

**Science Poster Abstracts
SNS-HFIR User Meeting
October 11-13, 2005**

Sponsored by:

**Oak Ridge National Laboratory, Spallation Neutron Source, High Flux Isotope Reactor, Center for Nanophase Materials Science and Office of University Relations
Oak Ridge Associated Universities
University of Tennessee / Joint Institute for Neutron Sciences**

Physicochemical Characterization of Mixed Ck2-13/AOT & Ck2-13/C₈βG₁ Microemulsions for Drug Delivery Applications

Mayson H. Alkhatib¹, Douglas G. Hayes², Javier Gomez del Rio³

¹*Biotechnology Science and Engineering Program, University of Alabama in Huntsville, AL 35899*

²*Department of Biosystems Engineering and Soil Science, and*

³*Chemical Engineering, University of Tennessee, Knoxville, TN 37996-4531*

Microemulsions are transparent, thermodynamically stable, isotropic mixtures of oil, water, surfactant, and frequently cosurfactant. However, the performance of mixed surfactants microemulsions over their individual components were improved resulting in a wide variety of drug delivery applications. In view of that, a pH-degradable nonionic cyclic ketal polyethylene oxide, Ck2-13, synthesized in our lab, is combined with bis(2-ethylhexyl) sulfosuccinate, AOT and n-octyl-β-D-glucopyranoside, C₈βG₁. The physicochemical behavior of Ck2-13/AOT and Ck2-13/C₈βG₁ microemulsion systems is performed before they can live up to their potential as multipurpose drug delivery vehicles. The phase diagrams of both mixed surfactants have showed large microemulsion region with temperature insensitivity and salinity as well. Along with the phase diagrams, Dynamic Light Scattering technique, electrical conductivity and Fourier Transform Infrared analysis, Small Angle Neutron Scattering, SANS will be utilized to reveal the microstructure of mixed surfactants in w/o (water droplets in oil) microemulsion. It will be used to figure out the molecular origins of how the two surfactants interact with each other by measuring the interfacial composition of both surfactants at oil/water interface with different contrast schemes. SANS could probe the nature of the oil penetration into the interfacial surfactant monolayer of the microemulsion. It could tell us what happens when the system comes in contact with acidic conditions. Are there any transient effects that occur as the surfactant system changes from Ck2-13-rich to AOT- or C₈βG₁-rich? The results of SANS would shed light on surfactant behavior in real-life situations.

Density Profiles of “Looped” Polymer Brushes Formed by Self Assembly of Poly (2-vinylpyridine)-d-polystyrene- poly (2-vinylpyridine) Triblock Copolymers at the Solid-Fluid Interface.

Jose Alonzo,[†] Zhenyu Huang,[‡] Michael Lay,[‡] Ming Liu,[‡] Haining Ji,[‡] Jimmy W. Mays,[§] Mark Dadmun,[‡] and S. Michael Kilbey II^{†*}

[†] *Department of Chemical and Biomolecular Engineering, Clemson University, Clemson, SC 29634*

[‡] *Department of Chemistry, University of Tennessee, Knoxville, TN 37996*

[§] *Chemical Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831*

Dense layers of end-tethered polymers, often called polymer brushes, are of interest for their ability to modify interfacial properties. Along these lines, creating brushes comprised of loops by tethering chains by both ends offers potential advantages in tailoring the adhesive or frictional properties of surfaces. Rigorously synthesized poly(2-vinylpyridine)-d-polystyrene-poly(2-vinylpyridine) (P2VP-dPS-P2VP) triblock copolymers were used as a model system to examine the equilibrium structure of looped brushes at the solid-liquid interface. Preferential assembly of the triblock copolymers from toluene creates PS loops tethered by the PVP end blocks. Neutron reflectivity (NR) was used to determine the equilibrium segment density profiles of the looped brushes. The density profiles were obtained in toluene at room temperature, a good solvent for the PS block, and then in cyclohexane at 20 °C (poor solvent), 32 °C, (near-theta solvent), and 50 °C (marginal solvent). The experiments provide important insights into the internal structure of the layer by showing how the structure of the looped brushes changes with changes in solvent quality and temperature. While the NR results qualitatively agree with

* Corresponding author. E-mail: mkilbey@clemson.edu

known results from singly-tethered brushes, there are important differences in the local structural details due to the extra degree-of-freedom that comes about from the loops being tethered by two ends (i.e. the distance between two tethering points). These differences are highlighted in the results showing how the structure changes from a stretched conformation under good solvent conditions to a collapsed conformation as solvent quality decreases. The thicknesses obtained from the NR profiles also are in good agreement with preliminary results from surface forces measurements.

International Materials Institute- Advanced Neutron Scattering Network for Education and Research (ANSWER) In Situ Neutron Diffraction Studies of a cobalt-based superalloy

M. L. Benson, P. K. Liaw, T. A. Salek, H. Choo, M. R. Dagmond, D. W. Brown, X.-L. Wang, A. D. Stoica, R. A. Buchanan, and D. L. Klarstron

Physical Properties of Gas Hydrate from Green Canyon, Gulf of Mexico

Bryan C. Chakoumakos,¹ Yoshinobu Ishii,² Claudia J. Rawn,¹ Hsin Wang,¹ Jane Y. Howe,¹ Michael J. Lance,¹ Adam J. Rondinone,¹ Camille Y. Jones,³ Roger Sassen⁴

¹*Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831*

²*Japan Atomic Energy Research Institute, Tokai, Japan*

³*Department of Chemistry, Hamilton College, Clinton, New York 13323*

⁴*Geochemical and Environmental Research Group, Texas A&M University, College Station, Texas 77845*

A high quality gas hydrate sample was recovered in the Green Canyon by a research submersible at a depth of 540 m. The sample is free of sediment. X-ray and neutron powder diffraction identify structure II gas hydrate along with ice (frozen pore water and the product of contamination from handling). Raman spectroscopy identifies cage occupants as predominately methane with minor ethane and high molecular weight alkanes. Analysis of SANS data yields a surface fractal with dimension 2.6, and a domain size of the two-phase (hydrate and ice) system of 70 nm. The thermal conductivity measured by the hot disk method is 0.20(4) W/mK at 77K. Oak Ridge National Laboratory is supported by the Division of Materials Sciences, U.S. D.O.E. (contract DE-AC05-00OR22725 with UT-Battelle, LLC).

Long Range Attraction between Like-Charge Dendrimeric Colloids

Wei-Ren Chen^{1,2}, Lionel Porcar^{1,3}, Yun Liu^{1,3}, Paul D. Butler¹ and Linda J. Magid^{1,2,4,*}

¹*The Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD 20899-8562, USA*

²*Department of Chemistry, the University of Tennessee, Knoxville, TN 37996-1600, USA*

³*Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, USA*

⁴*Division of Chemistry, the National Science Foundation, Arlington, VA, 22230, USA*

*: Author to whom the correspondence should be addressed: Email address: lmagid@nsf.gov

The effective interaction between charged poly(amido amine) (PAMAM) G4 dendrimers in dilute deuterium oxide solutions is investigated by small angle neutron scattering (SANS) and dynamic light scattering (DLS). Upon increasing the ionization of the terminal amines by adding DCI, upturns appear in the SANS intensity distributions at low Q within a certain range of pH value, then surprisingly disappear again when pH=2. Detailed data analysis suggests the upturns can be interpreted in terms of the presence of a weak long-range attraction between similarly charged dendrimeric colloids. It also shows that the range of this interaction is several times that of the diameter of a single dendrimer and much greater than the range of the screened electrostatic repulsion. Such long-range weak attractive interactions, probably due to the dynamic interaction between the counterions and the charged dendrimeric colloids, can not be explained by the well-accepted DLVO theory of colloidal stability and may be very important for the understanding the suspensions of the charged nanoparticles.

Small angle neutron scattering studies of flux-line lattice in CeCoIn₅

L. DeBeer-Schmitt, C. D. Dewhurst, B. W. Hagenboom, C. Petrovic, M. R. Eskildsen

Thermodynamics of Impurities in Vanadium

O. Delaire, M. Kresch and B. Fultz.

We investigated the effects of dilute alloying on the lattice dynamics and electronic structure of bcc vanadium. Using time-of-flight inelastic neutron scattering, we have measured the phonon density of states (DOS) and vibrational entropy of random solid solutions of vanadium with transition metal impurities. A clear trend was observed for solutes across the 3d-series. Ti caused a softening of the V phonons, while elements to the right of V induced an increasing stiffening. The stiffening observed for 6% Pt impurities is very large and induces a decrease of vibrational entropy that is larger than the gain in configurational entropy, resulting in a negative entropy of mixing. Using density functional theory, we calculated the electronic structure for all alloys and found that the electronic entropy of alloying follows the same trend as the vibrational part, although it is smaller in magnitude. We also performed high-temperature phonon DOS measurements, up to 1273K for the alloys V-7%Co, V-6%Pt and V-6%Nb and 1673K for pure vanadium. At elevated temperatures, the vanadium phonon DOS shows a pronounced anharmonic behavior, with minimal softening occurring up to 1273K. Alloying of V with a few percent impurities disrupts this behavior, and the softening between 293K and 1273K for the alloy V-7%Co is in good agreement with classical thermal expansion arguments. We discuss the consequences of these findings on the thermodynamics of impurities in vanadium.

