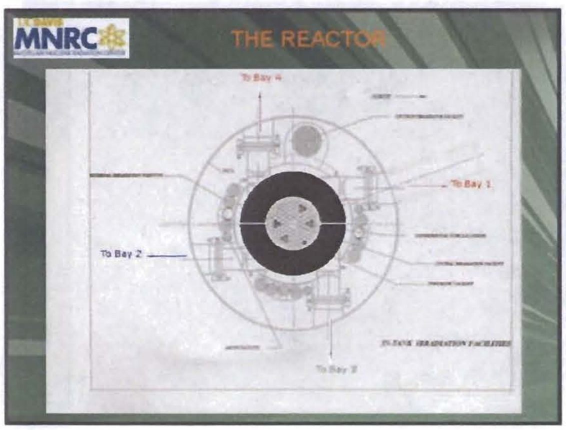
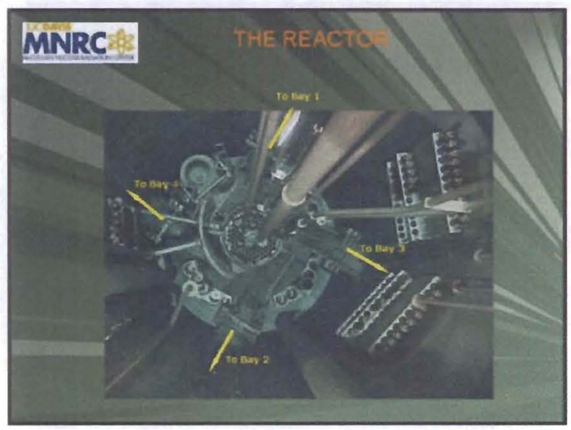
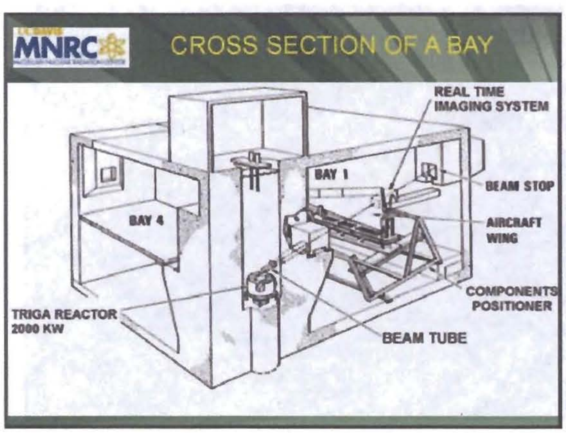

UC DAVIS
MNRC
M. Boussoufi, Ph.D
Experiment Coordinator/Nuclear Engineer
Development of a neutron scattering facility at the UC Davis/ McClellan Nuclear Radiation Center


MNRC
THE REACTOR
• The UCD/ MNRC's reactor is of the TRIGA type and is operated at a steady-state power of up to 2 MW with a pulsing capability to support various education and research applications.
• The reactor is moderated/ cooled by light water through natural convection.
portfolio.
• The reactor core is surrounded by a graphite reflector, which has been modified to accept the source ends of four tangential neutron beam tubes that deliver thermal neutrons to four (4) neutron radiography bays.


MNRC
THE REACTOR
To Bay 4
To Bay 1
To Bay 2
To Bay 3

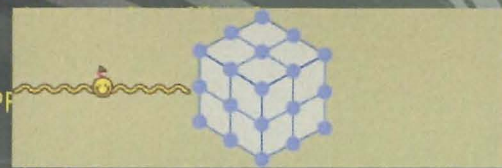

MNRC
THE REACTOR
To Bay 1
To Bay 4
To Bay 3
To Bay 2


MNRC
CROSS SECTION OF A BAY
REAL TIME IMAGING SYSTEM
BAY 1
BEAM STOP
BAY 4
AIRCRAFT WING
COMPONENTS POSITIONER
TRIGA REACTOR 2000 KW
BEAM TUBE


• Bay 1 with an aircraft wing

Facility	Thermal Flux (n/cm²·sec)	Beam Aperture (inch)	L/D Ratio
Bay 1	$\approx 4.2 \times 10^6$	1.40	200
Bay 2	$\approx 4.2 \times 10^6$	1.40	200
Bay 3	$\approx 5.6 \times 10^6$	1.54	175
Bay 4	$\approx 3.8 \times 10^5$	1.25 x 1.25	270

Implementing neutron scattering at MNRC



imaging

- Opportunity to combine neutron imaging systems with the emerging concept of Bragg reflection from bent crystals

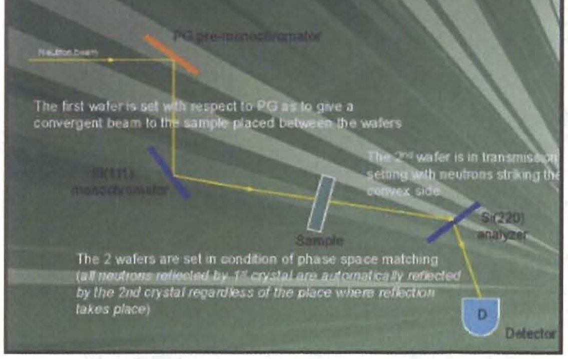
GENERAL CONSIDERATIONS

- Development of imaging for small angle neutron scattering (SANS) and neutron diffraction are being considered
- The handicap of low source would be overcome by using focusing monochromators.
- The existing detector systems of high spatial resolution would be used to implement neutron imaging techniques for SANS with PSD.

TECHNICAL DESCRIPTION

- A two-bent-crystal SANS technique will be used
- The use of different reflections from bent silicon wafers allows intensity gains at the expense of resolution (Q-resolution ~ 10^{-3} Å^{-1})
- Elements used would be:
  - *A medium-grade PG focusing pre-monochromator set up to extract a high-flux beam of 1.5 A neutrons (0.036 eV)*
  - *A pair of bent silicon wafers in succesive reflection [(111) reflection from the first and (220) from the second]*

SKETCH OF ARRANGEMENT

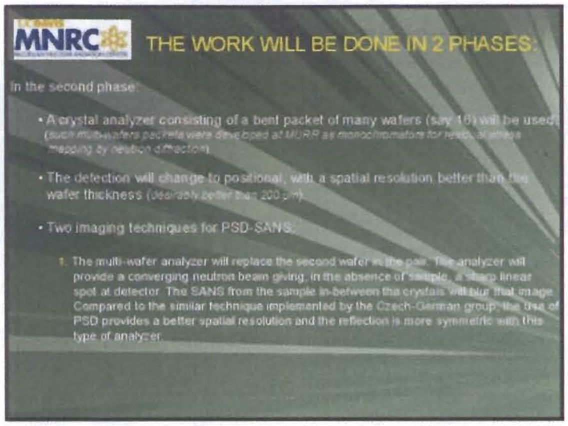


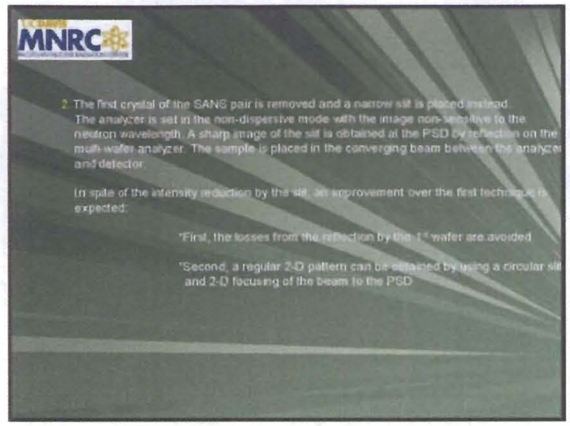
THE WORK WILL BE DONE IN 2 PHASES:

In the first phase:

- The SANS detector will be of normal type (He³)
- SANS will be measured sequentially at open detector by rocking the 2nd wafer against the 1st one.
- The width of the rocking curve at no sample defines the Q-resolution which in this case (bent crystals) depends also on the position of the sample

Boussoufi **1 of**





Vission Summary

National Perspectives and Vision for the Lujan Center

Moe Boussoufi, Phil Goldstone, Ken Herwig, Barry Klein, Alex Lacerda, Gunther Muhrer, Dan Neumann, Don Rej, Ray Teller, Guebre Tessema, Tonya Kuhl

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Echoes from Santa Fe Workshop

- **The SNS will be the nation's flagship neutron source**
- **Lujan Center has a vital role to play**
  - National Context, Los Alamos Context, Opportunities for Lujan, Science Priorties, Long Term Future
  - LANSCE-R > 150μA
    - 20Hz => long wave length, soft condensed matter, possible stroboscopic techniques
    - **National Security Mission**
    - UC connection
    - Fully instrumented (competitive) and staffed would satisfy *many* neutron scattering user needs that do not require flux of SNS
- **HFIR and NIST (reactors)**
  - Triple axis neutron spectrometers
  - SANS
  - Other complementary elastic and inelastic instruments
  - Major broad-based user programs
- **Lujan – The second BES Pulse source – An ISIS-class facility** (>100 μA reliable operation > peak intensity)

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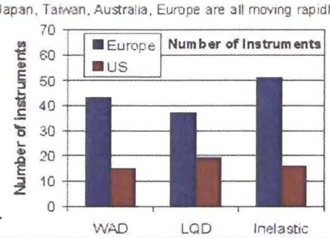
What has changed since Santa Fe Workshop

- **National and World Context has changed**
  - Passage of ACI was critical to maintain vitality of science
  - BUT ACI is not enough, must have continuing progress to regain/maintain world leadership
  - With SNS, HFIR, NCNR Expansion still only 50% of Europe, IPNS closure in 2009
  - China, Japan, Taiwan, Australia, Europe are all moving rapidly



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Lead Lujan in a mutually supportive role for the SNS and the national neutron landscape

- **Balance between special instruments and broad general tool instruments (Signature Concept for Lujan)**
  - Polarization
  - Long wavelength soft condensed matter
  - Inelastic low energy magnetism problems in the microV miliV
  - Hydrogen systems
  - Stroboscopic measurements (DAS is available to leverage) play to national security needs
  - Neutron resonance spectroscopy for EOS measurements
  - Correlated electrons
  - Powder diffraction grow synchrotron connect – dual neutron/x-ray characterization? High resolution instrument. Liquids
  - National security is a signature feature
  - Single crystal PCS – synchrotron connect
  - High pressure => Extreme environment Instrument (Laptron?)

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Complementarity of Lujan capabilities with the SNS, HFIR, NIST, and other neutron centers

- **Balance portfolio between World leadership in niche areas and broad user instruments**
- **DOE BES Needs Lujan to –**
  - grow users - more visiting academics faculty, postdocs, students
  - LANSCE-R Must get CD1,2,etc as soon as possible
  - BES will not wait - timing critical for successful LANSCE-R to ensure future BES funding to Lujan.
  - 3000Hrs, new instruments (aided by lower run time), >150μA
  - Defense Programmatic Mission, Homeland Security, competitive instruments, threat reduction chem-bio
- **DP Needs – BES satisfied, gateway (grow Users)**

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Complementarity of Lujan capabilities with the SNS, HFIR, NIST, and other neutron centers

- **Regional Focus**
  - Leverage UC connection better – LANS (addressed further in later slides)
  - Partnerships with West coast X-ray facilities, local structure theme XAFS, PDF analysis leverage with ASII
  - CINT
- **Partnerships with neutron facilities**
  - Integrated national approach to neutron science in this country
  - Continue to improve relations between facilities – Fractious neutron community is no longer true.
  - Continue to improve relations and leveraging across the community especially within DOE facilities – need convenient ways to share expertise across facilities.
  - Polarization is ripe for more synergy
  - Workshop and formation of IDTs NEEDED NOW to develop individual instrument proposals

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Vission Summary

Role of UC and Academic Institutions in Lujan Center

- Davis, San Diego, SB, and Santa Cruz all have joint LANL-UC Centers – can we improve the coupling between these centers and LANSCE
- Increase Joint LANL-UC Institutes
  - » Bay Area ENERGY Institute
  - » Materials Under Extreme Environments (UC, LLNL joint Center with LANL)
  - » UC-IDTs to tap non-traditional scatterers – e.g. hydrogen
    - + Example is LAPTRON
  - » UC-NUCLEAR Institute – imaging, irradiate seeds, I125, UC needs more heavy science component to use the reactor, cask fuel testing Possible LANL connection with radiation damage.
- How do we move forward to strengthen UC Connections
  - » Front load with faculty appointments
  - » Improve faculty / LANL staff exchanges (make it easier to do)
  - » PI-Lujan partnerships - need to partner/ split cost to get new instruments and smaller hardware. Additional Funding Opportunities with other Agencies.
- **Workshop and formation of IDTs NEEDED NOW to develop individual instrument proposals – UC-IDT**

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Future

1. **LANSCE-R critical component**
2. **ISIS class facility**
   - Fully instrumented
   - Fully staffed
   - 150 μA, 4000+Hrs, 90% reliability
   - Balance between general instruments and world recognized leadership
3. **Lujan Success in National Landscape**
   - LANSCE Signature capability – leverage long wavelength, 20Hz capabilities of Lujan
     - Sample Environment capabilities
     - National Security
     - Neutron Innovation non-flux limited – test bed
   - LANL Signature capabilities - Material Science expertise and theory
   - Alliances
     - Strategic around theme of National Security – Energy Science – Discovery Science
     - Synergies across agencies – e.g. CHRNS model, PCS
     - UC
     - West Coast Synergy – light sources, microscopy, etc. Regional Leadership
     - Coordination with sister neutron facilities

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Future

4. **Integrated complex of current facilities and capabilities to accomplish broad science mission**
   - Already good make it seamless to the User
   - Synergies of Material Science activities
     - MOUs to utilize all facilities – special needs for soft matter
   - CINT and Magnet Lab
   - Rad-Chem facilities and interface between facilities
   - Deuteration Facility
     - » Real-time, onsite, working facility
     - » Expansion will enable greater utilization of neutrons
     - » Example of UC partnership
5. **MaRIE –**
   Matter-Radiation Interactions in Extremes

Continuing Evolution of Physics Laboratory to Materials Laboratory

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Needs

- Operating funds to fully utilize the capabilities of Lujan – 13 instruments
- Funds for continuous upgrades
- Enhanced sample preparation facilities/access
- Development of future leaders and educational role of Lujan requires mid-career mentorship
- Concerted effort to expand neutron scattering as an important tool for broad scientific community in materials, energy, soft condensed matter, etc.
  - » Attract users who are not aware of neutron scattering – sufficient staff time is the main mechanism to accomplish this. Collaborative relationships are essential to enable novice users to obtain useful outcomes and become adept.
  - » Time and co-location aids the expansion. Visiting positions at a wide range of institutions
- Leveraging of the laboratory to grow User community
- **Continuing Evolution of Physics Laboratory to Materials Laboratory**

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Barriers

- **SNS is not a barrier – all facilities have to be run well to support national needs**
- **Operating funds to fully utilize the capabilities of Lujan**
  - Not an SC BES Lab and Lujan not an NNSA facility
  - Interface between NNSA and BES
  - Strengthen the Lujan – SC relationship
    - » Improvement in the relation over the last two years
    - » SC is very supportive of Lujan as the ISIS class facility
    - » More reaching out to strengthen role of Lujan in SC portfolio
    - » Strengthen the Lujan – NNSA relationship
- **Retention of high quality staff**
  - » Users go to facilities with the best staff and infrastructure
  - » Current support of facility is inadequate but strong potential for improvement in near term – clarity of vision from management will drive this to occur
  - » Long-term stability to operate as ISIS class facility
  - » Competition for staff by other worldwide facilities is a growing concern

