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RESEARCH

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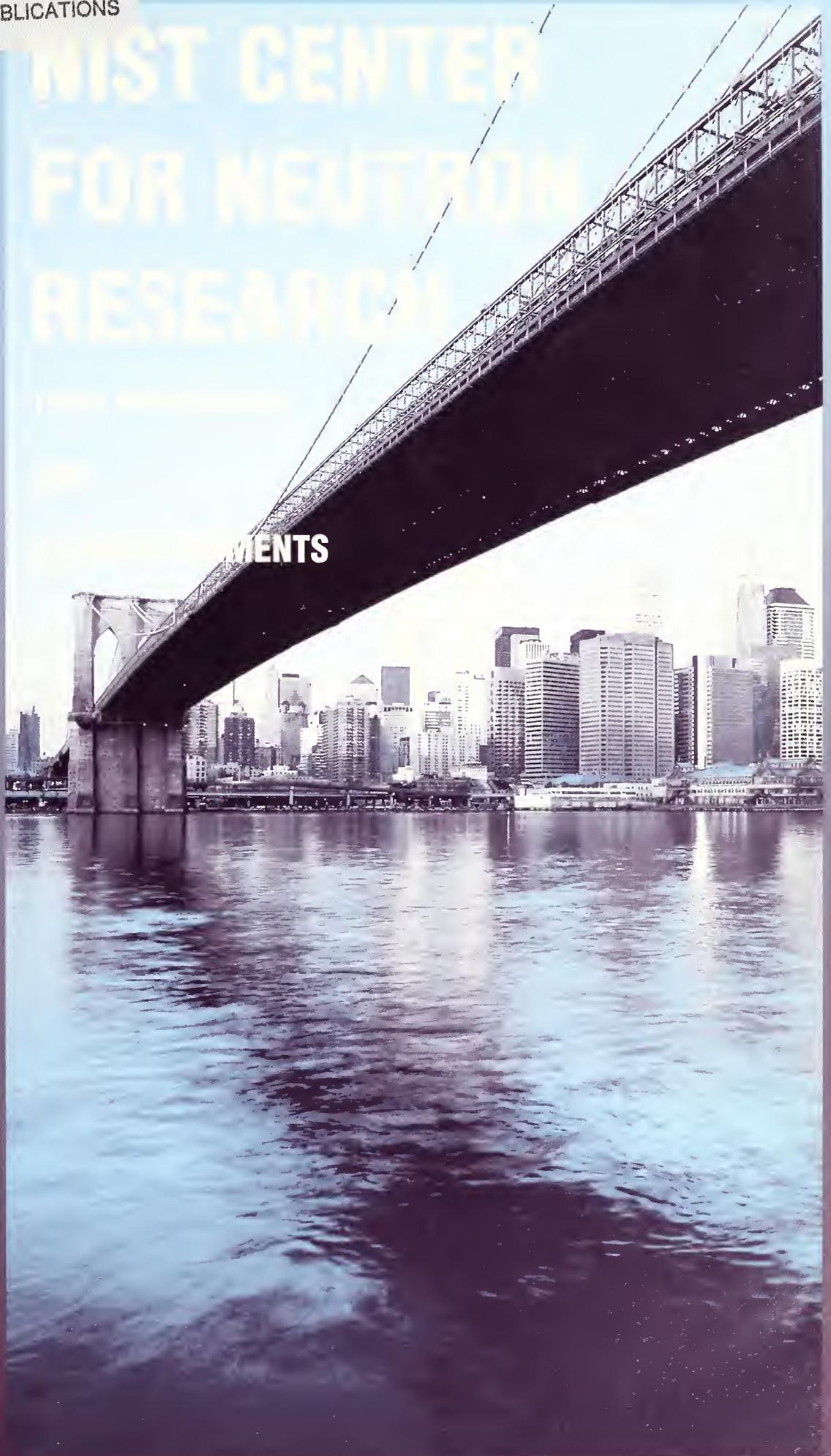
Unique Capabilities Provide Critical Data

The NIST Center for Neutron Research (NCNR) offers a bridge between the world of atoms, molecules and sub-microscopic structures and the macroscopic world of buildings, automobiles, efficient energy utilization, and the environment. Over 1500 researchers from 34 countries made use of the NCNR's world-class capabilities in the area of neutron-based research in 1998.