Condensate fraction and atomic kinetic energy of liquid ^3He - ^4He mixtures

S. O. Diallo¹ [email: sdiallo@udel.edu], J. V. Pearce², R. T. Azuah^{3,4} and H. R. Glyde¹ [email: glyde@udel.edu]

¹Physics and Astronomy, University of Delaware, Newark, DE USA 19716-2570

²Institut Laue-Langevin, BP 156, 38042 Grenoble, France

³Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742-2115

⁴NIST Center for Neutron Research, Gaithersburg, MD 20899-8562

Liquid ^3He - ^4He mixtures are the arch example of a mixed Bose and Fermi liquids in nature. New examples of Bose and Fermi gas mixtures are currently being actively created in trapped alkali atom systems. Taking advantage of the high energy neutrons available at ISIS spallation source and the high resolution of the MARI instrument, we have measured the Bose-Einstein condensate fraction and the momentum distribution of ^3He and ^4He atoms in ^3He - ^4He mixtures to new accuracy. We find that the condensate fraction increases only slightly above the pure ^4He value with increasing ^3He concentration x . This agrees with several calculations but is in contrast with the only single previous measurement of n_0 in ^3He - ^4He mixtures, thus resolving a longstanding disagreement between theory and experiment. We also find that the observed ^3He $n(k)$ is not well fitted with a Fermi step function alone. A high momentum tail in $n(k)$ is needed to get a good fit - a tail that is consistent with calculated tails in $n(k)$. The ^3He atomic kinetic energy, $\langle K_3 \rangle$, depends almost entirely on the tail. The tail is difficult to determine accurately in neutron scattering experiment. Thus $\langle K_3 \rangle$ is not a well determined quantity which explains why previous observed and calculated $\langle K_3 \rangle$ disagreed substantially. We find a ^4He kinetic energy which is largely independent x . Measurements of the dynamics of single atoms and molecules in materials are ideally done at spallation neutron sources and the SNS will greatly expand opportunities in this field.

Structural and magnetic studies of potential superconducting silver fluorides

M.R. Dolgos S.E. McLain, D.A. Tennant, T. Barnes, T. Proffen, and J. F. C. Turner

AgF₂-containing compounds are interesting given their structural similarity to the most commonly known superconducting materials, the cuprates. In a similar manner to the cuprates, the S= 1/2 ion displays square planar geometry and the ions also participate in strongly correlated magnetic behavior. Here we present structural and magnetic properties of Cs₂AgF₄ and its doped derivatives.

Incoherent Neutron Scattering Measurements of Hydrogen-Charged Zircaloy-4

E. Garlea¹, H. Choo^{1,2}, V. O. Garlea³, W. B. Bailey², J. R. Santisteban⁴,

P. D. Rack¹, P. K. Liaw¹, and C. R. Hubbard²

¹Materials Science and Engineering Department, The University of Tennessee, Knoxville, TN 37996

²Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

³Ames Laboratory and Iowa State University, Ames, Iowa, 50011, USA

⁴ *ISIS, Rutherford Appleton Laboratory, Chilton, United Kingdom*

Qualitative and quantitative phase measurements were conducted on Zircaloy-4 round bars using neutron scattering techniques. The specimens were charged using a 12.5 vol. % hydrogen in argon mixture in a tube furnace at 430 °C under 13.8 kPa for 1/2 hour, 1 hour, and 1.5 hour, respectively. The neutron diffraction mapping through the thickness of the specimens showed the presence of a face-centered-cubic delta (δ) zirconium hydride (ZrH_2) phase on the surface. The assessment of the background scattering due to the hydrogen incoherent process was carried out by performing inelastic scans (energy scans) around the zero energy transfer. To determine the relative amount of hydrogen in the Zircaloy-4 samples, the increase of the incoherent scattering with the hydrogen content was calibrated using standard samples for which the hydrogen content was known. For calibration, a polypropylene film with a thickness of 0.02 mm was cut into several sheets in a size of 40 mm x 50 mm. These sheets in sets of three were successively wrapped around a Zircaloy-4 specimen in as-received condition. The amount of the hydrogen in each sheet was calculated from its weight. Neutron energy scans were performed on the Zircaloy-4 sample wrapped with sets of polypropylene sheets in an energy range from -1.5 meV to 1.5 meV, with a step of 0.2 meV, and a counting time of 60 seconds per point. Moreover, "incoherent scans", were taken at a fixed two-theta value ($2\theta = 62$ deg) from an angular range with flat background such that no coherent scattering is present. Similarly, inelastic scans were carried out on the round-bar specimens charged with hydrogen gas to evaluate the hydrogen content in the bulk. Further, mapping of the background scattering through the thickness of the specimens was performed to evaluate the total hydrogen content within the round bar.

Topological relaxation of a shear-induced lamellar L_α phase to L_3 sponge equilibrium and the energetics of bilayer membrane fusion

W. A. Hamilton, L. Porcar, P. D. Butler, G. G. Warr

Current and future capabilities of the neutron reflectometer MIRROR at Oak Ridge National Laboratory's High Flux Isotope Reactor

W. A. Hamilton, G. S. Smith, G. B. Taylor, B. M. Larkins, and L. Porcar

Synthesis and Characterization of Calcium-Deficient Hydroxyapatite Biomimetically Incorporated into a Bacterial Cellulose Matrix

Stacy A. Hutchens¹, Roberto S. Benson², Barbara R. Evans³, Hugh M. O'Neill³, Claudia J. Rawn^{2,4}

¹ *Department of Mechanical, Aerospace, and Biomedical Engineering: University of Tennessee, Knoxville, TN 37996*

² *Department of Materials Science and Engineering: University of Tennessee, Knoxville, TN 37996*

³ *Chemical Sciences Division: Oak Ridge National Laboratory, Oak Ridge, TN 37831*

⁴ *Metals and Ceramics Division: Oak Ridge National Laboratory, Oak Ridge, TN 37831*

A novel composite material consisting of calcium-deficient hydroxyapatite biomimetically deposited in bacterial cellulose was developed for potential use as an orthopedic biomaterial. Crystalline cellulose produced by the *Gluconacetobacter hansenii* strain was sequentially incubated in aqueous calcium chloride followed by incubation in aqueous sodium phosphate. A thick deposition of apatite was homogeneously incorporated into the cellulose hydrogel. X-ray diffraction (XRD) confirmed that calcium-deficient hydroxyapatite had formed in the cellulose. Fourier Transform Infrared Spectroscopy (FTIR) demonstrated that the hydroxyapatite had chemically bonded with the hydroxyl groups of the cellulose. FTIR also showed that that hydroxyapatite had been produced with an octacalcium phosphate precursor similar to physiological bone. Scanning electron micrographs confirmed that uniform $\sim 1\mu\text{m}$ spherical hydroxyapatite particles comprised of nanosized crystallites within the cellulose. The limited resolution of the SEM prevented thorough examination of the crystallites, though needle and lamellar morphologies were observed. XRD confirmed that the hydroxyapatite was comprised of 10-40 nm anisotropic crystallites elongated in the c-axis much like natural bone apatite. The synthesis of the composite mimics natural biomineralization of bone indicating that the unique structure of bacterial cellulose provides an ideal template for biomimetic apatite formation. It is hoped that advanced characterization techniques, such as neutron diffraction and scattering, may be used to further evaluate the composite. Neutron technology may be used to determine the exact morphology of the hydroxyapatite

crystallites, ascertain the kinetics of the mineral formation, and determine the distribution of the crystallites throughout the cellulose matrix.