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Barriers

- **User barriers**
  - Training is reasonable level
  - Currently constrained staffing levels may impede ability to fully support users
    - » Computer security
    - » Enable users to get their data and analyze their data from anywhere
  - Foreign nationals timing issues – access to training 24/7?
    - Language Barriers
  - Streamline access and interface between CINT and LANSCE
    - » Travel – STONE funding should be renewed
    - » Guest-house – this will improve User access, comfort, and utilization of the beam 24/7
    - » Improved sample preparation facilities AND access to other facilities on the Mesa
- **New Instruments**
  - Funding
    - » ACI is a great start, continued investment over long term needed
    - » Potential of OP support for new instruments is affected by budgetary concerns
    - » Operating funds to utilize new instruments
  - **Materials under extreme environments is a cross-cutting theme and signature direction**

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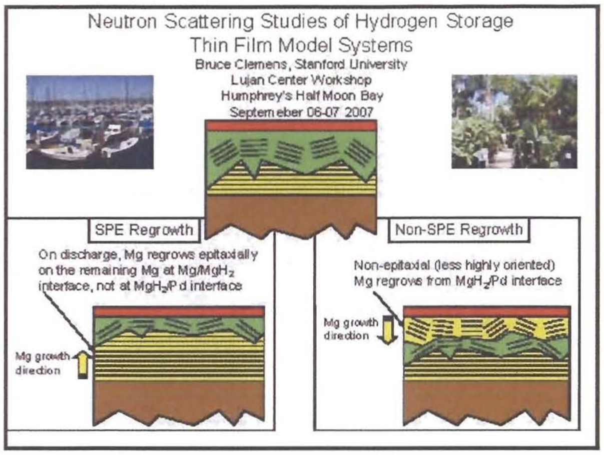
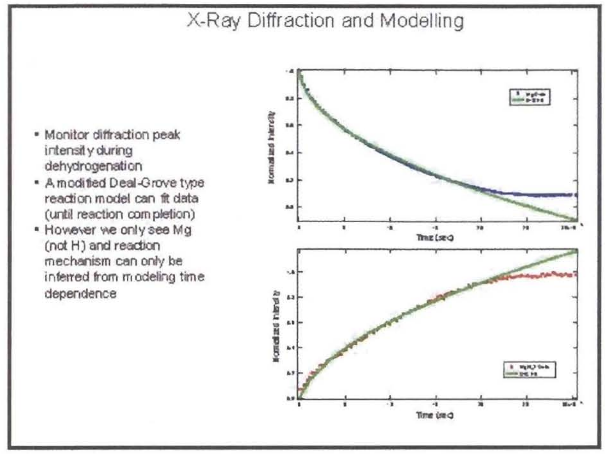
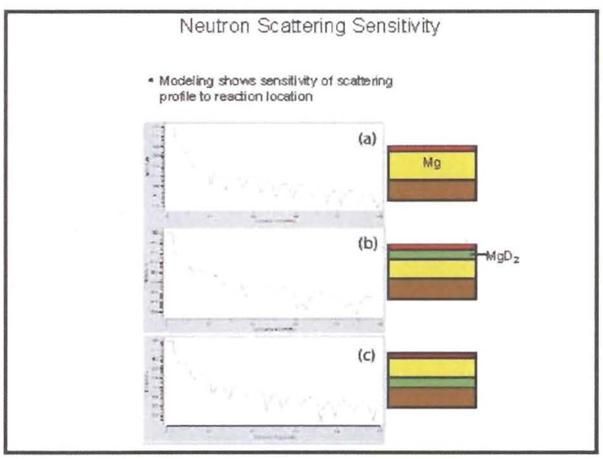
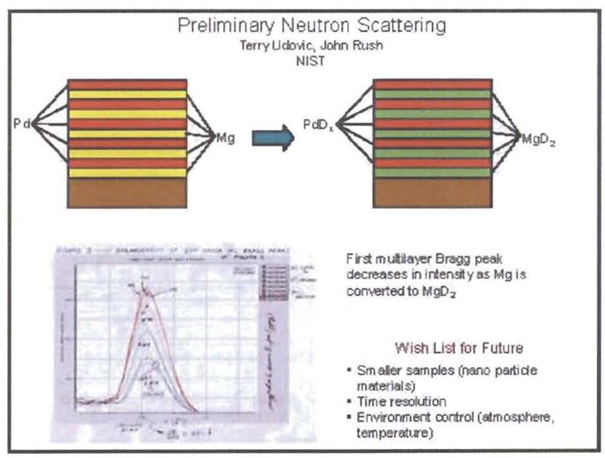

Neutron Scattering Studies of Hydrogen Storage
Thin Film Model Systems
Bruce Clemens, Stanford University
Lujan Center Workshop
Humphrey's Half Moon Bay
Septemeber 06-07 2007
SPE Regrowth
On discharge, Mg regrows epitaxially on the remaining Mg at Mg/MgH2 interface, not at MgH2/Pd interface
Mg growth direction
Non-SPE Regrowth
Non-epitaxial (less highly oriented) Mg regrows from MgH2/Pd interface
Mg growth direction


X-Ray Diffraction and Modelling
• Monitor diffraction peak intensity during dehydrogenation
• A modified Deal-Grove type reaction model can fit data (until reaction completion)
• However we only see Mg (not H) and reaction mechanism can only be inferred from modeling time dependence


Neutron Scattering Sensitivity
• Modeling shows sensitivity of scattering profile to reaction location
(a)
Mg
(b)
MgD2
(c)


Preliminary Neutron Scattering
Terry Udovic, John Rush
NIST
Pd
Mg
PdDx
MgD2
First multilayer Bragg peak decreases in intensity as Mg is converted to MgD2
Wish List for Future
• Smaller samples (nano particle materials)
• Time resolution
• Environment control (atmosphere, temperature)

Opportunities for polarized single-crystal diffraction in applied magnetic fields at the Lujan Center

Heinz Nakotte

Geometrical constraints of the magnets and negate much of the advantage of large detector coverage for many SNS instruments.

The design of present instruments (e.g. TOPAZ) only allows for limited magnetic fields. Magnetic stray fields may exclude fields in excess of 5 Tesla or so.

The recent developments of broad-band polarizers will allow magnetic studies that traditionally could be done only at reactor sourses (e.g. form-factor studies).

The Lujan Center a large opportunity to establish a niche area in the area of polarized single-crystal diffraction in applied magnetic field. There is an already strategic alliance with other LANL groups (MST, NHMFL)

SCD is clearly not equipped to do such experiments and an IDT should be formed to come up with a more suitable instrument design.

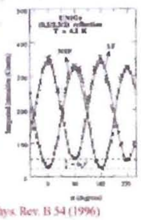
NNSA Los Alamos

Polarized Neutron Diffraction

Sensitive Detection of Moment Components

Spin-flip scattering tests the perpendicular and non-spin-flip scattering the parallel components to the moment.

Measuring the spin-flip and non-spin-flip response as function of neutron polarization within the b-c plane, x-component to the magnetic moment of UNiGe were confirmed



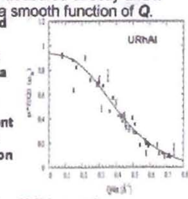
H. Nakotte et al., Phys. Rev. B 54 (1996)

Magnetic Form Factor Studies

The magnetic moments in a compound may differ from the free-ion moments, i.e. the orbital moments may be partly quenched.

$f(Q)$ can be measured directly and it should be a smooth function of Q.

The measured U magnetic formfactor in URhAl show a reduction of ~40% in the orbital moment compared to the U^{3+} free-ion value.



J.A. Paixao, H. Nakotte et al., J. Phys.-Cond. Matter 4 (1996)

NNSA Los Alamos

Polarized Neutron Diffraction - continued

Separation of Magnetic and Nuclear Intensities in Ferromagnets

Nuclear scattering is often much larger than magnetic scattering. The cross section for neutrons perfectly polarized parallel (+) or antiparallel (–) to the crystal magnetization are given by

$(d\sigma/d\Omega)^{+} \propto (b-C^{\eta})^2$ and $(d\sigma/d\Omega)^{-} \propto (b+C^{\eta})^2$

where b is the average nuclear scattering length and $C^{\eta} = \frac{1}{2}\gamma r_0 g F(Q) \langle S^{\eta} \rangle$ with $\langle S^{\eta} \rangle$ the mean spin in direction η. Measuring the so-called flipping ratio

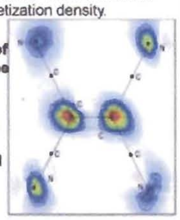
$$R = \frac{(d\sigma/d\Omega)^{+}}{(d\sigma/d\Omega)^{-}}$$

uses of the nuclear-magnetic interference term $\pm 2bC^{\eta}$ to determine the magnetic portion

Determination of Magnetization Densities

$M(Q)$ is the Fourier transform of the magnetization density.

Experimental spin density of an organic free radical-ion. Real-space density maps were reconstructed with model-enhanced Maximum Entropy method.



A. Zheludev, et al. J. Am. Chem. Soc. 116 (1994)

NNSA Los Alamos

Diffuse Magnetic Scattering

Scattering Response in Absence of Long-Range Magnetic Order

paramagnetic scattering

- entirely diffuse in zero magnetic field, i.e. it is continuously distributed over all scattering directions
- gives rise to an additional (but extremely small) 'magnetic background'

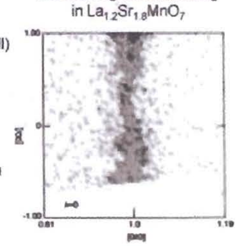
short-range magnetic fluctuations

- occur in the vicinity of magnetic transitions
- average net magnetic moment gives rise to Lorentzian-shaped magnetic peaks
- known as 'critical scattering'; the exponents in the temperature or field dependence can be related to the dimensionality of fluctuations

spin glasses

- for completely random spin distributions, there are no magnetic Bragg peaks
- reduced dimensionality in the randomness may allow for some Bragg diffraction, e.g. 'magnetic powder lines'.

Diffuse magnetic scattering in $La_{1.2}Sr_{1.8}MnO_7$



C.D. Ling et al., Phys. Rev. B 62 (2000)

NNSA Los Alamos

Powder vs. Single-Crystal Diffraction

Powder Diffraction

required sample size: > 1 cm^3

typical sensitivity^: >0.3μ_B/f.u.

Advantages:

- availability of 'good' samples
- 'simple' diffraction pattern
- substantially less problems with extinction, strain broadening etc.

Disadvantages:

- cannot resolve the moment configurations in some cases, e.g. for cubic structures
- does not distinguish between single-**q**, multi-domain and multiple-**q**, single-domain response
- relatively low sensitivity

^: depends on the magnetic structure

Single-Crystal Diffraction

required sample size: > 1 mm^3

typical sensitivity^: >0.05μ_B/f.u.

Advantages:

- substantially higher sensitivity
- allows 'unambiguous' determination of moment configurations (including domains)
- single crystals are required for studies of magnetic anisotroy, e.g. with external uniaxialpressure and/or magnetic field; magnetic form factor studies

Disadvantages:

- 'good-quality' single crystals are often hard to grow
- extinction corrections may be substantial
- experiments and the analysis of the data can be very time-consuming as one often needs to cover a large fraction of the reciprocal space

NNSA — Los Alamos

Spallation Neutron Sources vs. Neutron Research Reactors

Time-of-Flight Method

- spallation sources, such as LANSCE, utilizes the 'white beam' in a diffraction experiment
- position-sensitive area detectors cover large portions of the reciprocal space (similar to a Laue camera)
- coverage of the reciprocal space is typically achieved by a few rotations of the crystal

main advantages:

- no moving parts
- de**Monochromatic-Beam Experiment**res

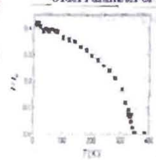
Data by Rotter et al.

- most diffractometers at reactors make use of monochromators to fix the wavelength
- in the resolution limit, only points in reciprocal space are explored

main advantage:

- far more efficient for the study of single reflections, e.g. to determine the order parameter

Order Parameter of $LaSrFeO_4$



M.H. Jung, H. Nakotte et al., J. Appl Phys (2005)

NNSA — Los Alamos

New science with Neutron Scattering at Extreme Conditions
(low T, high B, high p)

Magnetic transitions as function of T, B and p

Field-induced moment configurations

Metamagnetism and magnetic anisotropy

Magnetism in colossal magneto-resistance materials

Magnetism in low-dimensional magnets

Dimerization and incommensurability

Nanomagnetism

Magnetic multilayers, spin valves, exchange bias

Magnetic quantum dot arrays

Exchange coupling in permanent-magnet materials

Magnetic excitations and gap spectroscopy in high fields

Lifting crystal-field degeneracy by an applied field

Suppression of superconductivity, vortex kinematics

Spin wave dynamics

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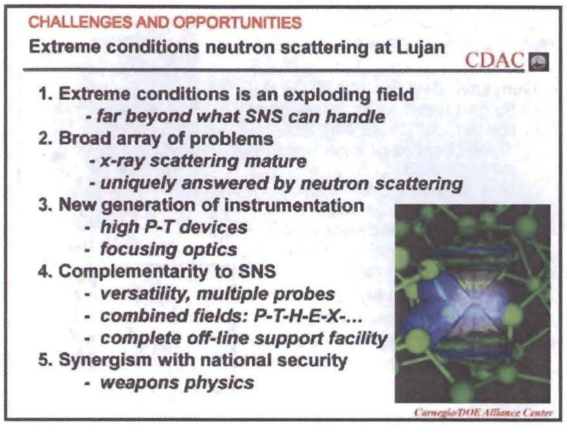
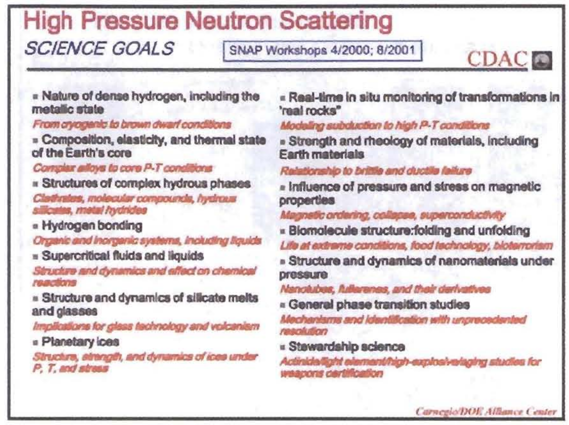
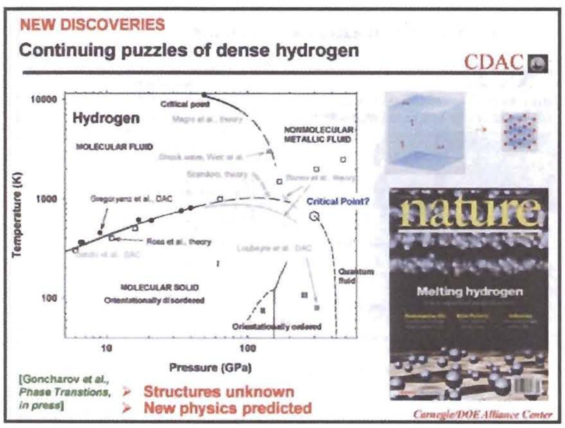
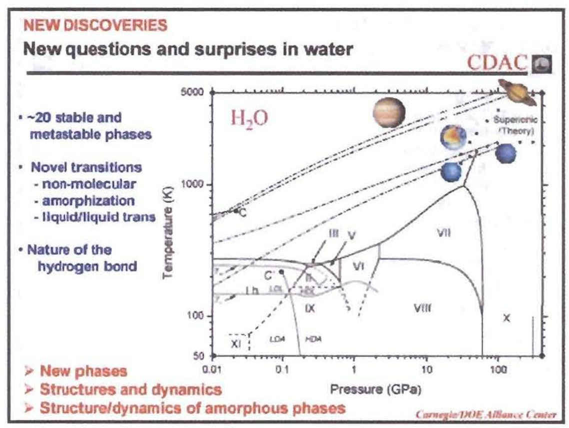
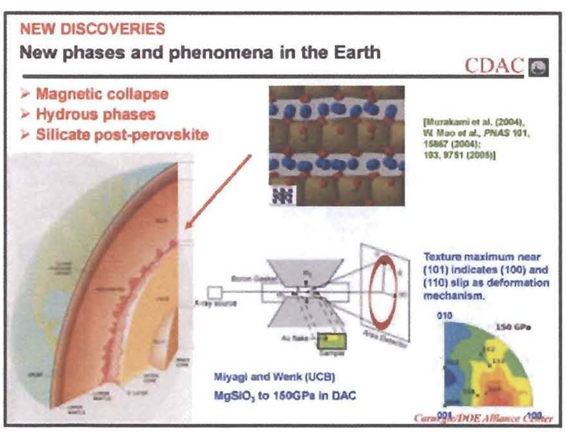
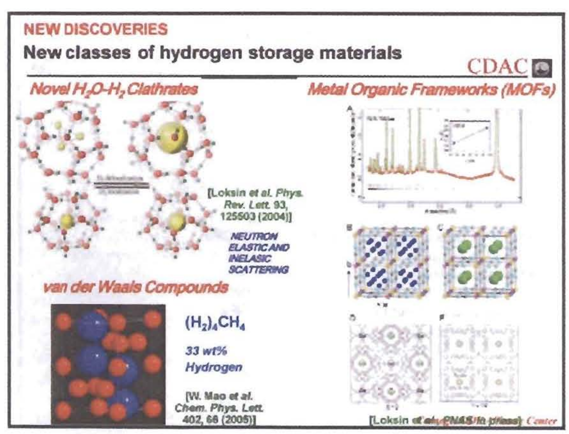