MATERIALS SCIENCE AND ENGINEERING LABORATORY

NIST CENTER FOR NEUTRON RESEARCH

1998 PROGRAMS

AND

ACCOMPLISHMENTS

J. Michael Rowe, Director

Tawfik M. Raby, Deputy

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Contents

Steve Kline (NCNR) helping Anne-Valerie Ruzette, MIT, to set up the pressure cell for a SANS experiment.

Joe Dura inspecting molecular beam epitaxy chamber.
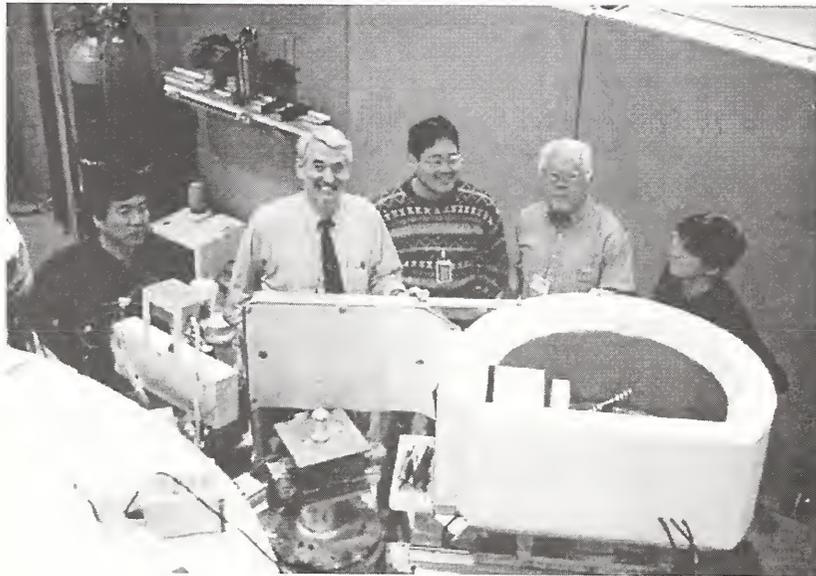
Kazu Yamada (Kyoto University), Bob Birgeneau (MIT), Suichi Wakimoto (Tohoku University), Gen Shirane (BNL), and Seung Hun Lee (NCNR) at the SPINS spectrometer.

Steve Kline and Paul Butler (NCNR) working with Lee Magid, University of Tennessee to set up a SANS experiment.
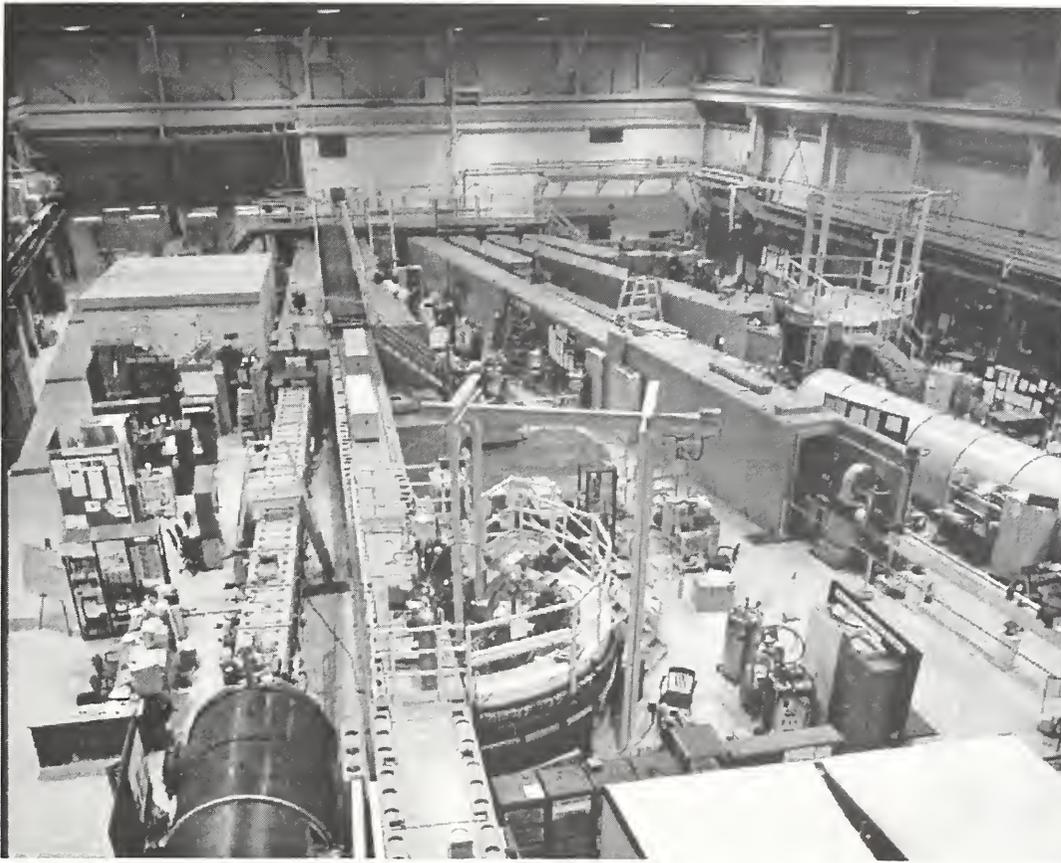
Guide hall at the NCNR, as of late 1997.