Spin Dynamics and Exchange Interactions in the A-type Antiferromagnetic State of Pr_{0.5}Sr_{0.5}MnO₃

V. V. Krishnamurthy¹, J. L. Robertson¹, R. S.

Fishman¹, M. D. Lumsden¹, and John F. Mitchell²

¹*Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6430, USA*

²*Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*

Both the undoped and heavily doped manganites exhibit antiferromagnetic ordering, but only the latter exhibits colossal magnetoresistance. In the half-doped manganites, colossal magnetoresistance occurs at the ferromagnetic metal to antiferromagnetic insulator transition, where a variety of magnetic phases compete for the ground state. The A-type antiferromagnetic ordering in the half-doped manganite Pr_{0.5}Sr_{0.5}MnO₃ below 140 K is associated with the dx_{2-y}^2 type orbital ordering as compared to the $d_{3x^2-y^2}/d_{3y^2-r^2}$ type orbital ordering in undoped manganites such as LaMnO₃. Inelastic neutron scattering is used to investigate the spin dynamics and excitations in the layered A-type antiferromagnetic state of Pr_{0.5}Sr_{0.5}MnO₃ at 20 K. Spin wave excitations from the manganese sublattice and two crystal field excitations of Pr are observed in the energy range between 2 and 20 meV. The spin wave dispersion for neutron momentum transfer, Q, parallel to the ferromagnetic planes is found to be much steeper than the dispersion when Q is perpendicular to the ferromagnetic planes, indicating strong anisotropy. Here we show that the 3D Heisenberg model with nearest neighbor exchange interactions, an interlayer antiferromagnetic coupling, and an intralayer ferromagnetic coupling and a single ion anisotropy can account for these dispersions. A comparison of the ratio of exchange interaction couplings in Pr_{0.5}Sr_{0.5}MnO₃ and LaMnO₃ shows that the anisotropy of exchange interactions strongly depends on the type of orbital ordering.

How Bad is Good? - A Critical Look at Iterative Fitting of Reflectivity Models using the Reduced Chi-Square Statistic

Charlie Laub and Tonya L. Kuhl, *UC-Davis Department of Chemical Engineering and Materials Science*

The origins of the chi-square statistic that is typically employed as a goodness of fit metric for iterative fitting of reflectivity data will be reviewed. The basis for the rule of thumb stating that a "good fit" is achieved with a reduced chi-square value of 1.0, will be derived, and it will be shown that, even for modestly larger errors, the "fit" is not significant in a statistical sense. We propose a new rule of thumb that states that the reduced chi-square error must be less than 1.5 to achieve a minimum level of significance, e.g. at the 0.1 percent level.

Spin-charge Coupling in Lightly Doped Nd_{2-x}Ce_xCuO₄

Shiliang Li, Stephen D. Wilson, David Mandrus, Bairu Zhao, Y. Onose, Y. Tokura, and Pengcheng Dai
UT, ORNL, ERATO (Japan), IPHY (China)

We use neutron scattering to study the influence of a magnetic field on spin structures of Nd₂CuO₄. On cooling from room temperature, Nd₂CuO₄ goes through a series of antiferromagnetic (AF) phase transitions with different noncollinear spin structures. While a c-axis aligned magnetic field does not alter the basic zero-field noncollinear spin structures, a field parallel to the CuO₂ plane can transform the noncollinear structure to a collinear one ("spin-flop" transition), induce magnetic disorder along the c axis, and cause hysteresis in the AF phase transitions. By comparing these results directly to the magnetoresistance (MR) measurements of Nd_{1.975}Ce_{0.025}CuO₄, which has essentially the same AF structures as Nd₂CuO₄, we find that a magnetic-field-induced spin-flop transition, AF phase hysteresis, and spin c-axis disorder all affect the transport properties of the material. Our results thus provide direct evidence for the existence of a strong spin-charge coupling in electron-doped copper oxides.

Pressure Effect on the Resonance of YBCO

Shiliang Li, Feng Ye, Jaime Fernandez-Baca, Rodney Hunt, and Pengcheng Dai, *UT, ORNL*

As one of the key features for understanding the mechanism of high-T_c superconductors, the magnetic resonance in YBCO has been studied a lot. It has been found that the intensity of resonance drops dramatically above T_c, which indicates a correlation between resonance and superconductivity. Several experiments have further tested this idea by tuning some parameters to affect the superconductivity, such as oxygen-doping, impurity-doping and magnetic field. We give a new method here, applying pressure, to study the correlation between resonance and superconductivity.

In-Situ Loading Neutron-Diffraction Studies of a Cobalt-Based Superalloy

P. K. Liaw¹, M. L. Benson¹, H. Choo^{1,2}, T. A. Saleh^{1,3}, D. W. Brown³, M. R. Daymond⁴, X.-L. Wang⁵, A. D. Stoica⁵, E. C. Oliver⁶, and D. L. Klarstrom⁷

¹*Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN 37996, USA.*

²*Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA.*

³*Los Alamos Neutron Science Center, Los Alamos National Laboratory, Los Alamos, NM 87545, USA.*

⁴*Department of Mechanical and Materials Engineering, Queen's University, Kingston, ON K7L3N6, Canada.*

⁵*Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA.*

⁶*ISIS Pulsed Neutron and Muon Source, Rutherford-Appleton Laboratory, Chilton, Didcot OX11 0QX.*

⁷*Haynes International, Inc., Kokomo, IN 46904, USA.*

ULTIMET[®] alloy is a cobalt-based superalloy that undergoes a stress-induced phase transformation from a face-centered-cubic (fcc) phase to a hexagonal-close-packed (hcp) phase. Several in-situ loading neutron-diffraction experiments were performed in order to investigate the behavior of this phase transformation under different loading conditions. The transformation was studied during monotonic loading and stress-controlled high-cycle fatigue (HCF) at the Spectrometer for Materials Research at Temperature and Stress (SMARTS) of Los Alamos Neutron Science Center. The HCF was performed at a maximum stress of $\sigma_{max} = 840$ MPa and a minimum stress of $\sigma_{min} = 84$ MPa, while the tensile experiment was terminated after reaching $\sigma_{max} = 890$ MPa. Low-cycle fatigue (LCF) experiments were conducted at the ENGIN-X instrument of the ISIS Pulsed Neutron and Muon Source in the United Kingdom. The LCF was performed at a maximum strain of $\epsilon_{max} = 1.25$ % and a minimum strain of $\epsilon_{min} = -1.25$ %. The monotonic-loading experiment revealed that the hcp phase forms after reaching the yield stress. During HCF, the hexagonal phase formed immediately upon the first fatigue cycle, with no further change in structure upon subsequent deformation. In contrast to HCF, the hcp phase forms gradually during LCF. In fact, fatigue cycle 12 is reached before the hcp phase is resolved by neutron diffraction. Diffraction patterns from subsequent fatigue cycles reveal that the hcp phase continues to accumulate as LCF progresses. These observations are related to previous work done on the alloy, in which the temperature evolution during HCF and LCF was measured and predicted. **Acknowledgements:** The author acknowledges the financial support of the National Science Foundation regarding the Combined Research-Curriculum Development (CRCD) Program, under EEC-9527527 and EEC-0203415, the Integrative Graduate Education and Research Training (IGERT) Program, under DGE-9987548, and the International Materials Institutes (IMI) Program, under DMR-0231320, to the University of Tennessee, Knoxville, with Ms. M. Poats, Dr. C. J. Van Hartesveldt, Dr. D. Dutta, Dr. L. Clesceri, Dr. W. Jennings, and Dr. C. Huber as contract monitors, respectively. Additional financial support from the Tennessee Advanced Materials Laboratory (TAML), with Prof. E. W. Plummer as director, is gratefully recognized.

Monte Carlo Simulation of ARCS Instrument Using Pyre Framework

Jiao Lin¹, Garrett Granroth², Michael Aivazis¹, Brent Fultz¹

¹*California Institute of Technology*

²*Spallation Neutron Source, Oak Ridge National Laboratory*

Instrument simulation can catch every detail of a neutron experiment. This kind of simulation will be helpful to both the design and the analysis of experiments. For example, we can perform quantum chemistry computations to obtain phonon dispersions of a material. These dispersions can be converted to a scattering kernel, which, in turn, can be inserted to a Monte-Carlo simulation application to produce detector signals. Because in such a simulation instrument characteristics are considered quite comprehensively, the detector signal calculated can be directly compared to experimental detector data in order to test our physical models. Another type of application would be, when researchers are preparing for an experiment, they can also run simulations first to confirm if the proposed experiment will produce discernable signals. In the last year, as part of the DANSE project, two software packages have been developed under pyre framework: "simulation" and

"pyre-mcstas". The "simulation" package provides a framework allowing very flexible integration of virtual neutron instruments for simulation. A simulation application can be conveniently constructed as a python class for a neutron instrument. Currently most neutron components that can be used in such a simulation application are provided by package "pyre-mcstas". This "simulation" package, however, has a collection of generic components, which provides a scheme for flexible and extensible simulation of samples and detectors. In this presentation we will report some preliminary results of simulation of ARCS instrument.