CHALLENGES AND OPPORTUNITIES
Extreme conditions neutron scattering at Lujan
CDAC
1. Extreme conditions is an exploding field
- far beyond what SNS can handle
2. Broad array of problems
- x-ray scattering mature
- uniquely answered by neutron scattering
3. New generation of instrumentation
- high P-T devices
- focusing optics
4. Complementarity to SNS
- versatility, multiple probes
- combined fields: P-T-H-E-X-...
- complete off-line support facility
5. Synergism with national security
- weapons physics
Carnegie/DOE Alliance Center

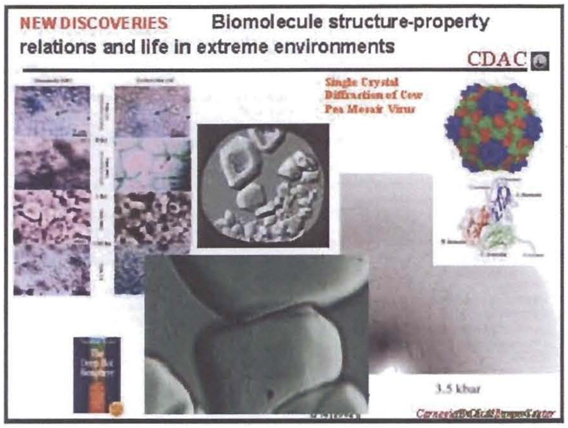

High Pressure Neutron Scattering
SCIENCE GOALS
SNAP Workshops 4/2000; 8/2001
CDAC
Nature of dense hydrogen, including the metallic state
From cryogenic to brown dwarf conditions
Composition, elasticity, and thermal state of the Earth's core
Complex alloys to core P-T conditions
Structures of complex hydrous phases
Clathrates, molecular compounds, hydrous silicates, metal hydrides
Hydrogen bonding
Organic and inorganic systems, including liquids
Supercritical fluids and liquids
Structure and dynamics and effect on chemical reactions
Structure and dynamics of silicate melts and glasses
Implications for glass technology and volcanism
Planetary ices
Structure, strength, and dynamics of ices under P, T, and stress
Real-time in situ monitoring of transformations in "real rocks"
Modeling subduction to high P-T conditions
Strength and rheology of materials, including Earth materials
Relationship to brittle and ductile failure
Influence of pressure and stress on magnetic properties
Magnetic ordering, collapse, superconductivity
Biomolecule structure:folding and unfolding
Life at extreme conditions, food technology, bioterrorism
Structure and dynamics of nanomaterials under pressure
Nanotubes, fullerenes, and their derivatives
General phase transition studies
Mechanisms and identification with unprecedented resolution
Stewardship science
Actinide/light element/high-explosive/aging studies for weapons certification
Carnegie/DOE Alliance Center

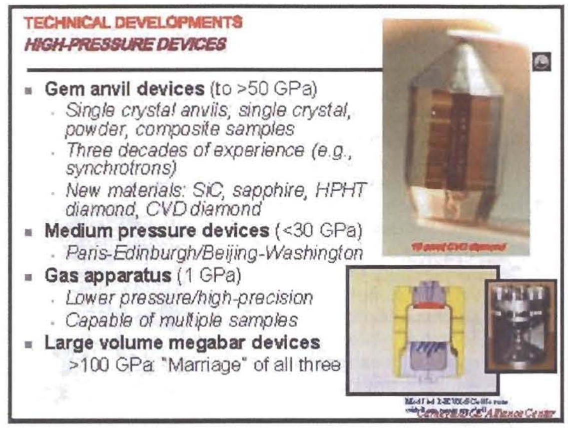

NEW DISCOVERIES
Continuing puzzles of dense hydrogen
CDAC
Hydrogen
Critical point
NONMOLECULAR METALLIC FLUID
MOLECULAR FLUID
Gregoryanz et al., DAC
Ross et al., theory
Critical Point?
Quantum fluid
MOLECULAR SOLID
Orientationally disordered
Orientationally ordered
Temperature (K)
10000
1000
100
10
100
Pressure (GPa)
nature
Melting hydrogen
[Goncharov et al., Phase Transtions, in press]
Structures unknown
New physics predicted
Carnegie/DOE Alliance Center

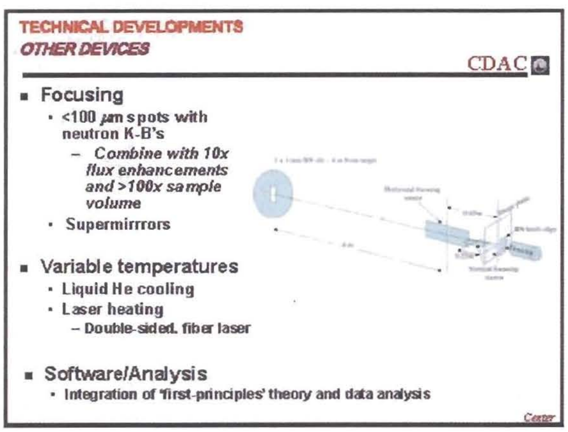

NEW DISCOVERIES
New questions and surprises in water
CDAC
~20 stable and metastable phases
Novel transitions
- non-molecular
- amorphization
- liquid/liquid trans
Nature of the hydrogen bond
H₂O
Superionic (Theory)
Temperature (K)
Pressure (GPa)
New phases
Structures and dynamics
Structure/dynamics of amorphous phases
Carnegie/DOE Alliance Center

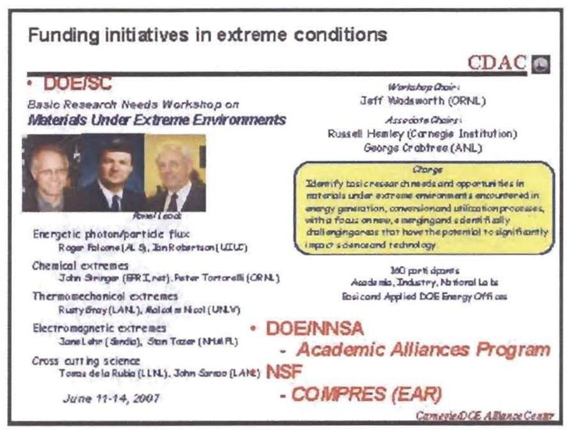

NEW DISCOVERIES
New phases and phenomena in the Earth
CDAC
Magnetic collapse
Hydrous phases
Silicate post-perovskite
[Murakami et al. (2004), W. Mao et al., PNAS 101, 15867 (2004); 103, 9751 (2005)]
Texture maximum near (101) indicates (100) and (110) slip as deformation mechanism.
010
150 GPa
Miyagi and Wenk (UCB)
MgSiO₃ to 150GPa in DAC
Carnegie/DOE Alliance Center

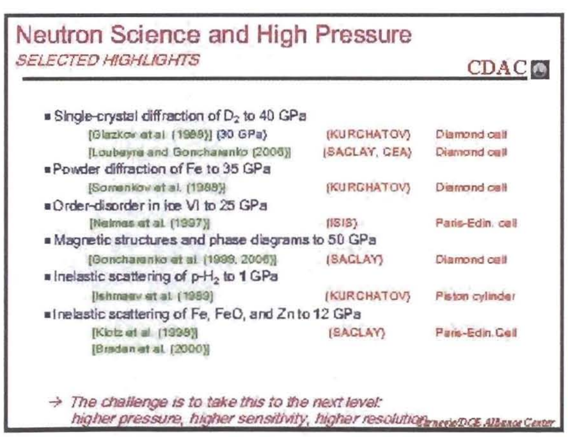

NEW DISCOVERIES
New classes of hydrogen storage materials
CDAC
Novel H₂O-H₂ Clathrates
Metal Organic Frameworks (MOFs)
[Loksin et al. Phys. Rev. Lett. 93, 125503 (2004)]
NEUTRON ELASTIC AND INELASIC SCATTERING
van der Waals Compounds
(H₂)₄CH₄
33 wt% Hydrogen
[W. Mao et al. Chem. Phys. Lett. 402, 66 (2005)]
[Loksin et al., PNAS in press]

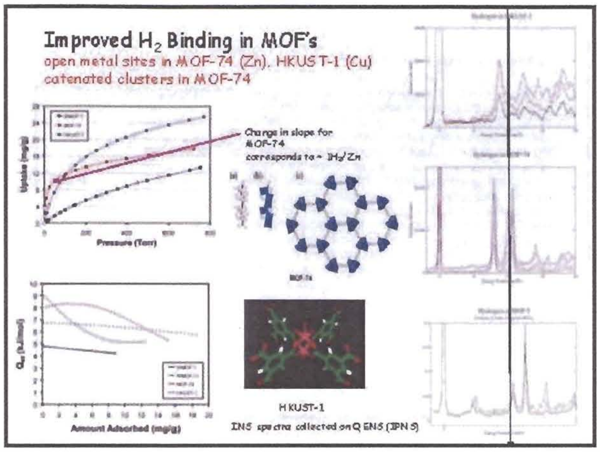

NEW DISCOVERIES Biomolecule structure-property relations and life in extreme environments
CDAC
Single Crystal Diffraction of Cow Pea Mosaic Virus
3.5 kbar

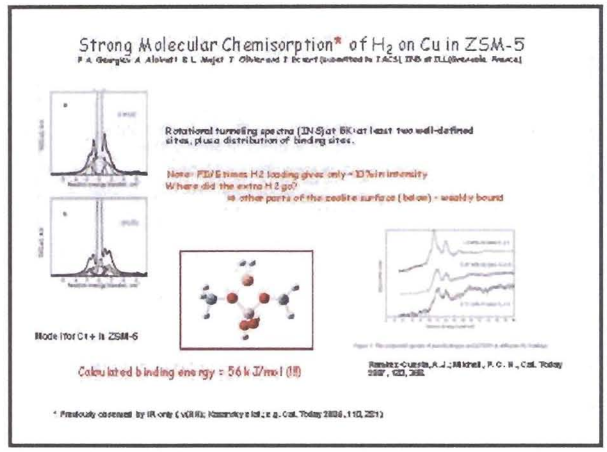

TECHNICAL DEVELOPMENTS
HIGH-PRESSURE DEVICES
Gem anvil devices (to >50 GPa)
Single crystal anvils, single crystal, powder, composite samples
Three decades of experience (e.g., synchrotrons)
New materials: SiC, sapphire, HPHT diamond, CVD diamond
Medium pressure devices (<30 GPa)
Paris-Edinburgh/Beijing-Washington
Gas apparatus (1 GPa)
Lower pressure/high-precision
Capable of multiple samples
Large volume megabar devices
>100 GPa: "Marriage" of all three

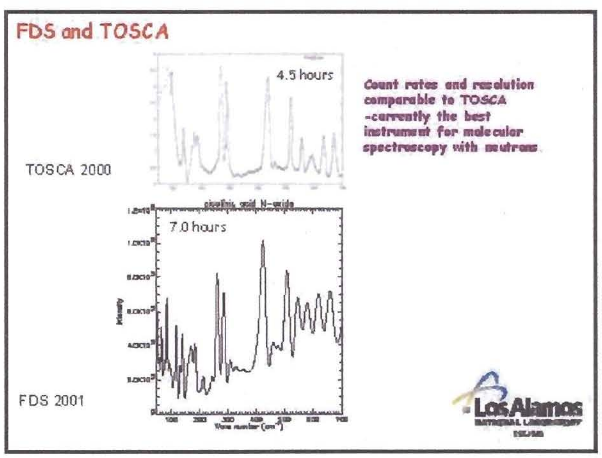

TECHNICAL DEVELOPMENTS
OTHER DEVICES
CDAC
Focusing
<100 μm spots with neutron K-B's
– Combine with 10x flux enhancements and >100x sample volume
Supermirrors
Variable temperatures
Liquid He cooling
Laser heating
– Double-sided. fiber laser
Software/Analysis
Integration of 'first-principles' theory and data analysis


Funding initiatives in extreme conditions
CDAC
• DOE/SC
Basic Research Needs Workshop on
Materials Under Extreme Environments
Workshop Chair:
Jeff Wadsworth (ORNL)
Associate Chairs:
Russell Hemley (Carnegie Institution)
George Crabtree (ANL)
Charge
Identify basic research needs and opportunities in materials under extreme environments encountered in energy generation, conversion and utilization processes, with a focus on new, emerging and scientifically challenging areas that have the potential to significantly impact science and technology
Energetic photon/particle flux
Roger Falcone (ALS), Ian Robertson (UIUC)
Chemical extremes
Thermomechanical extremes
Rusty Gray (LANL), Malcolm Nicol (UNLV)
Electromagnetic extremes
Cross cutting science
June 11-14, 2007
360 participants
Academia, Industry, National Labs
Basic and Applied DOE Energy Offices
• DOE/NNSA
- Academic Alliances Program
NSF
- COMPRES (EAR)
Carnegie/DOE Alliance Center


Neutron Science and High Pressure
SELECTED HIGHLIGHTS
CDAC
Single-crystal diffraction of D2 to 40 GPa
[Glazkov et al. (1988)] (30 GPa) (KURCHATOV) Diamond cell
[Loubeyre and Goncharenko (2006)] (SACLAY, CEA) Diamond cell
Powder diffraction of Fe to 35 GPa
[Somenkov et al. (1988)] (KURCHATOV) Diamond cell
Order-disorder in ice VI to 25 GPa
[Nelmes et al. (1997)] (ISIS) Paris-Edin. cell
Magnetic structures and phase diagrams to 50 GPa
[Goncharenko et al. (1999, 2006)] (SACLAY) Diamond cell
Inelastic scattering of p-H2 to 1 GPa
[Ishmaev et al. (1989)] (KURCHATOV) Piston cylinder
Inelastic scattering of Fe, FeO, and Zn to 12 GPa
[Klotz et al. (1998)] (SACLAY) Paris-Edin. Cell
[Braden et al. (2000)]
→ The challenge is to take this to the next level:
higher pressure, higher sensitivity, higher resolution
Carnegie/DOE Alliance Center


Improved H2 Binding in MOF's
open metal sites in MOF-74 (Zn), HKUST-1 (Cu)
catenated clusters in MOF-74
Change in slope for MOF-74 corresponds to ~ 1H2/Zn
Pressure (Torr)
Amount Adsorbed (mg/g)
HKUST-1
INS spectra collected on QENS (IPNS)


Strong Molecular Chemisorption* of H2 on Cu in ZSM-5
Rotational tunneling spectra (INS) at 5K: at least two well-defined sites, plus a distribution of binding sites.
Where did the extra H2 go?
Model for Cu+ in ZSM-5
Calculated binding energy = 56 kJ/mol (!!)