Heather Chen (NIST) aligning focusing capillary array.

Nobel Laureate Clifford Shull, inspecting NIST interferometer.

Foreword

This has been a productive and exciting year for the NIST Center for Neutron Research (NCNR), with many achievements in operation, instrumentation, and science. The reactor operated well through September, when an unscheduled shutdown was required to investigate a small leak in the vicinity of the thermal column. As a result of an excellent effort by the Reactor Operations and Engineering staff, this shutdown lasted no more than one complete cycle (14 % of availability). The reactor is now once again operating on our normal seven week schedule. We apologize to all those who were inconvenienced, and will work to make up as much of the time as possible. The next long scheduled shutdown, for replacement of shim control arms, is scheduled to begin in February, 2000 and will last 3-6 months.

During this year, commissioning of the high intensity back scattering spectrometer was begun, with very favorable results (see section later in this report), and the instrument should be available for user scheduling at the next program proposal period. Great progress was also made on the Spin Echo and Disc Chopper Spectrometers, with commissioning expected in the coming year. The reliability of operating instruments continues to be better than 95 %, with the average over all instruments being 98 %. The final engineering design of the second generation liquid hydrogen cold source is nearing completion, and fabrication and testing will begin in 1999. This source is calculated to provide approximately a factor of two gain over the present source.

This year we have changed the format of our report, and are featuring science highlights, chosen from the experiments done during the year. Thus, I will refrain from discussing science accomplishments here, except to say that productivity and quality remain exceptionally high. One of the great parts of my job is to be able to walk around the facility talking to experimenters, and I continue to be impressed by the breadth of the research and the enthusiasm of the researchers.

Finally, we continue to make good progress on preparing a request for a license renewal for the reactor for 20 years beyond 2004. Many different activities are underway towards this end, and we are fully confident that we will be successful. Neutron science as a whole is in a very exciting period, with the funding of the Spallation Neutron Source at Oak Ridge National Laboratory, and plans for new sources in several parts of the world. The NIST Center for Neutron Research is and will remain at the center of a renewed U.S. neutron research effort, working to provide the neutron measurement capabilities that are becoming ever more important.

Mike Rowe

Introduction to the NIST Center for Neutron Research (NCNR)

The modern technological society is dependent upon increasingly more sophisticated use of materials, many of whose properties are dictated by their sub-microscopic structural and dynamical properties. Our knowledge of these properties is provided by a wide range of scientific techniques, of which the many types of scattering (X-rays, light, electrons, neutrons, ...) are arguably the most important. Of these scattering probes, neutrons are perhaps least known, but they provide important advantages for many types of measurements.

Neutrons, as prepared for use at modern sources, are moving at speeds comparable to those of atoms moving at room temperature, thus providing the ability to probe dynamical behavior. At the same time, neutrons are well matched to measurements at length scales ranging from the distances between atoms to the size of biological or polymer macromolecules. Neutrons are sensitive to the magnetic properties of atoms and molecules, allowing study of the underlying magnetic properties of materials. They also scatter quite differently from normal hydrogen atoms than they do from heavy hydrogen (deuterium), allowing selective study of individual regions of molecular systems. Finally, neutrons interact only weakly with materials, providing the opportunity to study samples in different environments more easily (high pressures, in shear, in reaction vessels, etc.), and making them a non-destructive probe. These favorable properties are offset by the relative weakness of the best neutron sources, when compared to X-ray or electron sources, and by the relatively large facilities required to produce neutrons. As a result, neutron sources are operated as national user facilities, to which researchers come from all over the U.S. (and abroad), to perform small scale science using the special measurement capabilities provided.