Orbital Physics: Unusual Colossal Magnetoresistance and Quantum Oscillations in the Mott System

Ca₃Ru₂O₇*

X.N. Lin, V. Durairaj, and G. Cao, *Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506*,

P. Schlottmann, *National High Magnetic Field Laboratory, Tallahassee, FL 32310*

S.E. Nagler, M. Lumsden, Z.X. Zhou, *Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831*

The bilayered Ca₃Ru₂O₇ features a Mott transition, orbitally-driven colossal magnetoresistance and quantum oscillations. Transport and magnetic studies of Ca₃Ru₂O₇ for temperatures ranging from 0.4 K to 56 K and magnetic fields, B, up to 45 T display strikingly different behavior when the field is applied along the different crystal axes. A ferromagnetic (FM) state with full spin polarization is achieved for B||a-axis, but colossal magnetoresistance is realized *only* for B||b-axis by avoiding the ferromagnetic state. For B||c-axis, Shubnikov-de Haas oscillations are observed and followed by a less resistive state than for B||a. Hence, in contrast to standard colossal magnetoresistive materials where the spin polarization is the driving force, the FM phase is the least energetically *favorable* for electron hopping [1]. In addition, for B rotating within the *ac*-plane, slow and strong Shubnikov-de Haas (SdH) oscillations periodic in 1/B are observed for T≤1.5 K in the presence of metamagnetism. These oscillations are highly angular dependent and intimately correlated with the spin-polarization of the ferromagnetic state. For B||[110], oscillations are also observed but periodic in B (rather than 1/B) which persist up to 15 K. While the SdH oscillations are a manifestation of the presence of small Fermi surface (FS) pockets in the Mott-like system, the B-periodic oscillations, an exotic quantum phenomenon, may be a result of anomalous coupling of the magnetic field to the t_{2g}-orbitals that makes the extremal cross-section of the FS field-dependent. These properties together with highly unusual spin-charge-lattice coupling near the Mott transition (48 K) are driven by the orbital degrees of freedom. Preliminary results of our recent neutron study show sharp magnetic transitions consistent with thermodynamic results. All results will be presented and discussed along with comparisons drawn with other related systems.

Reference:

1. Colossal Magnetoresistance by Avoiding a Ferromagnetic State in Mott System Ca₃Ru₂O₇, X. N. Lin, Z.X.

Zhou, V. Durairaj, P. Schlottmann and G. Cao, *Phys. Rev. Lett.* 95, 017203 (2005)

* This work was supported by NSF grant No. DMR-0240813

Pressure Dependence of Fragile-to-Strong Transition and a Possible Second Critical Point in Supercooled Confined Water

Li Liu,¹ Sow-Hsin Chen,¹ Antonio Faraone,^{1,2} Chun-Wan Yen,³ Chung-Yuan Mou,³ Alexander Kolesnikov,⁴ Eugene Mamontov,² and Juscelino Leao²

¹*Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*

²*Department of Material Science and Engineering, University of Maryland, College Park, MD 20742 and NIST Center for Neutron Research, Gaithersburg MD, 20899-8562*

³*Department of Chemistry, National Taiwan University, Taipei 106, Taiwan*

⁴*Intense Pulsed Neutron Source Division, Argonne National Laboratory, Argonne, IL 60439*

We investigated, using quasi-elastic and inelastic neutron scattering, the slow single-particle dynamics of water confined in lab synthesized nanoporous silica matrices, MCM-41-S, with pore diameters ranging from 10 Å to 18 Å. Inside the pores of these matrices, the freezing process of water is strongly inhibited. We analyzed the neutron scattering spectra with a relaxing-cage model (RCM) and determined the temperature and pressure dependences of the Q-dependent translational relaxation time and the stretch exponent. The calculated Q-independent average relaxation time shows a fragile-to-strong (F-S) dynamic transition for pressures lower than

1600 bar. Above this pressure, it is no longer possible to discern the characteristic feature of the F-S transition. Identification of this end point with the predicted second low-temperature critical point of water is discussed. A subsequent inelastic neutron scattering investigation of the librational band of water indicates that this F-S transition is associated with a structural change of the hydrogen-bond cage surrounding a typical water molecule from a denser liquid-like configuration to a less-dense ice-like open structure. Remarks: Prof. Sow-Hsin Chen will speak on this subject, while detailed results will be shown in my poster. Some of the results have been recently published in *Phys. Rev. Lett.* 95, 117802 (2005).

Magnetic excitation spectrum in $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$

M. D. Lumsden, S. Wilson, P. Dai, S. E. Nagler, R. Jin, D. Mandrus

Study of Granular Materials in Compression Using NRSF2

Xin Luo¹, Dayakar Penumadu¹, Ke An², Fei Tang², Camden R. Hubbard²

¹ Civil and Environmental Engineering Department, University of Tennessee;

² Metals and Ceramics Division, Oak Ridge National Laboratory

Granular material such as silica sand is a hydrostatic pressure dependent frictional material. The global stress-strain relation of silica is complex, and depends on initial state of the specimen (for example, its porosity, particle morphology, and contact force arrangement) and the loading history (compression, extension, pure shear). This study aims to provide a fundamental understanding of macroscopic stress-strain relations to its microstructure, to study the magnitude of non-homogeneous and anisotropic of strain distribution within a deforming assemblage of particles, and to develop an understanding of the meaning of terms "stress" and "strain" in particle materials subjected to various types of loading conditions. Two types of the silica (Ottawa with round grain shape and Q-Rok with angular grain shape) are used in this research. Both these materials have very similar particle size distribution but different morphology and hardness. An assemblage of these particulate materials with controlled initial state of formation is subjected to 1-D compression with a cylindrical specimen geometry of 19 mm in diameter and 19 mm in height. The deforming specimens were studied by in-situ neutron diffraction at the High Flux Isotope Reactor using the recently developed load frame associated with NRSF2. For the continuous loading, a larger gage volume of $5 \times 10 \times 5 \text{ mm}^3$ was used with an axial deformation rate of 0.0004 mm/sec, and typical counting time of 60 sec per log was found to be adequate. For the strain mapping experiment, a smaller gage volume of $2 \times 5 \times 2 \text{ mm}^3$ was used with a loading rate of 0.005 mm/sec, and counting time of 40-70 minutes per log. A mono-chromator of Si400 ($\lambda=1.89 \text{ \AA}$) and the lattice plane SiO_2 (-321) with reflection at 2θ of 75.60° are used in this study. A novel approach for identifying elastic strains from elasto-plastic strain from the test results will be discussed along with other pertinent conclusions related to the possible use of this unique data for studying granular materials for wide ranging applications.

Nature of Antiferromagnetism in $\text{Fe}_{50}\text{Pt}_{50-x}\text{Rh}_x$ Films

P. Mani¹, Z. Lu¹, W. H. Butler¹, J. L. Robertson², V. V. Krishnamurthy² & G. J. Mankey¹

¹ MINT Center, The University of Alabama, Tuscaloosa, AL

² Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

The temperature and composition dependent antiferromagnetic spin structure of $\text{Fe}_{50}\text{Pt}_{50-x}\text{Rh}_x$ alloy films grown on MgO(100) were studied using neutron diffraction. FePt is a strong ferromagnet with $L1_0$ structure and is a prospective recording media owing to its high perpendicular anisotropy and controllable grain size. At room temperature, $\text{Fe}_{50}\text{Pt}_{50-x}\text{Rh}_x$ has a ferromagnetic-antiferromagnetic transition near $x=10$. Also, $\text{Fe}_{50}\text{Pt}_{50-x}\text{Rh}_x$ ($x \sim 10$) exhibits a temperature dependent antiferromagnetic-ferromagnetic-paramagnetic triple point near 400 K. In a heat assisted magnetic recording (HAMR) media, these films can be used as soft underlayers since they are ferromagnetic when heated. A thinner layer of Fe-Pt-Rh is sufficient to provide the same closure field as a lower anisotropy conventional underlayer like permalloy. In addition, since the film turns antiferromagnetic when cooled, it will help stabilize the FePt media via exchange interactions.

$\text{Fe}_{50}\text{Pt}_{50-x}\text{Rh}_x$ ($x=10, 17.5$ and 25) alloy films (200 nm) were grown on MgO(100) using co-sputtering. X-ray diffraction shows the formation of a highly epitaxial, centered tetragonal structure with nearly perfect chemical

ordering in these alloys. Neutron diffraction studies were carried out at the High Flux Isotope Reactor and confirm the presence of $(\frac{1}{2} 0 0)$, $(\frac{1}{2} \frac{1}{2} 0)$ and $(\frac{1}{2} \frac{1}{2} \frac{1}{2})$ antiferromagnetic spin orderings that are strongly dependent on the temperature and composition. Magnetization measurements indicate the presence of a temperature dependent ferromagnetic phase in the alloy with $x=10$. Future experiments are being planned to study the magnetic field induced antiferromagnetic to ferromagnetic phase transition in these alloys using neutron diffraction.