FDS and TOSCA
4.5 hours
TOSCA 2000
7.0 hours
FDS 2001
Count rates and resolution comparable to TOSCA -currently the best instrument for molecular spectroscopy with neutrons.
Los Alamos

F. Mezei
Aug. 26, 2007

Inelastic scattering capabilities at Lujan Center: quantitative estimates and special strengths in direct geometry TOF spectroscopy

The following comparison of instrument performance estimates for Lujan Center (at 100 KW power) and SNS (at 1.4 MW) are based on: a) analytical models fitted to the best available numerical results for the next, improved Lujan target to be installed within less than 2 years (current Lujan performance is comparable, the improvements to be expected are incremental), and b) analytical model estimates for SNS, which are expected to be correct within 20-30 %

1) Absolute beam intensities on sample

Figure 1 shows the instantaneous flux multiplied by the number pulses per second **f** as a function of the neutron wavelength. It takes into account the distance between source moderator and sample, which in turn determines the wavelength spread of the incoming beam at any instant in view of the source neutron pulse length. The data in Figure 1 assume no pulse shaping chopper upstream to improve resolution. Such chopper is feasible/foreseen for some of the instruments considered: it would imply a corresponding reduction of the instantaneous flux proportional to $\delta\lambda$. The duty factor of the main chopper in front of the sample is τf, where τ is the pulse width of the chopper. Thus is $\tau f \Phi_i$ is the absolute (time average) neutron beam flux on the sample. For the new FP 13 instrument (based on available guide and chopper system from the IN500 project) **f** is determined by assuming the use Repetition Rate Multiplication (RRM, 7 fold up to 7 Å wavelength and 5 fold beyond) and for a new FP 16 instrument (up-graded Pharos with converging supermirror guide and RRM capability) 3 fold pulse repetition was assumed.

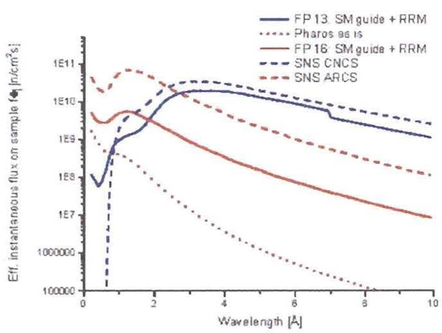
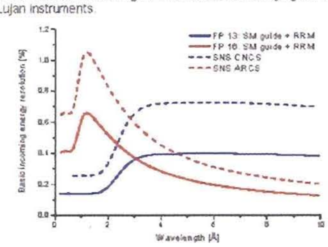


Figure 1. Comparison of beam intensities of TOF spectrometer options at Lujan Center and SNS.

2) Basic incoming energy resolution

The energy definition of the incoming neutron beam is primarily determined by the source moderator pulse length, if no pulses shaping chopper is used. This basic incoming energy resolution is shown in Figure 4 for the beam-lines considered above, obtained under the assumption of negligible pulse length for the chopper in front of the sample. Due to the longer moderator to sample distances at Lujan FP 13 and FP 16, they offer considerably better inherent energy resolution than the SNS counterparts. This also implies that the beam intensities shown in Figure 1 refer to considerably tighter wavelength resolution for the Lujan instruments.



3) Conclusions, special strengths

a) By using advanced TOF spectrometer technology (RRM and ballistic guide) a cold neutron spectrometer at Lujan Center FP 13 will be fully competitive with its counter-part at SNS. TOF instruments of more recent design than (at ISIS; J-PARC, ESS and SNS second target station) are built or planned based on the RRM technology developed at Lujan Center. The detector area coverage: some 30 m^2 is becoming standard with the newly developed 3 m long or longer position sensitive detectors. Only a question of availability of funds. (An acceptable minimum of about12 m2 is quite affordable).

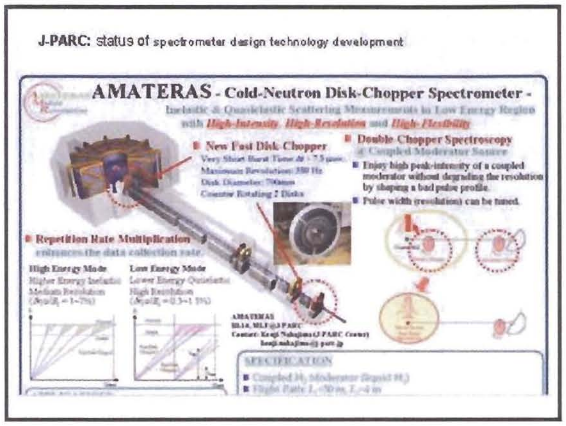
b) Without substantial up-grade Pharos is neither competitive with the SNS instruments (ARCS or SEQUOIA) nor for incoming neutron energies below some 200 meV with the FP 13 instrument with a neutron guide aligned to deliver hot neutrons too. (Pharos provides comparable flux to FP 13 above 50 meV incoming energy, but at much worse resolution.) The main draw-back of Pharos is the lack of neutron guide, which leads to fine incoming beam collimation. This, on the other hand, becomes an advantage for Brillouin scattering.

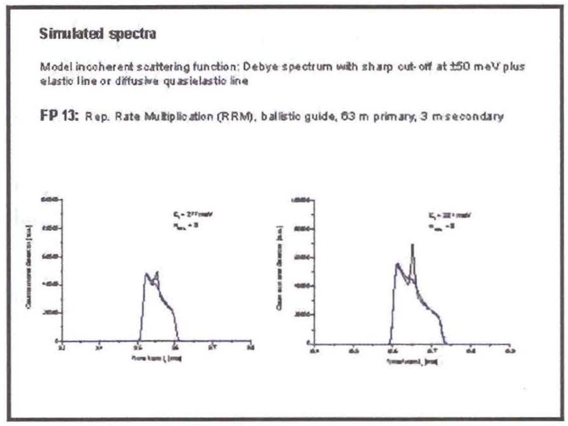
c) Up-grading Pharos by implementing RRM and supermirror neutron guide technology, both developed at Lujan Center, will make it reasonably competitive, reaching about 1/7 of the beam intensity of ARCS at 50 % better resolution. The large detector solid angle coverage of ARCS is hard to match though.

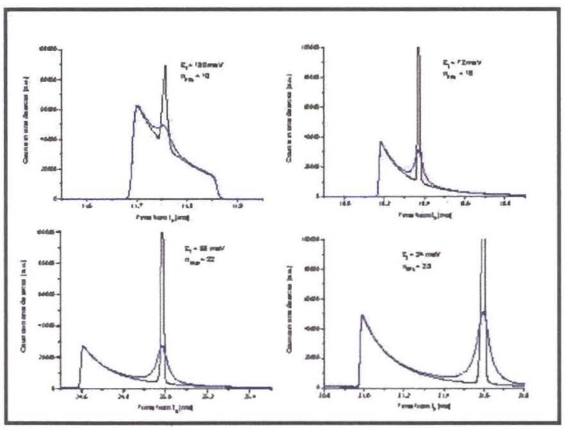
i) The longer incoming flight path of Pharos compared to ARCS and the lack of neutron guide offers better Q and E resolution, in particular for small angle Brillouin scattering work. This advantage can be maintained in an eventual up-grade, if the guide is made removable or by the use of a collimator system similar to the one developed for the new Brillouin scattering instrument BRISP at ILL. (The first option would probably offer lower background).

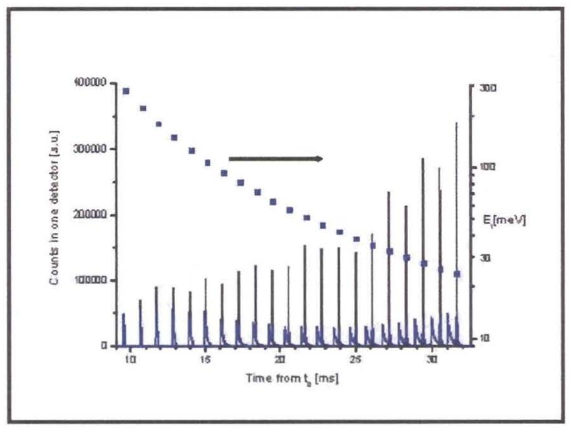
ii) The high incoming beam energy resolution for FP 13 (e.g. 150 μeV at E_i = 100 meV) opens up new opportunities in inelastic experiments with substantial neutron energy loss. This resolution could be matched in the analysis of the final neutron energy E_f for E_f < 16 meV ultimately providing optimized resolution conditions for high energy transfer (about 200 μeV at E_i-E_f > 84 meV in this example), as opposed to quasi-elastic scattering.

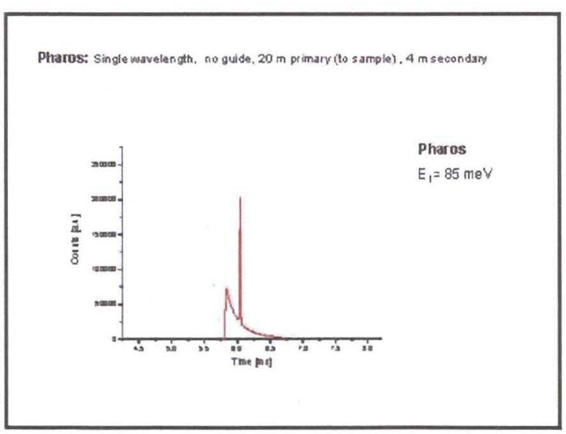
iii) TOF spectroscopy automatically provides a diffraction pattern of sample too, however in a too small Q domain, if the incoming neutron wavelength selected to provide the required energy resolution is long. Using Repetition Rate Multiplication a number of incoming wavelengths is used, which will allow for covering a larger Q range and also improve the resolution quality of the diffraction data. For example, for the FP 13 instrument operating in the second source pulse frame, neutrons with wavelengths from 3.15 about 6 Å will be available for simultaneous diffraction data collection, while in the first frame this range becomes 0.7 – 3 Å.

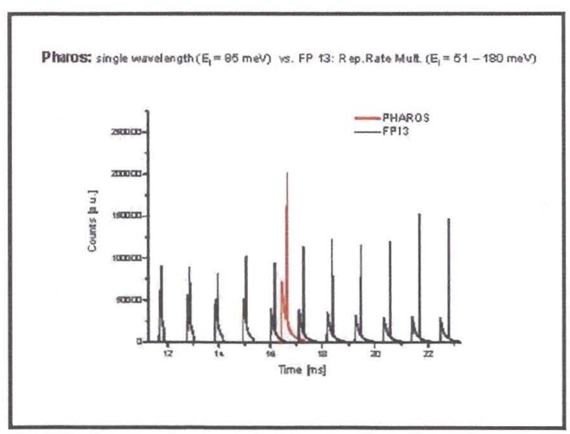

J-PARC: status of spectrometer design technology development
AMATERAS - Cold-Neutron Disk-Chopper Spectrometer -
New Fast Disk Chopper
Double Chopper Spectroscopy
Repetition Rate Multiplication
SPECIFICATION


Simulated spectra
Model incoherent scattering function: Debye spectrum with sharp cut-off at ±50 meV plus elastic line or diffusive quasielastic line
FP 13: Rep. Rate Multiplication (RRM), ballistic guide, 63 m primary, 3 m secondary

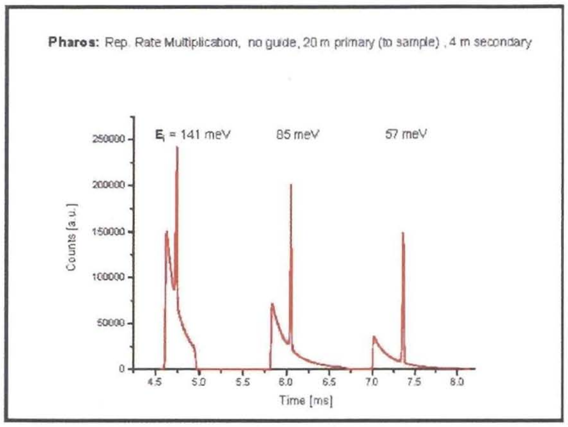


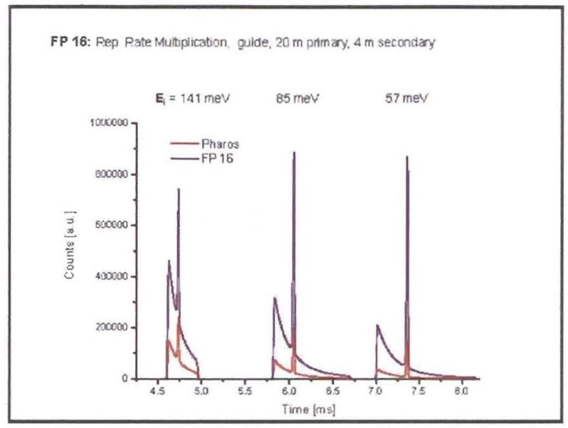

Counts in one detector [a.u.]
Time from t0 [ms]
E_i[meV]

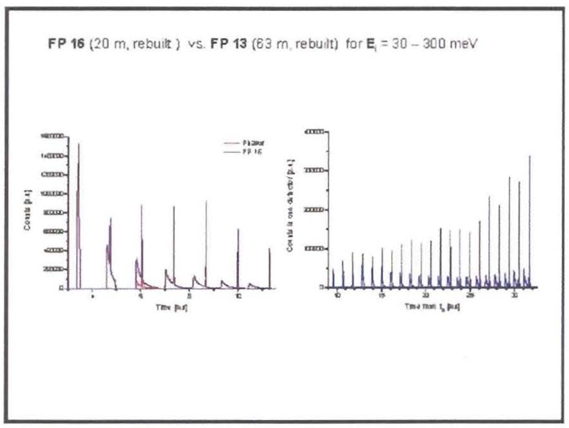

Pharos: Single wavelength, no guide, 20 m primary (to sample), 4 m secondary
Pharos
E_i = 85 meV
Counts [a.u.]
Time [ms]


Pharos: single wavelength (E_i = 85 meV) vs. FP 13: Rep.Rate Mult. (E_i = 51 – 180 meV)
PHAROS
FP13
Counts [a.u.]
Time [ms]

Mezei


Pharos: Rep. Rate Multiplication, no guide, 20 m primary (to sample), 4 m secondary
E_i = 141 meV
85 meV
57 meV
Counts [a.u.]
Time [ms]


FP 16: Rep. Rate Multiplication, guide, 20 m primary, 4 m secondary
E_i = 141 meV
85 meV
57 meV
Pharos
FP 16
Counts [a.u.]
Time [ms]


FP 16 (20 m, rebuilt) vs. FP 13 (63 m, rebuilt) for E_i = 30 – 300 meV

Lujan Workshop, San Diego 2007

Dynamics – the key to macroscopic properties of Soft Materials

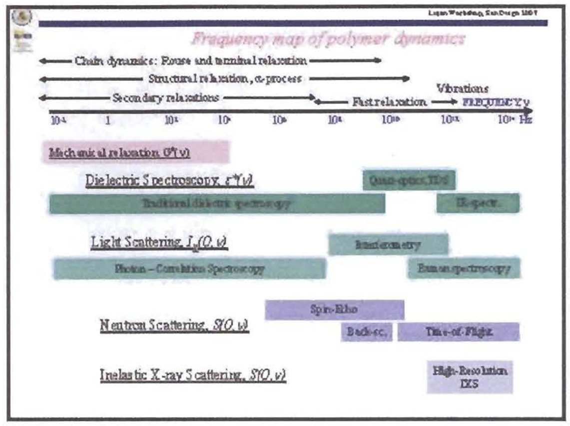
Scattering techniques have advantage of providing time and space correlation function through additional variable – Q.