In addition to scattering measurements, neutrons can be used to probe the atomic composition of materials, by means of capture and resultant radioactive decay. The characteristics of the decay act as "fingerprints" for particular atomic nuclei, allowing studies of environmental samples for pollutants (e.g. heavy metals), characterization of Standard Reference Materials, and many other essential measurements. While the scattering and capture users of neutrons are little concerned with the innate nature of neutrons, there are important areas in physics that can be well studied by observing the behavior of the neutron. Examples include the lifetime of the free neutron, an important ele-ment in the theory of astrophysics; the beta decay process of the neutron, the details of which are stringent tests of nuclear theory; and the effects of various external influences such as gravity or magnetic fields on neutrons.

The NCNR utilizes neutrons produced by the 20 MW NIST Research Reactor to provide facilities for all of the above types of measurements to a national user community. There are approximately 35 positions in the reactor and its associated beams which can provide neutrons for experiments. At the present time, there are 26 stations in active use, of which 6 provide high neutron flux positions in the reactor for irradiations, and 20 are beam facilities. A schematic layout of the beam facilities and brief descriptions of available instrumentation are given below. More complete descriptions can be found at http://rrdjazz.nist.gov.

These facilities are operated both to serve NIST mission needs and as a national user facility, with many different modes of access. Some of the instrumentation was built several years ago, and is not suited to general user access; however, user time is available for collaborative research. In some cases, NIST built new instrumentation, and reserves 1/3 of available time for mission needs, with the balance available to general users. In other cases, instrumentation was built and is operated by Participating Research Teams (PRT); in such cases, the PRT members have access to 75 % of available time, with the balance available to general users. In a special case, NIST and the National Science Foundation established the Center for High Resolution Neutron Scattering at the NCNR, with a 30-m Small Angle Scattering (SANS) instrument, a cold neutron triple axis spectrometer, annd a perfect crystal SANS under construction. For these facilities, most time is available for general users. While most access is for work which is freely available to the general public, proprietary research can be performed under full cost recovery. Each year, 1400 research participants (persons who participated in experiments at the facility, but did not necessarily come here) from all areas of the country, from industry, academe, and government use the facility to perform measurements not otherwise possible. The research covers a broad spectrum of disciplines, including chemistry, physics, biology, materials science, and engineering.

NG-3 30 m SANS

Disc Chopper Spectrometer

Neutron Physics Station

Fermi Chopper TOF Spectrometer

NG-7 30 m SANS

Back Scattering Spectrometer

Spin Echo Spectrometer

8 m SANS, Operated by Polymers Division

Prompt Gamma Activation Analysis

SPINS Spectrometer

Neutron Interferometry and Optics Station

Vertical Sample Reflectometer

Horizontal Sample reflectometer

BT-8 Residual Stress Diffractometer

Cold Neutron Depth Profiling

BT-9 Triple Axis Spectrometer

BT-4 Filter Analyzer Spectrometer

Thermal Column

BT-1 Powder Diffractometer

BT-2 Triple Axis Spectrometer

6

Horizontal Sample Reflectometer

Horizontal surface of sample allows reflectivity measurements of free surfaces, liquid vapor interfaces, as well as polymer coatings.

Neutron Interferometry & Optics Station

Includes perfect silicon interferometer; vibration isolation system provides exceptional phase stability and fringe visibility.

Prompt Gamma Activation Analysis

Cold neutron fluxes allow detection limit for H of 1-10 microgram. Focused beams available for profiling.

NG-7 30m SANS

Small Angle Neutron Scattering instrument for microstructure measurement sponsored by NIST, the Exxon Research and Engineering Co., the University of Minnesota, and Texaco R&D.

Neutron Physics Station

A cold neutron beam 150 x 60 mm^2, available for fundamental neutron physics experiments.

Fermi Chopper TOF Spectrometer

A hybrid time-of-flight spectrometer for inelastic scattering, with wavelengths between 0.23 and 0.61 nm. The wavelength is chosen by focusing pyrolytic graphite crystal, while the beam is pulsed by a simple Fermi chopper.

Spin Echo Spectrometer

A neutron spin echo spectrometer offering neV energy resolution, based upon Julich design, sponsored by NIST, Julich and Exxon.

SPINS Spectrometer

Spin Polarized Inelastic Scattering, a cold neutron triple axis spectrometer with spin polarization capabilities for high resolution studies, and position sensitive detector capability, sponsored by the National Science Foundation and NIST; part of Center for High Resolution Neutron Scattering (CHRNS).

Disc Chopper TOF Spectrometer

Versatile time-of-flight spectrometer, with beam pulsing and monochromatization effected by 7 disk choppers. Used for studies of dynamics in condensed matter, including macromolecular syatems.