Implications of structural features on magnetic properties of heavy fermion compounds: CePdGa₆, Ce₂PdGa₁₀ and Ce₂PdGa₁₂

Robin T. Macaluso, Jasmine Millican, Hanoh Lee, S. Nakatsuji, Z. Fisk, Julia Y. Chan

Universal aspects of macromolecules in blends, organic and supercritical solvents

Y. B. Melnichenko, G. D. Wignall (ORNL)

D. Schwahn, (Forschungszentrum Jülich)

Crystal Growth and Structure and Property Relationships of Pr-Ni-Ga Phases

Jasmine N. Millican, D. P. Young, M. Moldovan, Julia Y. Chan, *Louisiana State University*

Single crystals of two new ternary compounds, Pr₂NiGa₁₀ and Pr₂NiGa₁₂ were synthesized by flux methods. Single crystal X-ray diffraction data were collected and structures were solved for Pr₂NiGa₁₀ and Pr₂NiGa₁₂. Pr₂NiGa₁₀ crystallizes in a tetragonal space group $I4/mmm$, $Z = 2$, with the lattice parameters: $a = 4.2330$ (4) and $c = 26.364$ (3), Rfactor = 2.71%, and is isostructural to Ce₂PdGa₁₀. Pr₂NiGa₁₂ crystallizes in a tetragonal space group $P4/nbm$, $Z = 2$, with the lattice parameters: $a = 6.0080$ (7) and $c = 15.454$ (3), Rfactor = 4.2%, and is isostructural to Ce₂PdGa₁₂. The structure, transport, and magnetic properties of these compounds will be compared to other Ln_2PdGa_{10} ($Ln = La, Ce$) and Ln_2PdGa_{12} ($Ln = La, Ce$) phases.

Structure of Polymer Brushes Under Confinement Using Catalyst Matching

D. J. Mulder, T. L. Kuhl, G. S. Smith, W. A. Hamilton, and J. Majewski

The Neutron Spin Echo Spectrometer for the SNS

M. Ohl, M. Butzek, T. Kozielski, M. Monkenbusch, Ch. Tiemann, D. Richter

Research Centre Jülich, Leo-Brandt-Strasse, 52425 Jülich, Germany

The Research Centre of Jülich is going to install a new high resolution neutron spin echo spectrometer at the Spallation Neutron Source (SNS). Here we present the design of this instrument. In detail we will report on the neutron guide system, polarizing bender with revolver drum, chopper system, radiation shielding, magnetic enclosure, and the spectrometer itself. The unique feature of this instrument shall be the highest field integral of more than $J > 1 \text{ Tm}$. Subsequently, we will focus on the key technologies the superconducting main precession coils and correction elements to achieve this goal. To use superconducting coils (SC) the hysteresis effects have to be taken into account and the coils design must render them negligible and reproducible. Control of the exact position and vibration of the solenoid pack with respect to the cryostat is another important issue. The real challenge of this project is to correct the field integral inhomogeneities within a wide divergent beam in the large field of the main coils down to values of the order $\Delta J < 10^{-6} \text{ Tm}$. This task will be performed by "Fresnel-coil" type correction elements that have to carry a high radial current density. Our current design of shaped Al coils with an outer thickness of 20mm implies a maximum dissipation of about 800W in the largest of these coils. They must be positioned within a few 10 microns and being cooled to a maximum temperature of 60°C. Here we report on the tests of prototypes which accomplish these design goals. Also we will discuss new frontiers in science to be explored with this new generation of neutron spin echo experiments.

Magnetic Properties of Metal Cyanide Networks Assembled at Interfaces.*

Ju-Hyun Park,^a Franz Frye,^b Jeffrey T. Culp,^b Sarah Lane,^b Young-Duk Huh,^{b,c} Daniel R. Talham,^b Mark W. Meisel.^a

^a Department of Physics and Center for Condensed Matter Sciences, University of Florida, Gainesville, FL 32611-8440, USA; corresponding author e-mail : juhyun@phys.ufl.edu;

^b Department of Chemistry, University of Florida, Gainesville, FL 32611-7200, USA;

^c permanent address: Department of Chemistry, Dankook University, Seoul, Korea

The magnetic properties of metal cyanide thin films generated directly at interfaces have been studied. Prussian blue analogues, Fe-CN-Ni networks are prepared at the air/water interface and transferred to solid supports using Langmuir-Blodgett film methods. The process allows us to study the evolution of magnetic properties in the films ranging from structurally isolated magnetic monolayer to multiple bilayer (multilayer) systems [1]. Films of bulk materials are also prepared directly on the solid supports using sequential deposition method. In the case of Fe-CN-Co bulk film, we observed anisotropic photo-induced magnetism, where photo-induced magnetization increases or decreases depending on the orientation of the film with respect to the external magnetic field [2].

* This work was supported, in part, by NSF DMR-0305371.

[1] J.T. Culp, J.-H. Park, M.W. Meisel and D.R. Talham, *Inorg. Chem.* 42 (2003) 2842.

[2] J.H. Park, E. Čížmár, M.W. Meisel, Y.-D. Huh, F. Frye, S. Lane and D.R. Talham, *Appl. Phys. Lett.* 85 (2004) 3797.

Spin Density Wave Antiferromagnetism in Cr/CrV

Lee Robertson, Kaya Shah, and Eric Fullerton

Residual Strains Under Torsion Using Hollow Cylinder Steel Specimens and Neutron Diffraction

Dayakar Penumadu¹, Xin Luo¹, Amal Dutta¹, Ke An², Fei Tang², Camden R. Hubbard², Hahn Choo³, Peter K. Liaw³

¹ Civil and Environmental Engineering Department, University of Tennessee

² Metals and Ceramics Division, Oak Ridge National Laboratory

³ Material Science and Engineering Department, University of Tennessee

Use of neutron diffraction for studying residual strains developed in metallic specimens under tension has been well studied in the past four decades. However, the study of materials subjected to pure torsion or a combination of axial loading and torsion has not been reported in the past literature. The present study was performed to evaluate the role of torsion in residual strain evolution for hollow cylinder specimens. Torsion provides unique opportunity to probe mechanical behavior of materials under pure shear stress, and in combination with axial load, provides a mechanism to rotate principal stresses in a controlled fashion. Thus, complete three dimensional mechanical behavior can be investigated by controlling the major principal stress rotation to characterize anisotropic materials. In this research, hollow cylinder specimens made of 12L14 steel with an outer diameter 10.8 mm, inner diameter 6.8 mm, and a wall thickness of 2 mm are used. These specimens are then subjected to either pure torsion or pure tension tests in which the steel specimens experience the same magnitude of equivalent octahedral shear strain using combined axial-torsional testing system available at the University of Tennessee, Knoxville. These specimens are then studied (ex-situ) using the neutron residual stress facility 2 (NRSF 2) at Oak Ridge National Laboratory (ORNL). Changes in the lattice spacing are measured in radial and circumferential direction with a gage volume of $1 \times 2 \times 1 \text{ mm}^3$, and along axial direction with a gage volume of $2 \times 1 \times 2 \text{ mm}^3$. Two mono-chromaters of Si220 (2.67Å) and Si331AF (1.73Å), and two lattice planes Fe(110) and Fe(211) with reflection at 2θ of 82.23° and 95.37° , respectively, are used in this study. The test results are analyzed for Fe(110) and Fe(211), which are reported to be both weakly affected by intergranular strain for tension stress path from prior literature. Considerable difference in terms of the measured residual strain variation between the steel specimens subjected to torsion and tension for similar invariant strain history was observed and implications will be presented. An immediate goal of this study is also to demonstrate the need for having a multi-axial testing system (axial and torsional) for the anticipated testing facility at VULCAN for the Spallation Neutron Source (SNS) users.

Neutron Scattering Studies of Short-Range Order and Atomic Displacements in a Null Matrix $^{62}\text{Ni}_{0.52}\text{Pt}_{0.48}$ Crystal.