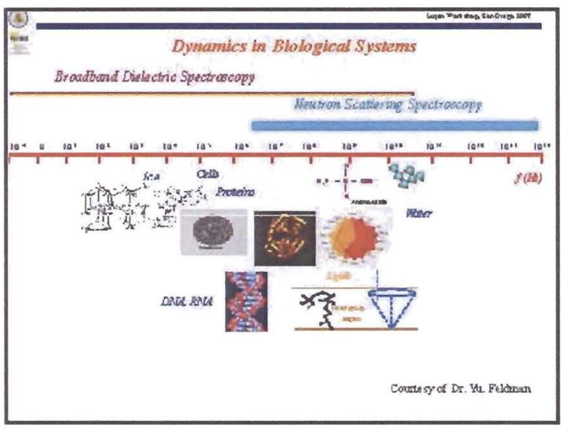
Light scattering – Broad frequency/time range, from 10^{-5} Hz up to 10^{14} Hz with a small gap. However, very low Q-range: $Q<5*10^{-2}$ nm^{-1}. Molecular scale motions are not accessible.

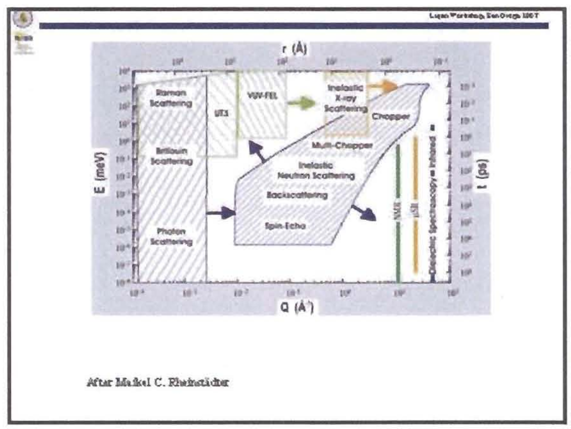
X-ray scattering – Right Q-range, but very limited frequency (time window): IXS E>1 meV~$2*10^{11}$ Hz, X-PCS t > ms.

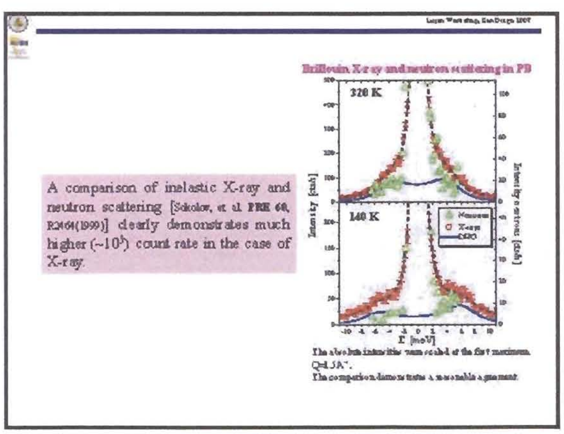
Neutron scattering – Has significant advantage by combining the right Q-range (0.5 $nm^{-1}<Q<100$ nm^{-1}) with the reasonable frequency/time window (from 10^{6} Hz up to 10^{14} Hz, from ~10 neV to eV).

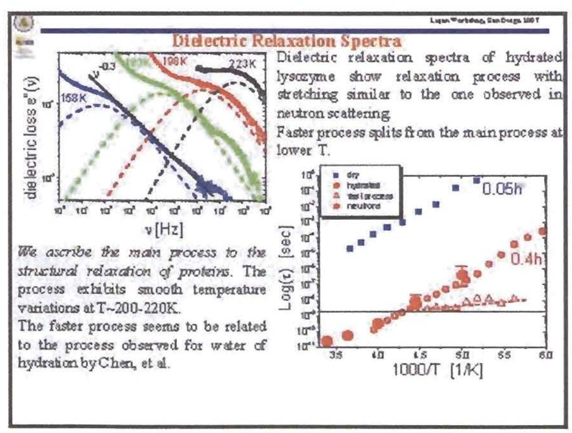
Required directions:
- *Lower Q (down to 0.1 nm^{-1} and lower)*
- *Longer times (μsec and longer)*
- *Higher Statistics*

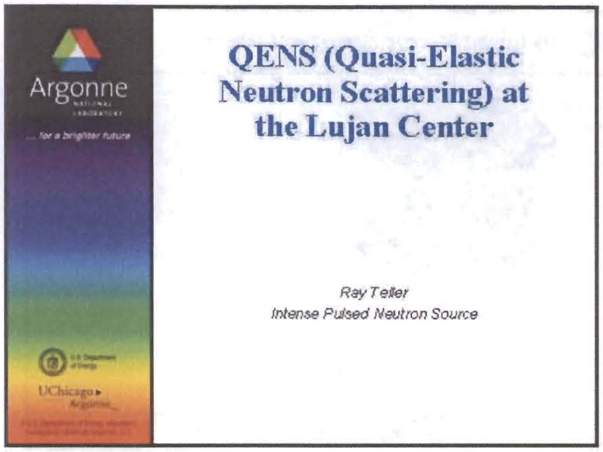


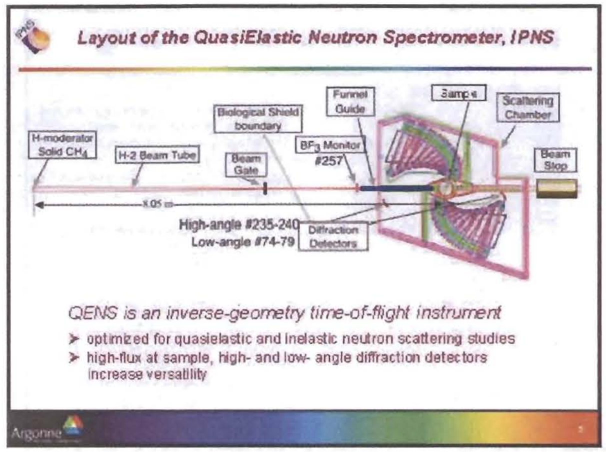


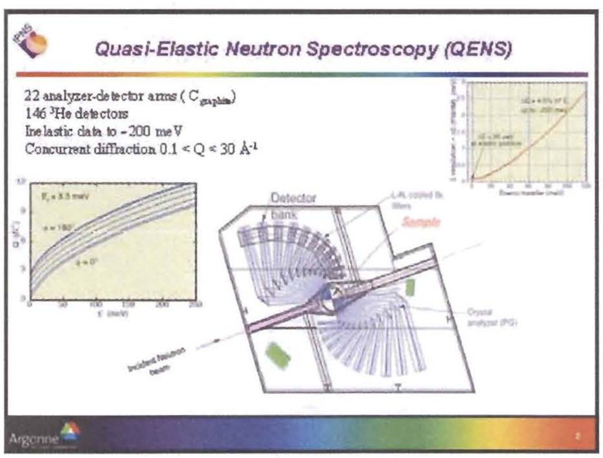


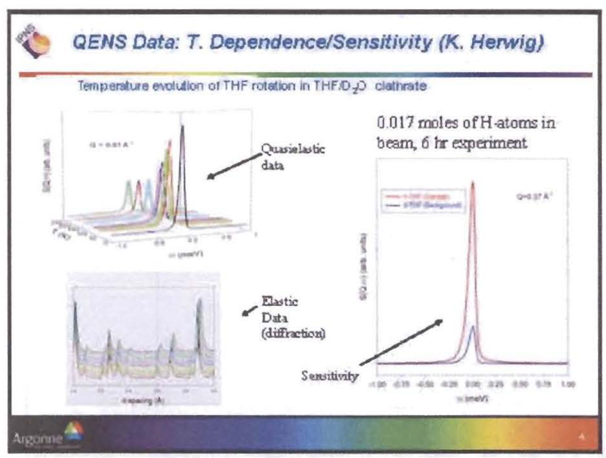


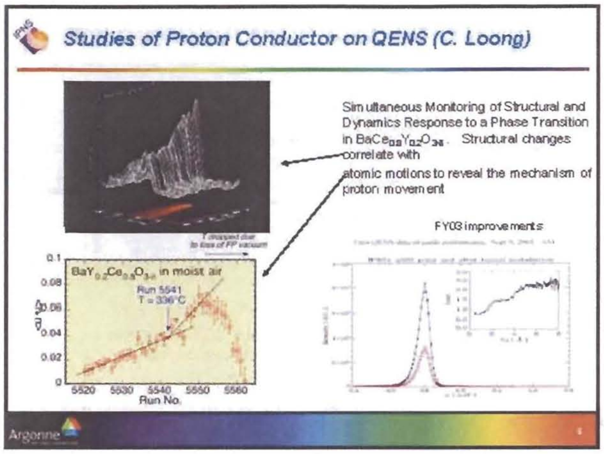


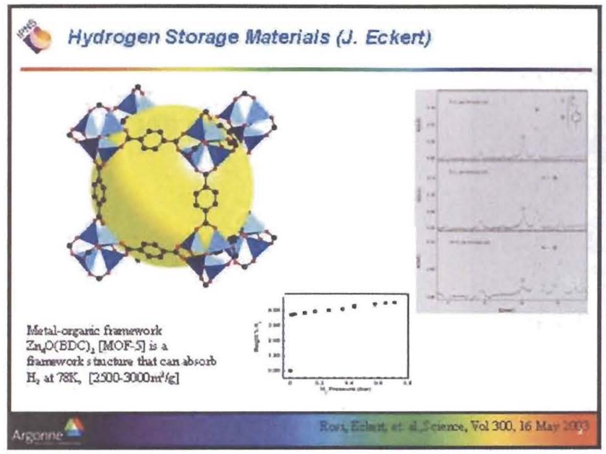

Argonne
QENS (Quasi-Elastic Neutron Scattering) at the Lujan Center
Ray Teller
Intense Pulsed Neutron Source
UChicago
Argonne


Layout of the QuasiElastic Neutron Spectrometer, IPNS
H-moderator Solid CH4
H-2 Beam Tube
Biological Shield boundary
Beam Gate
Funnel Guide
BF3 Monitor #257
Sample
Scattering Chamber
Beam Stop
High-angle #235-240
Low-angle #74-79
Diffraction Detectors
QENS is an inverse-geometry time-of-flight instrument
optimized for quasielastic and inelastic neutron scattering studies
high-flux at sample, high- and low- angle diffraction detectors increase versatility
Argonne


Quasi-Elastic Neutron Spectroscopy (QENS)
22 analyzer-detector arms (C graphite)
146 3He detectors
Inelastic data to ~200 meV
Concurrent diffraction 0.1 < Q < 30 Å-1
Detector bank
Sample
Incident Neutron beam
Argonne


QENS Data: T. Dependence/Sensitivity (K. Herwig)
Temperature evolution of THF rotation in THF/D2O clathrate
0.017 moles of H-atoms in beam, 6 hr experiment
Quasielastic data
Elastic Data (diffraction)
Sensitivity
Argonne

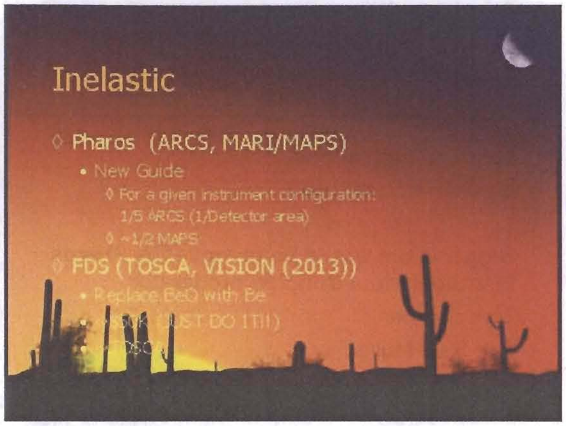


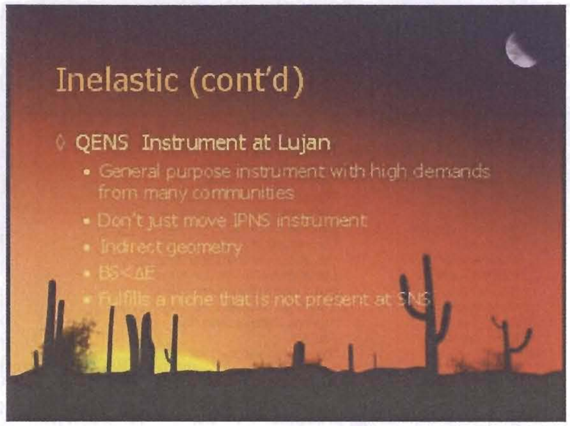


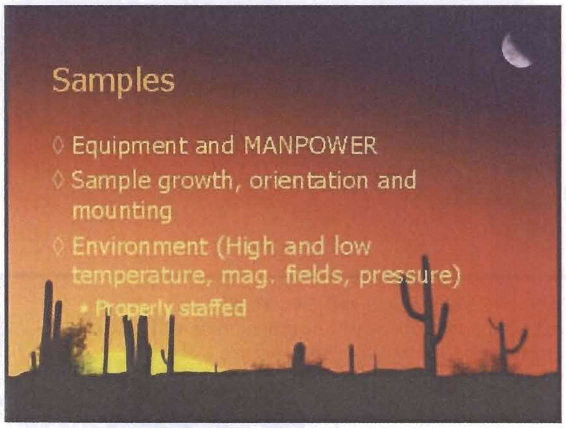
Scientific-user program of QENS

QENS facilitates investigations of the following classes of materials, through the IPNS proposal system (averages per proposal round):	proposals accepted (acceptance rate)	research groups
➤ Hydrogen-economy related materials, especially hydrogen storage; *e.g.* metal organic frameworks.	3.3 (85%)	5
➤ Magnetic materials, new field of investigation on QENS (2006) *e.g.* frustrated-spin magnets.	1.3 (80%)	1.7
➤ Proton conductors *e.g.* ceramic materials and model materials for proton quantum delocalization.	1.5 (70%)	2.7
➤ (Macro)molecular solids and fluids *e.g.* minerals, water-sensitive materials, metals, molten salts...	3.3 (65%)	5

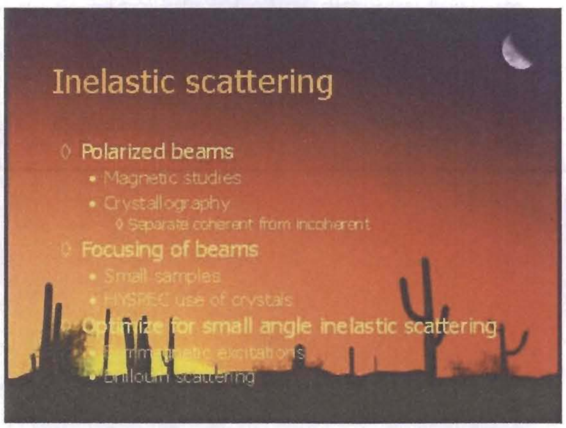
Argonne


Inelastic
Pharos (ARCS, MARI/MAPS)
New Guide
For a given instrument configuration: 1/5 ARCS (1/Detector area)
~1/2 MAPS
FDS (TOSCA, VISION (2013))
Replace BeO with Be


Inelastic (cont'd)
QENS Instrument at Lujan
General purpose instrument with high demands from many communities
Don't just move IPNS instrument
Indirect geometry
Fulfills a niche that is not present at SNS


Samples
Equipment and MANPOWER
Sample growth, orientation and mounting
Environment (High and low temperature, mag. fields, pressure)
Properly staffed


New Instrument Concepts
Multipurpose instrument for studies of hydrogen
Multianalyzers
....