Jose A. Rodriguez, S. C. Moss, University of Houston;
J. L. Roberson, ORNL;

J. R. D. Copley, D. A. Neumann, *NIST*;
J. Major, H. Reichert, H. Dosch, *MPI für Metallforschung-Stuttgart*.

The best known exception to the Heine-Samson and Bibier-Gauthier arguments for ordering effects of transition metal alloys (similar to the Hume-Rothery rules) is a NiPt alloy, where the phase diagram is similar to the CuAu system. Using the Disk Chopper Spectrometer (DCS) at NIST, we have investigated a Null-Matrix Crystal $^{62}\text{Ni}_{0.52}\text{Pt}_{0.48}$, (^{62}Ni has a negative scattering length, nearly equal in magnitude to Pt). Its composition has therefore been chosen whereby all effects depending on the average lattice scattering vanish. The only remaining contributions to the diffuse scattering are the Short Range Order (SRO) and Size Effect (SE) terms. Such data permit the extraction of the SRO parameters (concentration-concentration correlations) as well as the displacement parameters (concentration-displacement correlations). Using the Krivoglaz-Clapp-Moss theory, we obtained the Effective Pair Interactions (EPI). The results can be used to model the alloy in the context of electronic theory of alloy phase stability, including the very important aspect of charge transfer and ionicity.

Organizing Immiscible Polymers with Balanced Diblock Copolymer Surfactants

Megan Ruegg¹, Ben Reynolds¹, and Nitash Balsara¹, Min Lin², David Lohse²

¹*University of California, Berkeley*

²*ExxonMobil Research and Engineering*.

A balanced A-C diblock copolymer surfactant was used to organize mixtures of immiscible A and B homopolymers. The C-block of the copolymer exhibits repulsive and attractive interactions with the A and B homopolymers, respectively, leading to rich phase behavior. Small angle neutron scattering (SANS) experiments indicate the existence of a microphase separated state at low temperatures, a homogeneous phase at intermediate temperatures, and macrophase separation at high temperatures. It is unusual for a microphase separated blend to exhibit a homogeneous phase prior to macrophase separation. We use a combination of self-consistent field theory (SCFT) and the random phase approximation (RPA) to understand the origin of our observations. All of the parameters needed for the SCFT and RPA calculations were obtained from independent measurements utilizing SANS experiments on binary homogeneous blends. The measured length scale of the periodic concentration fluctuations in the homogeneous state, and the domain spacing of the microphase separated blends were in close agreement with RPA and SCFT, respectively. The transition temperatures between phases predicted with theory were in reasonable agreement with the experimental measurements.

Jahn-Teller distorted manganite frameworks: geometric modeling and interpretation of experimental results

Sartbaeva A., Wells S.A., Bozin E.S. Billinge S.J.L., *Arizona State University, Michigan State University*

The manganese-based perovskite compounds have recently received considerable interest because of the discovery of their colossal magnetoresistance. The interpretation of experimental data on these materials is often difficult – with disagreement, for example, between determination of average and local structure [1]. A new method of geometric modeling [2] with inclusion of JT-distortion is presented. It allows the simulations of large cells containing thousands of polyhedra. This allows us to simulate different patterns of local order for comparison with the experimental data. We present geometric frustration as a novel mechanism for stripe formation [3]. We also present results on polarons in doped manganites and polaronic defects.

1. Qiu X. et al. PRL, 94, 177203, 2005

2. Sartbaeva A. et al. JPCM, 16, 8173, 2004; Gatta D. and Wells S.A., PCM, 31, 1, 2004

3. Loudon J. et al. PRL, 94, 097202, 2005

Conformational Changes in Guanylate Kinase Studied by Osmotic Stress and SANS

Christopher Stanley¹, Susan Krueger¹, V. Adrian Parsegian², and Donald C. Rau²

¹*NIST Center for Neutron Research, Gaithersburg, MD*; ²*NICHHD, National Institutes of Health, Bethesda, MD*

Protein conformational changes induced by ligand binding are accompanied by a change in the number of water molecules sequestered in pockets, cavities, and grooves. The significance of hydration to protein-ligand interactions has been illustrated using the osmotic stress technique. We are using small-angle neutron

scattering (SANS) coupled with the osmotic stress technique to directly probe the connection between protein structural change and thermodynamics for guanylate kinase. We chose this enzyme because it is known to undergo a large conformational change upon binding the ligand GMP. We are able to follow this conformational change using SANS to determine the radius of gyration, R_g , and the pair-distribution function, $P(R)$, and now we are investigating protein mechanics by using osmotic stress to induce the conformational change in the absence of ligand. This should offer new opportunities for protein structure research by allowing the energetics of the conformational change to be measured apart from the ligand binding energy.

Temperature Dependent Bilayer Ferromagnetism in $\text{Sr}_3\text{Ru}_2\text{O}_7$

M. B. Stone, M. D. Lumsden, R. Jin, B. C. Sales, D. G. Mandrus, S.E. Nagler
Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

The Ruthenium based perovskites exhibit a wide range of interesting physical behaviors, including exotic superconductivity, metal insulator transitions, and strong quantum fluctuations. Exciting magnetic phenomena have been identified in several ruthenates, but a clear understanding of the underlying magnetic excitation spectrum in these layered perovskites is far from complete. We present results of detailed inelastic neutron scattering measurements of $\text{Sr}_3\text{Ru}_2\text{O}_7$ performed at the HFIR neutron scattering facility. Measurements were performed using the HB1 triple-axis spectrometer to probe the ferromagnetic fluctuations of the bilayer structure. A magnetic response is clearly visible for a range of temperatures, $T = 3.8$ K up to $T = 100$ K, and for energy transfers between $\hbar\omega = 2$ and 14 meV. These measurements indicate that the ferromagnetic fluctuations explicitly shown in the bilayer magnetic form-factor persist to temperatures large compared to the energy-scales of the fluctuations. This high temperature behavior is proposed as a manifestation of the proximity of the system in zero magnetic field to the metamagnetic/ferromagnetic transition.

Changes in Lattice Strain Profiles around a Fatigue Crack through the Retardation Period after Overloading

Y. Sun^a, K. An^b, F. Tang^b, C. R. Hubbard^b, Y. L. Lu^a, H. Choo^{a, b}, and P. K. Liaw^a,

^a *Materials Science and Engineering Department, The University of Tennessee, Knoxville, TN 37996.*

^b *Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831.*

An overload was applied during a fatigue crack-growth experiment, resulting in a temporary decrease in crack-growth rates, i.e., a retardation period. Neutron diffraction was used to investigate the retardation phenomenon by mapping the changes in the lattice strain profiles around the fatigue-crack tip in a series of compact-tension (CT) specimens, which were fatigued to various stages through the retardation period after the overload. Following the overload, compressive-strain fields were observed along the loading direction close to the crack tip. As the crack grows out of the retardation period, the residual compressive strains decreased.

Effect of Welding Process on the Residual Stress Distribution in Welded Cruciform Parts

Fei Tang, Andrew Payzant, Suresh Babu, Camden Hubbard, Ke An, and William Barton Bailey

Unusual magnetic properties of the orbitally degenerate triangular lattice LiVO_2

W. Tian^a, M.B. Stone^b, D.G. Mandrus^b, B.C. Sales^b, R. Jin^b, D.T. Adroja^c, S.E. Nagler^b

^a *Department of Physics and Astronomy, The University of Tennessee, Knoxville, TN 37996, USA*

^b *Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*

^c *ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon., OX11, OQX, United Kingdom*

LiVO_2 contains a two dimensional triangular lattice of $S = 1$ V^{3+} ions with threefold t_{2g} orbital degeneracy. Magnetically, at $T \approx 500$ K, LiVO_2 changes from a high temperature Curie-Weiss paramagnet state to a low temperature non-magnetic state with no indication of magnetic long range order down to $T = 2$ K. It has been proposed that V^{3+} ions form isolated trimers by a special type of orbital ordering in the low temperature phase that removes the frustration inherent in the triangular lattice. We report here the bulk properties and especially inelastic neutron scattering studies of LiVO_2 . Our low temperature inelastic neutron scattering experiments detect an excitation at ~ 58 meV which we identify as a candidate for the principal singlet to triplet magnetic

transition. Additional excitations are also observed at lower and higher energies. Our results suggest that orbital degeneracy plays an important role in understanding the unusual magnetic properties of LiVO_2 .

Inelastic neutron scattering investigation of medium cycloalkanes: a test of theory in conformation identification from vibrational spectra

Nina Verdal, Jeremiah J. Wilke, Bruce S. Hudson

Department of Chemistry, 111 College Ave, Syracuse University, Syracuse, NY 13244-4100

Inelastic neutron scattering (INS) spectra of a series of medium sized cycloalkanes: C_6H_{12} , C_7H_{14} , C_8H_{16} , $\text{C}_{10}\text{H}_{20}$, $\text{C}_{12}\text{H}_{24}$ and $\text{C}_{14}\text{H}_{28}$ are presented. Optimized geometry and normal mode frequencies have been calculated for the lowest energy conformers of these cycloalkanes using the B3LYP/6-311G(d,p) functional and basis set. The observed spectra are compared with the calculated normal modes of conformers that are predicted to be lowest in energy or thermally accessible at the experimental temperature of 30 K to determine the dominant conformation present in a potentially conformationally rich system. The results of this analysis are compared with the results of analysis of low temperature diffraction data available for C_6H_{12} , $\text{C}_{10}\text{H}_{20}$, $\text{C}_{12}\text{H}_{24}$ and $\text{C}_{14}\text{H}_{28}$. The conformers that are calculated to have the lowest energy are consistent with those determined from diffraction studies and the observed INS spectra are in good agreement with the conformer spectra of the lowest calculated energy. INS spectra simulated using the higher energy conformations have a much poorer fit to the observed spectra than those lowest in energy. These results indicate that inelastic neutron scattering spectroscopy may be a useful tool in determining the dominant conformation in a crystal lattice in cases like this in which the intermolecular interactions are weak and the different conformers are calculated to have differing spectra. Such an analysis is applied to the cases of C_7H_{14} and C_8H_{16} for which no low temperature x-ray analysis is available. Clear structure predictions result and, again, the conformer observed is that computed to be of lowest energy.

Increasing the alignment of PS-b-PMMA thin films through adding lithium ions under electric field

Jia-Yu Wang, Suresh Gupta, Julie Leiston-Belanger, Ting Xu and Thomas P. Russell, *University of Massachusetts - Amherst*

The long-range ordering of microdomains in thin films of diblock copolymers is requisite for applications that require spatial definition of structure in three dimensions. Xu's result exhibited the impurity of lithium ions from anionic polymerization may be a significant drive for the formation of long-range ordering nanostructure in thin films of diblock copolymers under electric field. In this poster, we successfully introduced lithium ions into PS-b-PMMA thin films. The results show that when lithium ions were bonded to PMMA chains, dielectric constant increased about four times so that the critical electric field strength may be reduced to a quarter. The cross-sectional TEM images of PS-b-PMMA thin films with and without bonded lithium ions also support above results. Furthermore, they showed two different reorientation dynamics of lamellar microdomains normal to the surface. In the presence of bonded lithium ions, the transition occurred from grain rotation. Otherwise, the lamellae locally broke up and then reformed under the condition of no bonded lithium ions. In conclusion, lithium ions markedly increased the alignment of block copolymer thin films under electric field through overcoming interfacial interaction.

VULCAN – Roman God of Fire and Metalworking at the Spallation Neutron Source

X.-L. Wang, T. M. Holden, G. Q. Rennich, A. D. Stoica, P. K. Liaw, H. Choo, and C. R. Hubbard

Global and local textures in Ni_2MnGa Ferromagnetic Shape-Memory Alloy

Y. D. Wang, Y. Ren, H. Li, D. Y. Cong, H. Choo, P. K. Liaw, R. Lin Peng, and L. Zuo

The Biodeuteration Laboratory at Oak Ridge National Laboratory

K. L. Weiss, D. A. Pelletier, D. A. A. Myles

Direct Microscopic Evidence for a Quantum Critical Point in the Electron-Doped Cuprate $\text{Pr}_{1-x}\text{LaCe}_x\text{CuO}_4$

Stephen Wilson, *Department of Physics and Astronomy, The University of Tennessee*

Shiliang Li, *Department of Physics and Astronomy, The University of Tennessee*

Pengcheng Dai, *Department of Physics and Astronomy, The University of Tennessee\ Condensed Matter Sciences Division, Oak Ridge National Laboratory*

Wei Bao, *Los Alamos National Laboratory*

Jae-Ho Chung, *NIST Center for Neutron Research*

Seung-Hun Lee, *Department of Physics, University of Virginia*

A quantum critical point (QCP) has been shown to render profound effects on the electronic properties of a material over a wide parameter region at finite temperatures providing in particular a mechanism for unconventional superconductivity. In high-transition temperature (high- T_c) copper oxides, a variety of experiments have already provided varying degrees of indications for QCPs near "optimal doping", where superconductivity is the most robust [1-4]. Here we report inelastic neutron scattering measurements on the electron-doped superconducting compound, $\text{Pr}_{0.88}\text{LaCe}_{0.12}\text{CuO}_{4-\delta}$ (PLCCO), which demonstrate that the energy and temperature dependence of the dynamical spin susceptibility χ'' satisfy an χ''/T scaling. These measurements on a series of samples demonstrate this scaling regime's evolution as the doped proximity of the QCP changes. Moreover, this scaling regime is directly correlated with the gradual suppression of an antiferromagnetic (AF) order as optimal superconductivity is achieved [5,6]. These results thus provide direct microscopic evidence for a magnetic QCP in the electron-doped superconductors.

[1] S. M. Hayden *et al.*, *Phys. Rev. Lett.* **66**, 821 (1991).

[2] B. Keimer *et al.*, *Phys. Rev. B* **46**, 14034 (1992).

[3] G. Aeppli *et al.*, *Science* **278**, 1432 (1997).

[4] W. Bao *et al.*, *Phys. Rev. Lett.* **91**, 127005 (2003).

[5] P. Dai *et al.*, *Phys. Rev. B* **71**, 100502 (R) (2005).

[6] H. J. Kang *et al.*, *Phys. Rev. B* **71**, 214512 (2005)

The US-Japan Triple Axis Spectrometer

Barry Winn, *Field Representative for the Center for Neutron Science at Brookhaven National Lab*

Cold neutrons (typical energies, <5 meV), in contrast to thermal neutrons, provide higher energy resolution and momentum resolution for triple-axis spectrometers. Cold neutrons also provide greater sensitivity to magnetic phenomena, due both to larger magnetic scattering intensities for smaller Q and a matching energy scale to achievable magnetic fields at the sample. The US-Japan Triple Axis Spectrometer exploits these cold neutrons, and is an important component of the HFIR User Program, the US-Japan Cooperative Research Program on Neutron Scattering, and Brookhaven National Laboratory's Neutron Scattering Group. Parts of this spectrometer were once part of BNL's H4M triple-axis spectrometer at the High Flux Beam Reactor and are finding new life at HFIR

The Optic and Acoustic magnetic excitations in optimum-doped superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{6.95}$

Hyungje Woo¹, Pengcheng Dai^{1,2}, S. M. Hayden³, Herb A. Mook², T. G. Perring⁴, T. Dahm⁵, D. J. Scalapino⁶ and Doğan⁷

¹ *Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996*

² *Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831*

³ *H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, UK*

⁴ *ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon, OX11 0QX, UK*

⁵ *Institut für Theoretische Physik, Universität Tübingen, Tübingen, Germany*

⁶ *Department of Physics, University of California, Santa Barbara, CA 93106*

⁷ *Department of Ceramic Engineering, University of Missouri-Rolla, Rolla, Missouri 65409*

An ultimate goal in understanding high-transition temperature superconductors (HTSC) is to search for the pairing mechanism of superconductivity. Since the discovery of HTSC some 19 years ago, magnetic excitations have been one of the strong candidates for mediating electron pairing. We use inelastic neutron scattering to map out the full spin excitations spectra in $\text{YBa}_2\text{Cu}_3\text{O}_{6.95}$ (YBCO, $T_c = 93$ K), probably the most studied HTSC. In the bi-layer systems such as YBCO, there are two magnetic ions per unit cell. This means that the magnetic excitations have two distinct symmetries: odd (acoustic) and even (optical). Recent work on the bi-layer

YBa₂Cu₃O_{6.6} [1] and single layer La_{1.875}Ba_{0.125}CuO₄ [2] showed that magnetic excitations in these two families of materials are remarkably similar. Our analysis of YBa₂Cu₃O_{6.95} reveals the difference and similarity comparing those systems. By using the total magnetic spectra, we can calculate whether spin fluctuations are sufficient to account for the superconducting condensation energy in YBCO.

[1] S. M. Hayden, H. A. Mook, Pengcheng Dai, T. G. Perring & F. Doğan, *Nature* **429**, 531 (2004).

[2] J. M. Tranquada, H. Woo, T. G. Perring, H. Goka, G. D. Gu, G. Xu, M. Fujita & K. Yamada, *Nature* **429**, 534 (2004).

Comparison between in-situ time-resolved neutron diffraction measurements based on quasi-steady state phenomenon and direct real-time experiment

W. Woo^{a, b}, Z. Feng^{b*}, K. An^b, X-L. Wang^c, H. Choo^{a, b}, C. R. Hubbard^b, and S. A. David^b

^{a)} *Materials Science and Engineering Department, University of Tennessee, Knoxville, TN 37996, USA*

^{b)} *Metal and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*

^{c)} *Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA*

The material state changes (e.g., temperature, stress and microstructure) are one of the issues in the severe thermo-mechanical processing. Deep penetrating capability of neutrons enables to understand the mechanical properties and structures for the changes of the material states. However, it has been limited to the “static” behavior due to the insufficient time to reach adequate neutron fluxes in the rapid changes of material state. Thermal stresses were imposed on a local area of the 6061-T6 aluminum alloy plates using an electric heat source. A new technique was performed using in-situ time-resolved neutron diffraction measurement technique based on the quasi-steady state (QSS) phenomenon. The results show the equivalency of the lattice parameter changes between the QSS and direct real-time measurements in the transient response by the localized moving heat source. The developed QSS technique suggests that neutron collecting time associated with the neutron flux and sampling volume can be independent to the change rate of material states in the transient processes.