Inelastic scattering
Polarized beams
Magnetic studies
Crystallography
Separate coherent from incoherent
Focusing of beams
Small samples
HYSPEC use of crystals
Optimize for small angle inelastic scattering

Lessons from Vertex Concept

B. Fultz (Caltech) and R.J. McQueeney (Iowa State)

VERTEX Spectrometer Development Team

Gabe Aeppli	NEC Research Institute
Collin Broholm	The Johns Hopkins University
Brent Fultz	California Institute of Technology
Bernhard Keimer	Max-Planck-Institut
Sandy Kern	Colorado State University
Thom Mason	Oak Ridge National Laboratory
Rob McQueeney	Los Alamos National Laboratory
Herb Mook	Oak Ridge National Laboratory
Steve Nagler	Oak Ridge National Laboratory
Ray Osborn	Argonne National Laboratory
Rob Robinson	ANSTO
Frans Trouw	Los Alamos National Laboratory

VERTEX Proposal had Innovations that Could be Upgrades to Pharos

Fast and high impact

Guide in incident beam

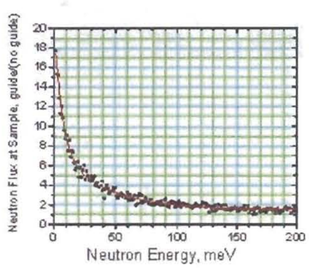
Bigger issue would be to move the Pharos instrument to a Coupled moderator

Disk chopper

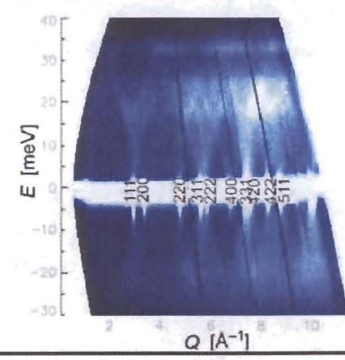
Rep Rate Multip.

Supermirror Guide

The addition of a 13 meter $3\theta_c$ neutron supermirror guide further increases the flux at the sample for thermal neutrons

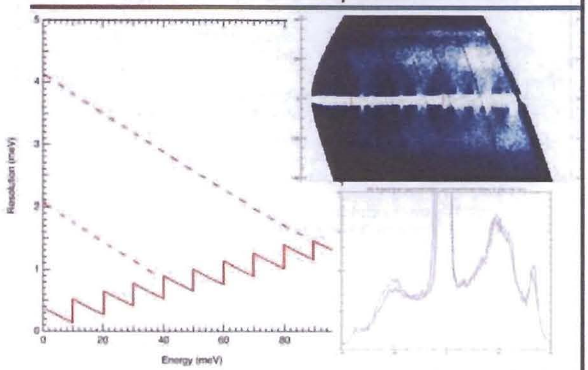


With ARCS at the SNS, the Q information will be much more important for inelastic scattering research. Not so practical on Pharos with a good sample (Ni) run in 36 hours.



Fultz

**Multiple Energies Give Higher Resolution
ARCS has Potential to be Explored**



Sample
Environments
Are High Payoff.
Modest temperature
furnace

Best Buys in Pharos Upgrades

* Guide in Pharos Incident Beam
* Sample Environments

New Instrument Concepts and Upgrades for Inelastic Scattering

Science opportunities / mission:

- National / regional user facility
- User community building / training
- Innovation and development
- Special / unique / topics oriented capabilities and strengths

Means to achieve these

- Enhance share of capacity and capability in inelastic spectroscopy: 4 instruments at least
- Use strengths of Lujan source: 5 kj/pulse (vs 23 at SNS), low rep. rate
- Upgraded / new instrument: competitive for most hot experiments
- Innovative approaches, special / unique features
- Strong / integrated (extreme) sample environment
- Enhanced staff in condensed matter
- Involve university community, in particular West Coast

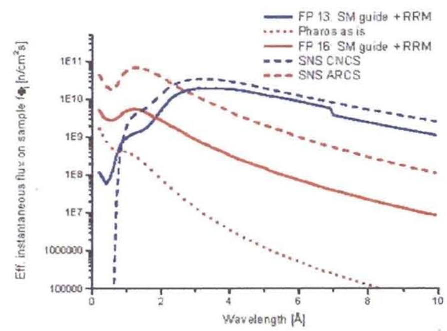
Competitive inelastic scattering opportunities in SNS era

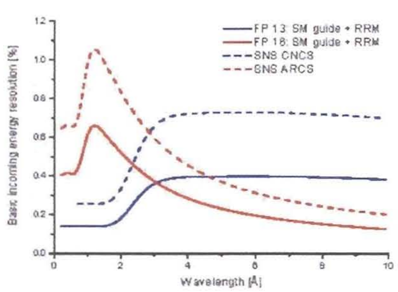
- Chemical spectroscopy: FDS upgrade (strengths: large solid angle, adjustable resolution by filter edge)
- Thermal spectroscopy: PHAROS upgrade (strengths: advanced chopper system, RRM, correlation chopper, high angular resolution)
- Cold-thermal spectroscopy: FP 13 new / completion (strengths: advanced guide, RRM, long flight-path, broad dynamic range, high resolution in ~ 30 – 80 meV down scattering)
- Cold neutron inverted geometry "QENS" new (strength: designed for special / dedicated sample environment, innovative development)

Special scientific needs / strengths

- Soft matter: Brillouin scattering for c = 2 -3 km/s, as good resolution as possible, 0.1 $Å^{-1}$ range
- Magnetism: work around (000), high resolution in substantial down scattering
- Polarized neutrons for magnetism and incoherent scattering
- Life sciences, radiological effets
- Hydrogen science

Illustration of competitive opportunities to SNS: example of TOF spectrom.





Lujan Futures: Small-angle Scattering and Neutron Reflectometry Instruments

Rex P. Hjelm
hjelm@lanl.gov

Lujan Neutron Scattering Center
Los Alamos National Laboratory

2007 San Diego Workshop on Lujan Center
San Diego, California
5-8 September 2007

Los Alamos NNSA

Lujan Small-angle and reflectometry committee members:

- Monika Hartl
- Rex Hjelm
- Mike Fitzsimmons
- Jarek Majewski
- Günther Müller
- Hillary Smith
- Eric Watkins

Los Alamos NNSA

Addressing needs, opportunities and the future

- Issues:
  - Neutron and γ background.
  - Faster data rates: new detector and DAQ technology.
  - Better optics.
  - Improved instrument flexibility.
  - Multi-measurement instruments (*e.g.* SANS & Diffractometry)
- Opportunities:
  - 20 Hz well suited for measurements using cold neutrons (16 Å bandwidth).
  - Currently the brightest cold neutron source.
  - A path forward exists for for a brighter cold source:
    - Be filter (Mark III TMRS):
      - 2x increase $\lambda > 4$ Å.
      - 2x decrease $\lambda < 4$ Å.
      - Softer γ spectra.
    - Other future developments:
      - Advanced fully coupled moderator: 1.5 - 2x increase.
      - Accelerator upgrade: 2x increase protons per pulse on target.
- Unique opportunities using pulsed source: pulse-probe measurements.
- Advanced polarization and spin echo techniques.

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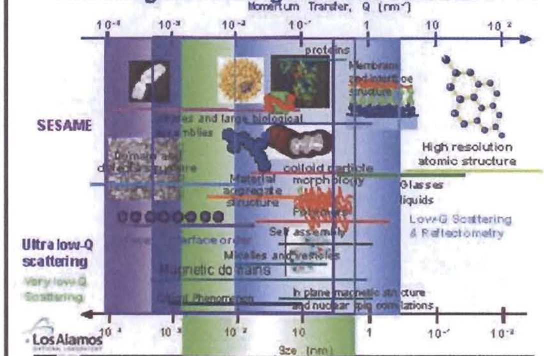
Small-angle scattering instrument scales



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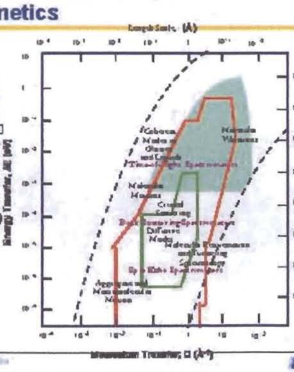
SANS and neutron reflection probes of dynamics & kinetics

□□i□□□□□, electronic chopping□□e□□□□□□□□□□□□□□□□□□□□□□□□□□□□□low energy spectroscopy (10 μeV- neV) and in □□□□□□□□□□□□□□□□□□□□□ (to 10s of seconds)



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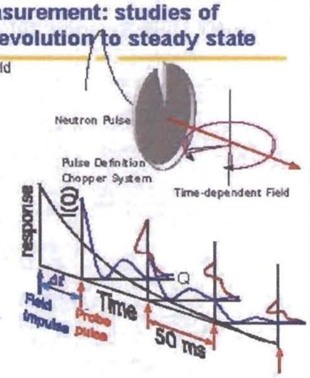
The pulse-probe measurement: studies of transient states and evolution to steady state

- Pulsed or continuously varying field types:
  - mechanical.
  - photon.
  - electrical.
  - magnetic.
  - temperature.
  - Pressure.
  - *Etc.*
- Neutron measurements:
  - I or R vs Q and t.
  - Offset, Δt, adjusted to probe time points $t = \Delta t + n/f$.
  - Q-domain depends on probing measurement.
  - f = 20 Hz gives good Q dynamic range.
  - Time scales: ~50 μs - seconds.
- Requires multi-dimensional, time-stamped data.



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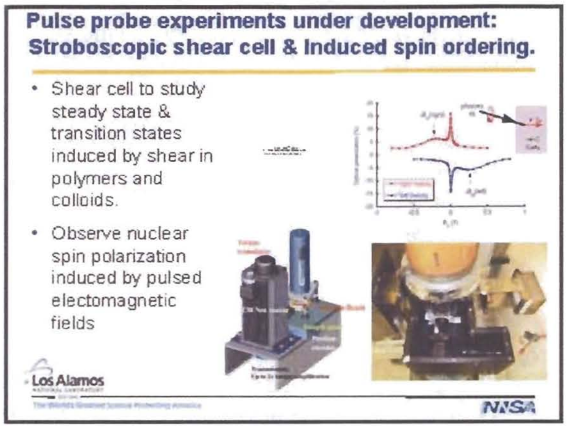
Pulse probe experiments under development:
Stroboscopic shear cell & Induced spin ordering.
Shear cell to study steady state & transition states induced by shear in polymers and colloids.
Observe nuclear spin polarization induced by pulsed electomagnetic fields
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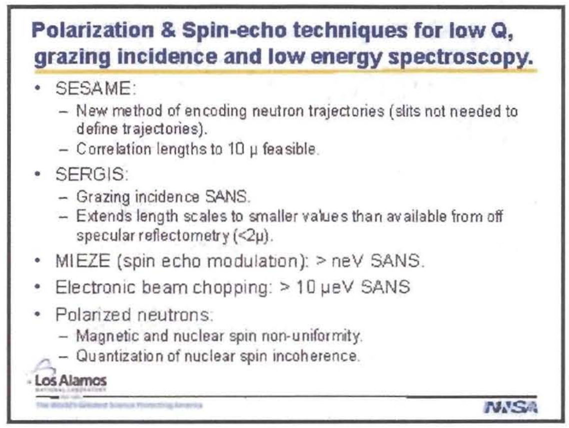
NNSA


Polarization & Spin-echo techniques for low Q, grazing incidence and low energy spectroscopy.
SESAME:
– New method of encoding neutron trajectories (slits not needed to define trajectories).
– Correlation lengths to 10 μ feasible.
SERGIS:
– Grazing incidence SANS.
– Extends length scales to smaller values than available from off specular reflectometry (<2μ).
MIEZE (spin echo modulation): > neV SANS.
Electronic beam chopping: > 10 μeV SANS
Polarized neutrons:
– Magnetic and nuclear spin non-uniformity.
– Quantization of nuclear spin incoherence.
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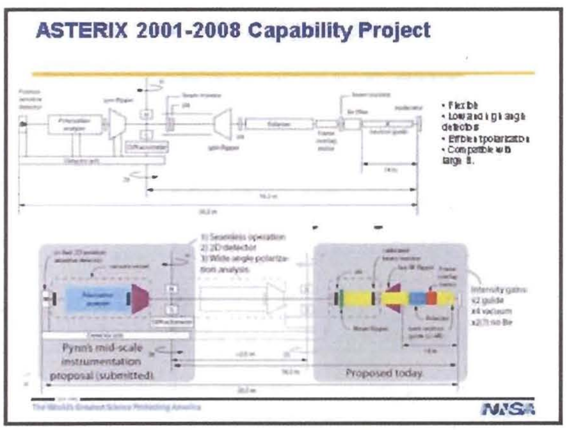
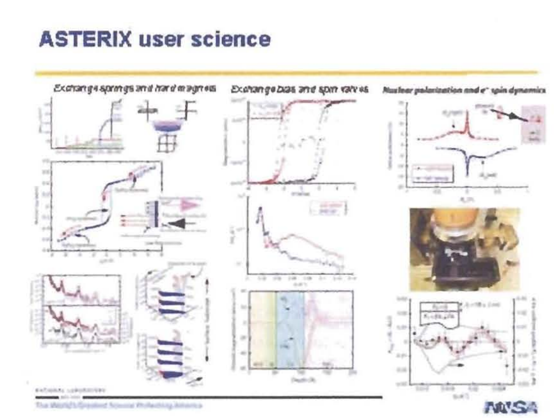
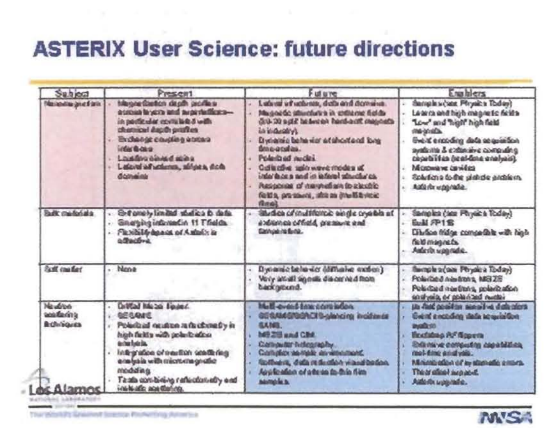
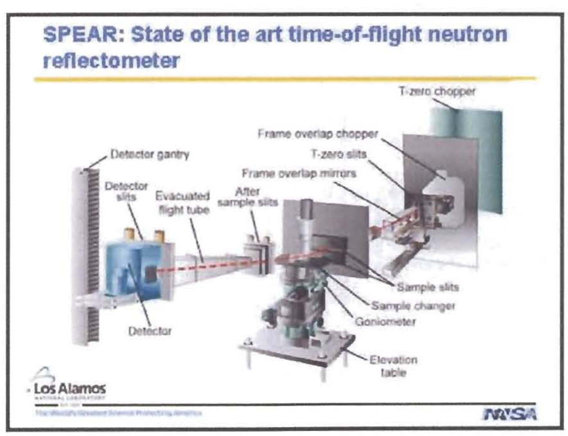

ASTERIX 2001-2008 Capability Project
Pynn's mid-scale instrumentation proposal (submitted)
Proposed today
NNSA


ASTERIX user science
NNSA

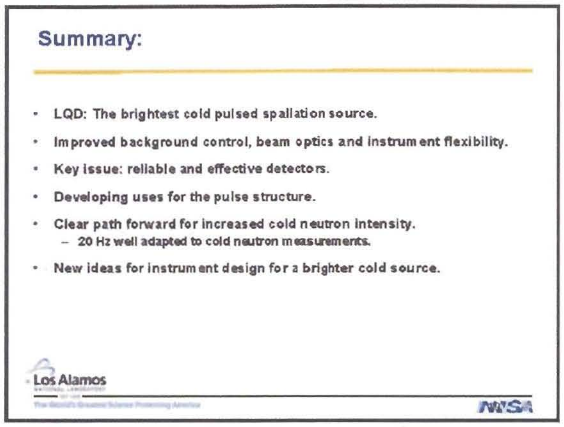

ASTERIX User Science: future directions
Subject
Present
Future
Enablers
Los Alamos
NNSA


SPEAR: State of the art time-of-flight neutron reflectometer
T-zero chopper
Frame overlap chopper
Detector gantry
T-zero slits
Frame overlap mirrors
Detector slits
Evacuated flight tube
After sample slits
Sample slits
Sample changer
Goniometer
Detector
Elevation table
Los Alamos
NNSA

Hjelm **1 of**

Hjelm

1 of


Summary:
• LQD: The brightest cold pulsed spallation source.
• Improved background control, beam optics and instrument flexibility.
• Key issue: reliable and effective detectors.
• Developing uses for the pulse structure.
• Clear path forward for increased cold neutron intensity.
– 20 Hz well adapted to cold neutron measurements.
• New ideas for instrument design for a brighter cold source.
Los Alamos
NNSA

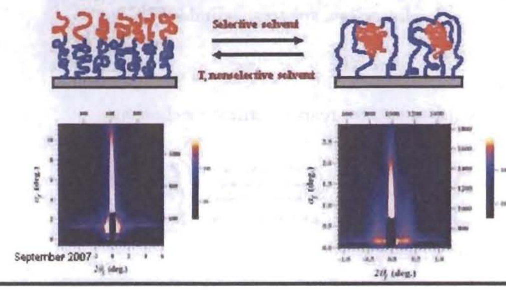
Future Polymer Areas

- Supramolecular assemblies
- Biologically relevant structures
- Dependence of properties on architecture
- High performance materials, composites, hybrids
- Interfacial dynamics
- heterogeneous/complex interfaces/films
- integrated study over multiple length scales

September 2007
M. Foster U. Akron

In-plane Structure and Dynamics in Switchable Brushes

Mark D. Foster U. Akron



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Needs

- Define details of in-plane structure, particularly in presence of solvent (GISANS)
- Determine dynamics of change in structure in "switching" due to solvent and temperature
- Look at fluctuations of brush surface next to layer of free chains (GISANS)

September 2007
M. Foster U. Akron

In-plane Structure and Dynamics in Switchable Brushes

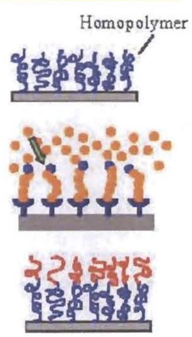
Mark D. Foster

Department of Polymer Science, The University of Akron

September 2007

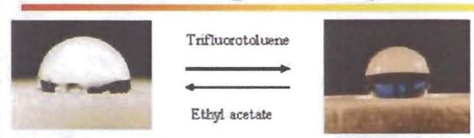
What a Polymer Brush Is

- Features: Monomolecular
  End grafted
  Densely Grafted
  Strongly stretched
- Ours made by "Grafting from"
- Special Case: diblock copolymer



September 2007

Diblock Brushes to Create Stimuli-responsive Surfaces



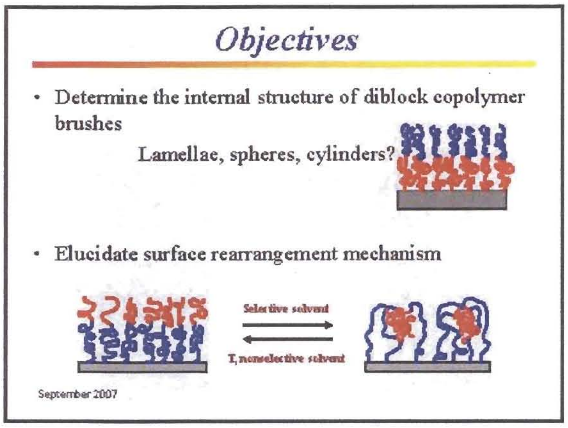
PMA-b-PPFA $\theta_A = 90°$ PMA-b-PPFA $\theta_A = 135$

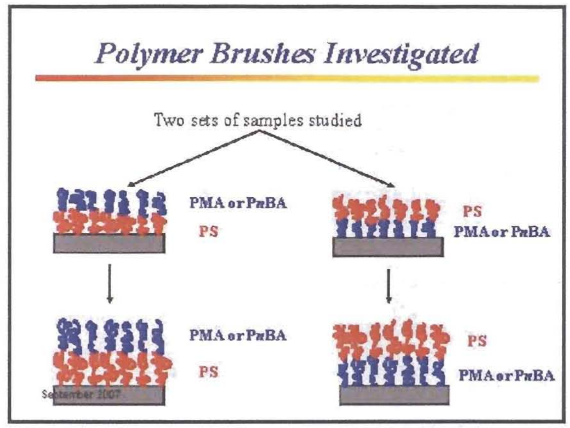
Water passes through frit — Solvent, T — Not readily adhered to Hydrophobic

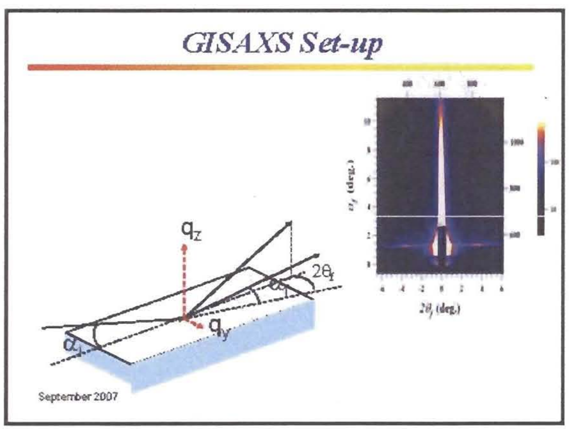
Flow can be controlled in microchannels

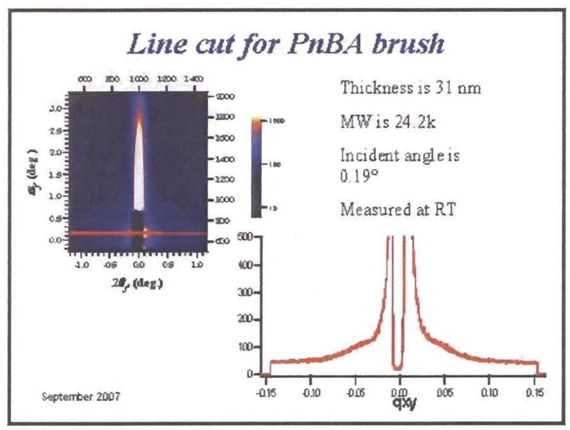
Chemical Gating

September 2007
Granville, A. M., Brittain, W. J. *Macromol. Rapid Comm.* 2004, 25, 1298.


Objectives
Determine the internal structure of diblock copolymer brushes
Lamellae, spheres, cylinders?
Elucidate surface rearrangement mechanism
Selective solvent
T, nonselective solvent
September 2007

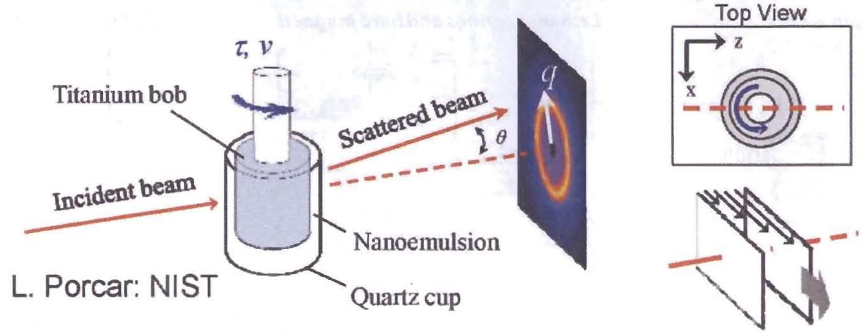

Polymer Brushes Investigated
Two sets of samples studied
PMA or PnBA
PS
PS
PMA or PnBA
PMA or PnBA
PS
PS
PMA or PnBA
September 2007


GISAXS Set-up
q_z
q_y
$2\theta_f$
α_f
α_i
$2\theta_f$ (deg.)
α_f (deg.)
September 2007


Line cut for PnBA brush
Thickness is 31 nm
MW is 24.2k
Incident angle is 0.19°
Measured at RT
$2\theta_f$ (deg)
α_f (deg)
qxy
September 2007

Opportunities for Lujan: Rheo-SANS

T.G. Mason - UCLA Chemistry and Physics



L. Porcar: NIST

See nanostructural changes in response to applied stress and strain

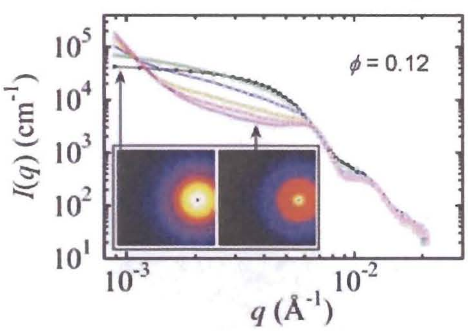
Few sample geometries exist: ILL and NIST offer Rheo-SANS
- U.S.-based Rheo-SANS is controlled shear stress only (w/ temp)
- Needs: reduced sample volume, controlled shear strain
- Other opportunities: extensional Rheo-SANS, solids failure

Opportunities for Lujan: SANS+SALS

T.G. Mason - UCLA Chemistry and Physics

Extend q-range to lower q by performing SALS and SANS together

Example: Time-Resolved Slippery Aggregation of Nanoemulsion



Silicone oil nanodroplets in Water quenched into attractive regime by T

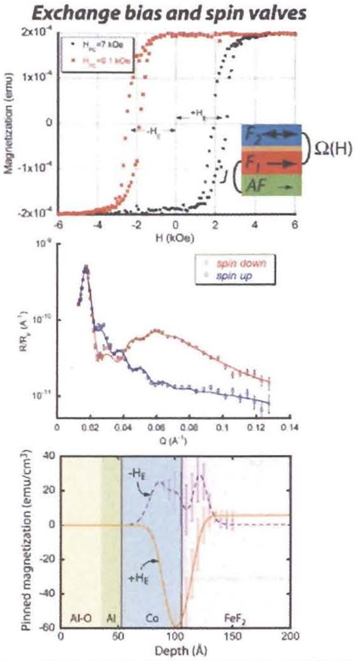
J.N. Wilking, ... T.G.M., *Phys. Rev. Lett.* **96** 015501 (2006)

USANS would require separate experiments

Advantage: exact same sample and a broader $I(q)$
- No need to repeat the experiment
- Software could match LS and NS intensities
- Possibilities for orienting sample perp. to gravity?

Asterix User Science

Exchange bias and spin valves

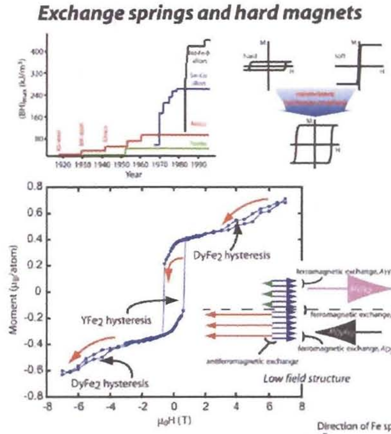


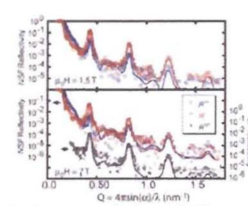
The resistance Ω across a spin valve (inset top panel) depends upon whether the magnetizations of ferromagnets F_1 and F_2 are parallel (low resistance) or antiparallel. The variation of Ω with field H provides a means to detect small fields, such as stray fields from magnetic domains. Key to the operation of a spin valve, F_1 must remain fixed for reasonable H. This can be accomplished by coupling F_1 with spins in an antiferromagnet AF, causing the hysteresis loop to be shifted about H=0 (top panel). The shift is the exchange bias H_E. The sign of H_E can be controlled by the size of the field in which the AF is cooled H_{FC}. Extensive neutron scattering (representative data middle panel) has shown that the AF contains uncompensated spins[1] that couple to the F_1. Since the spins of the AF can not move, the interfacial coupling pins spin on both sides of the F_1/AF interface (lower panel). The direction and magnitude of the pinned magnetization throughout the interfacial region determines the sign and strength of HE.[2]

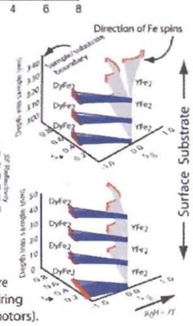
[1] S. Roy et al., PRL **95**, 047201 (2005).

[2] M.R. Fitzsimmons et al., PRB **75**, 214412 (2007).

Exchange springs and hard magnets



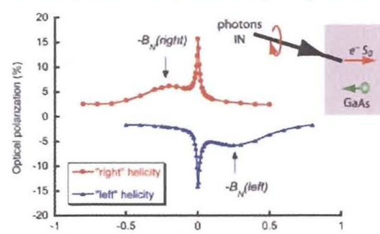


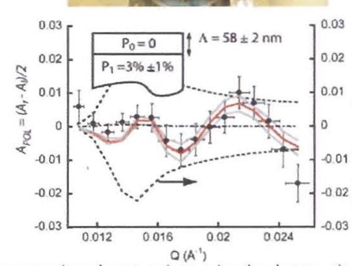


The large magnetization and ability to resist magnetization reversal typical of magnetic alloys (left top panel) are attractive properties in applications requiring 'hard' magnetic materials (as in electric motors). Nanoengineered materials offer opportunities to wed layers of soft and hard materials such that the properties of the composite exceed the sum of the components (right top panel). A superlattice of $DyFe_2$ and YFe_2 layers is a framework to understand the behavior (middle panel) of such materials, because the anisotropy of $DyFe_2$ is strongly temperature dependent, and the magnetizations of the individual layers compete against the forces of exchange coupling at the atomic scale (inset middle panel). Polarized neutron reflectometry (left lower panel)[3] in fields up to 11 T have elucidated the magnetic structure of this compound (right lower panel), and the response of this material to temperature, cooling and applied field.

3 M.R. Fitzsimmons et al., PRB **73**, 134413 (2006).

Nuclear polarization and e⁻ spin dynamics





Future computing schemes envisage using the electron spin to convey information rather than charge. However, fields of only a couple Oersted are sufficient to reorient electron spins, consequently, the effective fields from polarized nuclei (several kOe large) can profoundly influence electron spin dynamics. Polarized electron spin populations induce nuclear polarization in GaAs (inset top panel) from which the effective nuclear field can be observed with photoluminescence (top panel). Owing to the sensitivity of the neutron polarization to nuclear polarization, a neutron scattering experiment (middle panel) yielded data (lower panel) which suggests the nuclear polarization is suppressed near the surface of GaAs- presumably due to the lack of electrons in the depletion layer.

Asterix capabilities 2001-2008

- z-structures: $\vec{M}(z)$ across interfaces, bilayers, superlattices. Includes detection of very small pinned magnetization in the presence of unpinned magnetization.
- Lateral structures: $\vec{M}(x)$ (off-specular reflectometry) in superlattices and anti-dots (of the right dimension μm's!).
- Lateral structures: $\vec{M}(y)$ (glancing incidence SANS) from one layer of Fe dots (60 nm diameter, 110 nm spacing).
- Integration of neutron scattering with moderately complex sample environments, including: 11 T magnet and laser light.
- Depth profiling nuclear polarization.
- Some success with on-site model refinement.

Asterix emerging capabilities

- SESAME
- Single crystal diffraction

Title?