* Author to whom correspondence should be addressed; electronic mail: fengz@ornl.gov

Design, synthesis and characterization of artificial proteins for biomolecular materials

Ting Xu^{1,2}, Shixin Ye¹, Joe Strzalka¹, Sophia Wu¹, Micheal J. Therien¹, Thomas P. Russell³, J. Kent Blasié^{1,2}

¹Department of Chemistry, University of Pennsylvania,

²Cold Neutrons for Biology and Technology (CNBT) at NIST,

³Department of Polymer Science and Engineering, University of Massachusetts, Amherst.

Artificial protein models (or “maquettes”), based on both alpha-helical bundle and beta-sheet structural motifs, can now be designed to incorporate biological cofactors and retain a range of specific functional elements of their natural counterparts by design, but within much more simple structures. Amphiphilic 4-helix bundle peptides have been previously designed and synthesized to selectively incorporate heme and other natural cofactors within both the hydrophilic and hydrophobic domains and have proven to possess characteristic electronic and optical properties of the kind familiar in natural electron-transfer proteins. The design of artificial proteins with synthetic non-biological cofactors could potentially lead to artificial protein-based systems with novel properties not exhibited by the biological systems. For example, extended pi-electron systems can now be designed and tailored, with appropriate donors, acceptors and constituents, to exhibit selected light-induced electron transport and/or proton translocation over large distances. These non-biological groups have the advantage of including the electron donor and the electron acceptor within the same prosthetic group. We studied the binding between a series of non-biological metalloporphyrin cofactors and the designed amphiphilic 4-helix bundles at selected locations. The interior of the artificial protein scaffolding can be used to control the solubility, position, orientation of the cofactors within the peptide, while the exterior can be used to control the artificial protein's macroscopic orientation. The binding selectivity depends on hydrophobicity and steric hindrance of the cofactors. Artificial proteins monolayer, both the apo- and holo-form, can be oriented vectorially at the air/water interface. Incorporation of the non-biological cofactors into the 4-helix bundle via bis-histidyl ligation did not change the secondary structure of the proteins. The amphiphilic protein/cofactor complexes have good thermal stability up to 80 degree. This development may potentially lead to functional biomaterials with novel electron transfer properties.

To generate useful biomaterials, the artificial proteins must be assembled into one-, two- or three-dimensional order. Although 1-dimensional order has been achieved by designing the exterior of the artificial proteins, control over their 2-D ordering has yet to be realized, not to mention 3-D ordering. It has proven difficult

to engineer technologically important biomaterials solely from these *de novo* designed artificial proteins. Recent developments in controlling the microdomain orientation and generating long-range order makes copolymer thin films ideal platforms as templates, masks and scaffolds for nanodevices. I am working on incorporating the artificial proteins into copolymer assemblies and generate biomaterials exhibiting macroscopic functions. Using copolymers as a scaffold will enable us to make 1, 2, or 3-D ordered assemblies with features ranging from 1nm cofactors, to 2-5nm α -helical bundles, to 10-100nm microdomains. My future research will focus on the fundamental understanding of the assembly mechanism, with an emphasis on the thin films, and the contributions from different factors governing the assembly process from all levels including cofactor, artificial proteins and copolymers. They will, in turn, guide the design of the artificial proteins and block copolymers and finally lead toward technologically important biomaterials. The systems require structural characterization, as related to their macroscopic functionality. Combinations of various scattering techniques are essential and synchrotron and neutron sources are required to study the complex in thin films. X-ray scattering techniques such as grazing incidence small angle x-ray scattering, small/wide angle x-ray scattering, x-ray reflectivity and resonance x-ray reflectivity will be used to characterize the hierarchical assembly at different size scales. Neutron sources offer great advantages as the contrast variation with neutrons can be afforded by the deuteration of selected components at all levels, upwards from the single residue level (for the peptides) while avoiding beam damage and maintaining the protein integrity.

Electronically smectic-like phase in a nearly half-doped manganites $\text{Pr}_{0.55}(\text{Ca,Sr})_{0.45}\text{MnO}_3$

F. Ye, J. A. Fernandez-Baca, P. Dai, J. W. Lynn, H. Kawano-Furukawa, H. Yoshizawa, Y. Tomioka, and Y. Tokura

Relaxation study of polarized ^3He nuclei at low temperatures for the neutron EDM experiment

Qiang Ye¹, Haiyan Gao¹, Dipankar Dutta¹, Kevin Kramer¹, Xin Qian¹, Xing Zong¹, Lars Hanneliu², Bernadette Heyburn, Robert D. McKeown², Scott Singer², Lars Hanneliu², Bernadette Heyburn, Robert D. McKeown², Scott Singer², Bob Golub³, Ekaterina Korobkina³

¹Duke University, Durham, NC

²California Institute of Technology, Pasadena, CA

³North Carolina State University, Raleigh, NC

The search for the existence of a nonzero neutron electric dipole moment (EDM) has the potential to reveal new sources of T and CP violation beyond the Standard Model and may have a significant impact on our understanding of baryogenesis. This experiment presented a new way to measure the neutron EDM with unprecedented sensitivity. A fluid composed of polarized ultra-cold neutrons (UCN), polarized ^3He atoms and super-fluid ^4He at 300mK is formed and put in a small fixed uniform magnetic field. By applying a strong electric field parallel and anti-parallel to a weak magnetic field, the precession frequencies of the neutron are measured. The neutron EDM can then be determined by monitoring the difference of the neutron and ^3He spin precession frequencies. Highly spin-dependent nuclear reaction $n+^3\text{He}\rightarrow p+t+764\text{keV}$ is used to compare the ^3He and neutron precession frequencies. This nuclear reaction and the use of ^3He as a co-magnetometer both require that the ^3He polarization to have little or negligible loss during the measurement time period. The ^3He relaxation time under neutron EDM experimental surface conditions at low temperatures is being studied at Duke and preliminary results are obtained. A double-cell glass/acrylic system has been built and the Spin Exchange Optical Pumping (SEOP) process is performed in the oven at the temperature of 180 degrees Celsius with Rubidium as the spin-exchange medium. The whole system sits in a large area of uniform B-field created by a pair of large Helmholtz coils. Spin polarized ^3He can then be transferred from the optical pumping cell to a test cell either made of glass or acrylic cell embedded in a liquid ^4He bath inside a dewar. Temperatures as low as 1.8K can be reached by pumping the ^4He vapor. The system allows the test cell to be coated with ^4He and/or d-TPB wavelength shifting material. Preliminary results from both glass and acrylic test cells will be presented.

Nonlocal effects in High-K Superconductors: V_3Si

Mohana Yethiraj, D. K. Christen, ORNL

D. McK. Paul, University of Warwick

C. Dewhurst and R. Cubitt, ILL

Dimer gap vs. Haldane gap in S=1 chains

A. Zheludev, Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA.

L.-P. Regnault, CEA-Grenoble, DRFMC-SPSMS-MDN, Grenoble, France.

M. Hagiwara, KYOKUGEN, Osaka University, Japan

A comparison of inelastic neutron spectra measured for the S=1 quasi-1D bond-alternating antiferromagnet NTENP and the uniform-chain Haldane-gap compound NDMAP reveals key differences in the spin dynamics of these distinct types of quantum spin liquids. In modest applied fields the spectra of NDMAP [A. Zheludev et al., Phys. Rev. Lett. 88, 077206 (2002)] features three sharp gap excitations. In contrast, in NTENP the highest mode is anomalously weak already at H=0 and rapidly broadens and vanishes when the field is turned on. Above the critical field of 1D Bose condensation of magnons the spectral differences become even more pronounced. NDMAP retains a triplet of massive long-lived excitations [A. Zheludev et al., Phys. Rev. B 68, 134438 (2003)]. In NTENP only one sharp excitation branch is observed in this regime [Hagiwara et al., Phys. Rev. Lett. 94, 177202 (2005)], but there is new evidence of additional low-lying excitation continua. Work at ORNL was carried out under DOE Contract No. DE-AC05-00OR22725.

Magnetic Properties of Coupled Ni/Gd Bilayers

I. Zoto, Gary J. Mankey, A. M. Alsmadi, and S. G. E. te Velthuis