1 of

Asterix User Science: future directions

Subject	Present	Future	Enablers
Nanomagnetism	• Magnetization depth profiles across layers and superlattices—in particular correlated with chemical depth profiles • Exchange coupling across interfaces • Locating pinned spins • Lateral structures, stripes, dots domains	• Lateral structures, dots and domains. • Magnetic structures in extreme fields (80-20 split between hard-soft magnets in industry). • Dynamic behavior at short and long time-scales. • Polarized nuclei. • Collective spin wave modes at interfaces and in lateral structures. • Response of magnetism to electric fields, pressure, stress (multiferroic films).	• Samples (see Physics Today) • Lasers. • "Low" and "high" high field magnets. • Event encoding data acquisition systems & extensive computing capabilities (real-time analysis). • Microwave cavities • Solutions to the pinhole problem. • Asterix upgrade.
Bulk materials	• Extremely limited studies to date. • Emerging interest in 11 T fields. • Flexibility/space of Asterix is attractive.	• Studies of multiferroic single crystals at extremes of field, pressure and temperature.	• Samples (see Physics Today) • Build FP11B • Dilution fridge compatible with high field magnets. • Asterix upgrade.
Soft matter	• None, see SPEAR.	• Dynamic behavior (diffusive motion). • Very small signals discerned from background.	• Samples (see Physics Today) • Polarized neutrons, MIEZE • Polarized neutrons, polarization analysis, or polarized nuclei
Neutron scattering techniques	• Drifted Mezei flipper. • SESAME. • Polarized neutron reflectometry in high fields with polarization analysis. • Integration of neutron scattering analysis with micromagnetic modeling. • Tests combining reflectometry and inelastic scattering.	• Multi-event-time correlation. • SESAME/SERGIS-glancing incidence SANS. • MIEZE and CIM. • Computer holography. • Complex sample environment. • Software, data reduction visualization. • Application of stress to thin film samples.	• μs-fast position sensitive detectors • Event encoding data acquisition system • Bootstrap RF flippers • Extensive computing capabilities, real-time analysis. • Minimization of systematic errors. • Theoretical support. • Asterix upgrade.

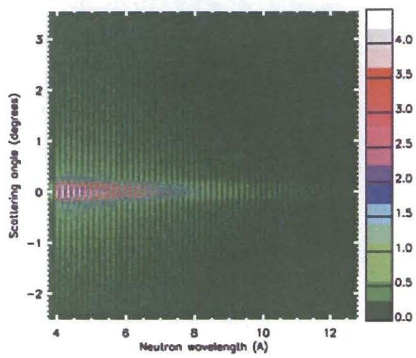
M.R. Fitzsimmons et al., Neutron scattering studies of nanomagnetism and artificially structured materials, *J. Magn. Magn. Mat.*, **271**, 103 (2004).

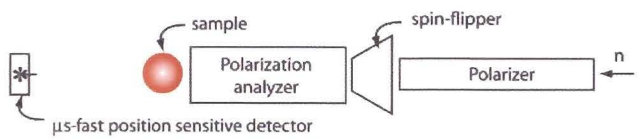
Next generation polarized neutron reflectometer workshop (organization in progress).

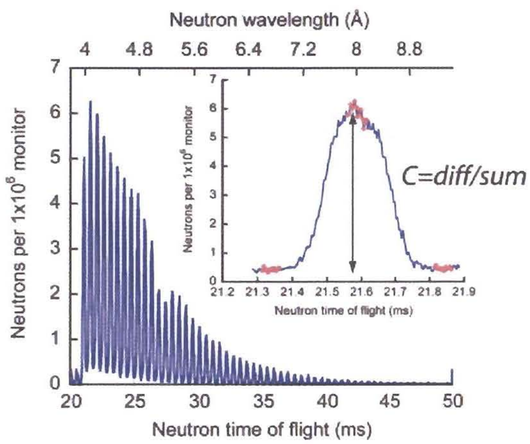
Title?

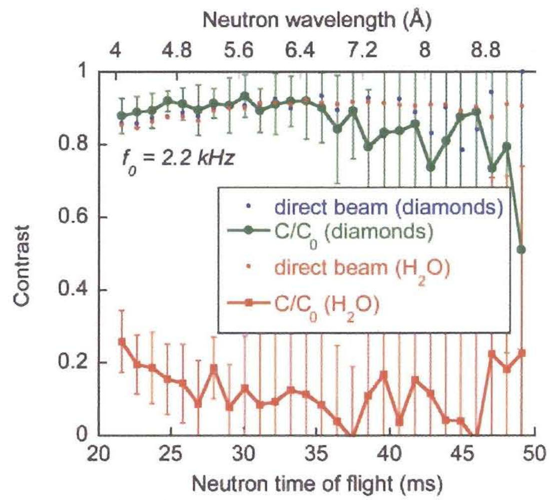
Electronic chopping and dynamics

Bleuel (ANL) and Fitzsimmons (LANL)



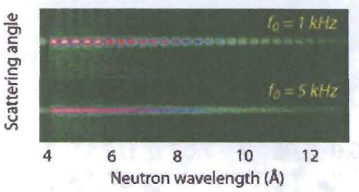


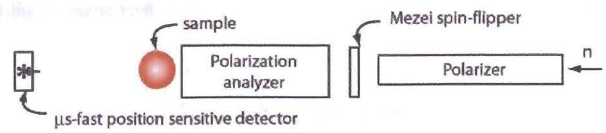


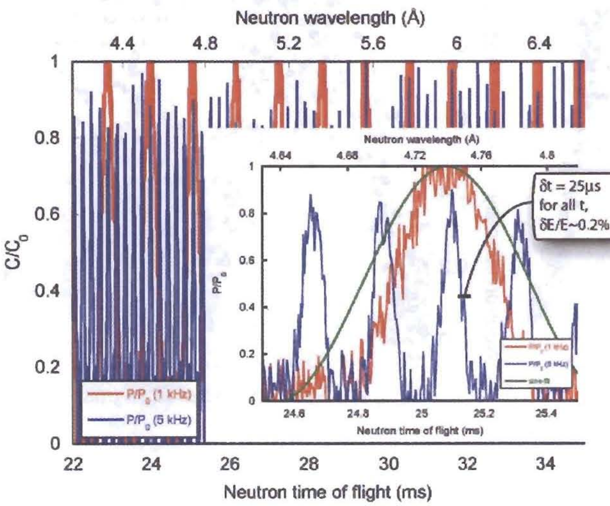


Have we observed dynamics of water?

Can we do better? Yes, perhaps 10's of kHz.







E_i = 5.2 meV to 0.6 meV
To avoid "mini-frame-overlap":
$\Delta t = 0.1/f_0$ to $0.5/f_0$
For 100 Hz operation:
Δt = 1 ms to 5 ms
For sample-to-detector distance of 2.5 m
E_f = 1.3 meV to 33 meV
For δt = 25 μs, δE~0.2%E

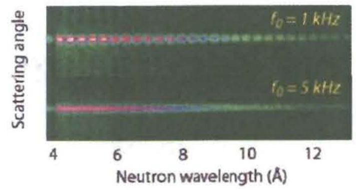
Downscatter (neutron energy loss)
E_i(max) 5.2 meV to E_f(min) = 1 meV (or less)
[Compare to FDS E_i = 5.2 to 500 meV to E_f = 5.2 meV]
Chemisorption
Physisorption
Hydrogen storage
Acoustic phonos
-'ve thermal expansion
Small Q means low momentum transfer (good for liquids and perhaps soft matter). biology

Upscatter (neutron absorbs energy)
E_i(min) = 0.6 meV to E_f(max) 33 meV (or more)
Excitations must exist in sample, e.g., FMR

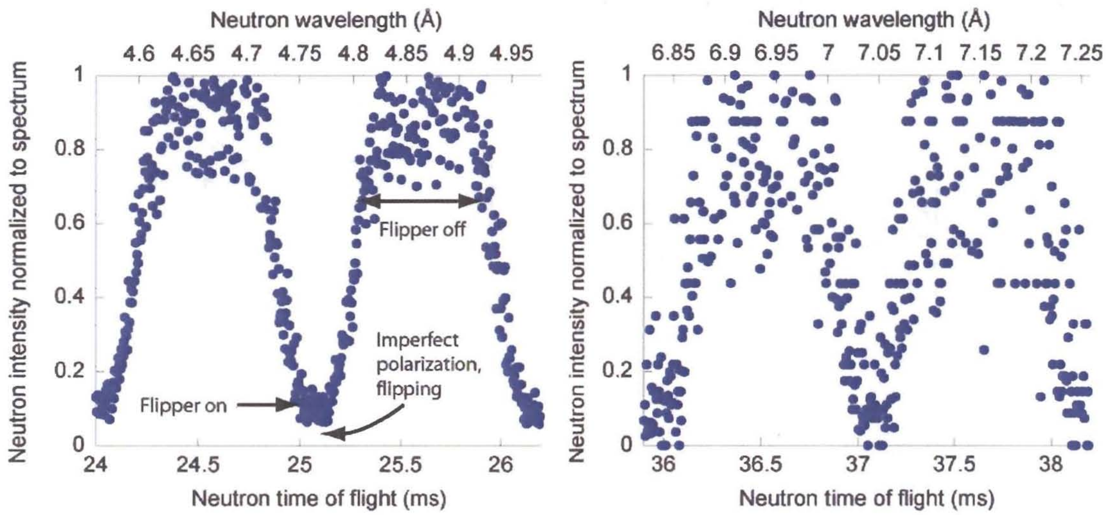
Advantages: (1) Inexpensive, and (2) Bolt-on in front of the sample.

Title?

1 of



$f_0 = 1\ kHz$
$f_0 = 5\ kHz$
Scattering angle
4
6
8
10
12
Neutron wavelength (Å)



Neutron wavelength (Å)
4.6 4.65 4.7 4.75 4.8 4.85 4.9 4.95
Neutron intensity normalized to spectrum
1
0.8
0.6
0.4
0.2
0
Flipper off
Imperfect polarization, flipping
Flipper on
24
24.5
25
25.5
26
Neutron time of flight (ms)
Neutron wavelength (Å)
6.85 6.9 6.95 7 7.05 7.1 7.15 7.2 7.25
Neutron intensity normalized to spectrum
1
0.8
0.6
0.4
0.2
0
36
36.5
37
37.5
38
Neutron time of flight (ms)

Writing Team Notes

September 5-7, 2007
Humphrey's Half Moon Bay Hotel
San Diego, California

Writing Team Meeting

- **Agenda for Friday-Saturday**
  - **Dinner on Friday 7 pm**
  - **Explore overlaps and outbrief comments**
- **Schedule agreement**
  - **Draft:** **Circulate by Sept 30**
  - **Final:** **CD and publication by Oct 30**
    - **Circulation plan: Audience?**
- **Process plan proposal**
  - **Chapters:** **by breakout chairs (2)**
  - **Overview:** **by Lujan managements**
  - **Figures:** **photographer, contributors**

Los Alamos — NNSA

Writing team discussion

- Audience includes LANL management. Shall there be recommendations to them?
  - Synergies within the lab
  - Policy issues–ammo
- NNSA as the audience?
  - Put in community needs and BES needs
  - National security needs is less of a priority
  - Lujan has moved beyond demonstrating need and value to LANL and NNSA management
- Roll this workshop up to a business plan built on the strategic plan
- Cater to certain groups in LANL (e.g. condensed matter community)
  - Work on synergies, e.g. biothreat, CINT, Shreve,...
  - CINT: Need to refresh that relationship

Los Alamos — NNSA

Writing team discussion (Friday)

- Add executive summary to chapters
- Aim for 5 page text single spaced
- Each chapter should address sample environments
- Provide a prioritized list.
  - Indicate interest in community if possible and have group address the sketch
  - Roll up the investment list up front including staffing
  - Suggestion: immediate and mid-term lists.
  - Indicate basis of priority (scientific interest, time sequence, etc)
  - IDT push is important
- Discuss real estate, moderator, staffing, user, and other global implications

Los Alamos — NNSA

Staffing

- Opportunity:
  - Define the staffing plan without whining
  - Strategy drives staffing—even for proposal writing
  - Will be captured in all chapters: flow from vision chapter down to science area chapters including sample environment team
  - Invoke the OSTP IWG report that cites number of unique users per scientific staff member including all direct technical support.
  - Look at ISIS and ILL metrics
  - Maxed out such that we are limited in users by staffing
- Team formation check
- INS reflectometry and USANS
  - Lo Q will address
  - Teams to coordinate
  - Techniques for Asterix—crystals, NSE,.. be careful with being complementary to the exclusion of success
  - Pulse probe and other synergies

Los Alamos — NNSA

- **BES session will be captured by Vision report**
  - Travel, Programmatic Proposals, Mail-ins, training students, fast access,
  - LANSCE-R down time aspects
  - Synchrotron issue: Take this up within the neutron community exp facilities directors' meeting in February
  - Emphesize complementarity
- **Diffraction with energy analysis: INS will take this up in Pharos discussion; Diffraction will include where valued.**

Los Alamos — NNSA

Addresses of Attendees

First	Last	Email	Institution
Ward	Beyerman	beyerman@citrus.ucr.edu	UCR
Moe	Boussoufi	mboussoufi@ucdavis.edu	
UCD			
Colin	Broholm	broholm@jhu.edu	
Johns Hopkins			
Leilani	Conradson	leilani@lanl.gov	
LANL			
Steve	Conradson	conradson@lanl.gov	
LANL			
Pengcheng	Dai	pdai@utk.edu	
UTenn			
Juergen	Eckert	juergen@mrl.ucsb.edu	UCLA
Mike	Fitzsimmons	fitz@lanl.gov	
LANL			
Mark	Foster	mfoster@uakron.edu	
UAkron			
Eric	Fullerton	efullerton@ece.ucsd.edu	
UCSD			
Brent	Fultz	btf@caltech.edu	
Cal Tech			
Henry	Glyde	glyde@physics.udel.edu	U Del
Rus	Hemley	hemley@gl.ciw.edu	
Carnegie			
Tanya	Herrera	tanyah@lanl.gov	
LANL			
Ken	Herwig	herwigkw@ornl.gov	
ORNL			
Rex	Hjelm	hjelm@lanl.gov	
LANL			
Alan	Hurd	ajhurd@lanl.gov	
LANL			
Barry	Klein	bmklein@ucdavis.edu	UCD
Tonya	Kuhl	tlkuhl@ucdavis.edu	UCD
Despina	Louca	louca@virginia.edu	U Va
Christian	Mailhiot	mailhiotl@llnl.gov	
LLNL			
Tom	Mason	mason@chem.ucla.edu	UCLA
Feri	Mezei	mezei@lanl.gov	
LANL			
Dan	Neuman	dan@nist.gov	
NIST			
Atul	Parikh	anparikh@ucdavis.edu	UCD
Thomas	Proffen	tproffen@lanl.gov	LANL
Roger	Pynn	pynn@mrl.ucsb.edu	Univ Ind
Ramamoorthy	Ramesh	rramesh@berkeley.edu	UCB
Don	Rej	drej@lanl.gov	LANL
Jim	Rhyne	rhyne@lanl.gov	LANL

Addresses of Attendees (cont.)

First	Last	Email	Institution
John	Sarrao	sarrao@lanl.gov	LANL
Dale	Schaefer	schaefdw@email.uc.edu	Univ Cinn
Kurt	Schoenberg	kurts@lanl.gov	LANL
Ivan	Schuller	ischuller@ucsd.edu	UCSD
Steve	Shapiro	shapiro@bnl.gov	BNL
Sunny	Sinha	ssinha@physics.ucsd.edu	UCSD
Alexei	Sokolov	alexei@uakron.edu	U Akron
Ray	Teller	rteller@anl.gov	ANL
Guebre	Tessema	gtessema@nsf.gov	NSF
Doug	Tobias	dtobias@uci.edu	UC Irvine
Frans	Trouw	trouw@lanl.gov	LANL
Jacob	Urquidi	jurquidi@nmsu.edu	NMSU
Jianzhong	Zhang	jzhang@lanl.gov	LANL