NG-3 30m SANS

Instrument for microstructure measurement sponsored by the National Science Foundation and NIST; part of CHRNS.

Back Scattering Spectrometer

High intensity, very high resolution back scattering spectrometer, with many innovative features, and energy resolution of approximately 1 μeV.

8M SANS

Instrument for polymer characterization, sponsored by Polymers Division.

Vertical Sample Reflectometer

Instrument for measuring subsurface structure with polarization analysis capability. Capable of measuring reflectivities down to 10^{-8}.

BT-8 Residual Stress Diffractometer

Diffractometer optimized for depth profiling of residual stress in large components.

BT-9 Triple Axis Spectrometer

Triple axis crystal spectrometer for measurements of excitations and structure.

BT-1 Powder Diffractometer

Powder diffractometer with 32 detectors; incident wavelengths of 0.208, 0.154, and 0.159 nm, with highest resolution of $\delta d/d = 8 \times 10^{-4}$.

BT-2 Triple Axis Spectrometer

Triple axis crystal spectrometer with polarized beam capability for measurement of magnetic dynamics and structure.

BT-4 Filter Spectrometer

A triple axis crystal spectrometer with a Be or Be/Graphite filter analyzer option for chemical spectroscopy.

Cold Neutron Depth Profiling

A station for quantitative profiling of subsurface impurities and coatings, based on neutron capture and emission of a charged particle.

Thermal Column

A very well-thermalized beam of neutrons used for radiography, tomography, dosimetry, and other experiments.

Solids that Shrink when Heated

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Thermal expansion is the reason that cracks between railroad tracks are largest in the winter and that the Sears tower grows by 15 cm in the summer. The reason that solids generally expand when heated is that atoms move apart to make room for each other when the amplitude of their thermal motion increases. There are however exceptions to this rule; i.e. solids that *contract* when heated. Such materials can be of great technological significance because they allow engineers to create composites that retain their dimensions irrespective of temperature. One example of a solid that contracts as temperature increases is ZrW_2O_8. Discovered by Martinek and Hummel in 1968[1] this cubic material shrinks by 9 ppm/K from cryogenic temperatures until its decomposition temperature of 1050°C (see Fig. 1). Because the material is a transparent dielectric Lucent Technologies is using ZrW_2O_8 to compensate for thermal expansion of standard dielectrics in fiber optic gratings that must maintain their optical dimensions over a large range of temperatures. Before ZrW_2O_8 arrives at a telephone exchange near you we wanted to understand its unusual behavior through a series of neutron scattering experiments[2].

Figure 1 shows the reduction of the lattice
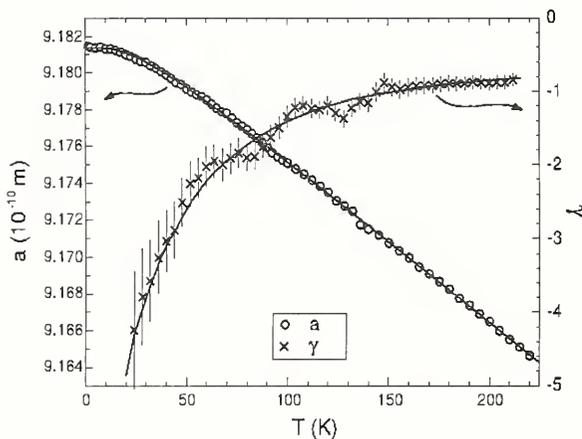
Figure 1. Temperature dependence of the cubic lattice parameter, a, and Grüneisen parameter γ(T) for ZrW_2O_8. Solid lines are based on a model described in the text.

parameter of ZrW_2O_8 with increasing temperature as measured with cold neutron diffraction on SPINS. The

Grüneisen theory of thermal expansion relates the thermal expansion coefficient $\alpha = d \ln a / dT$, to the specific heat as follows:

$$\alpha = \frac{1}{3B} \sum_i \gamma_i c_i \qquad (1)$$

The summation is over normal modes, $B = -dP/d \ln V$ is the bulk modulus ($B = 4.8 \times 10^{10}$ Nm^{-2} for ZrW_2O_8), c_i is the specific heat of a single mode, and $\gamma_i = -(\partial \ln \omega_i / \partial \ln V)$ is the Grüneisen parameter which modulates the contribution of each mode to thermal expansion. The overall Grüneisen parameter is defined as $\gamma(T) = 3B\alpha / C$ where $C = \sum_i c_i$ is the total specific heat. Clearly γ(T) is temperature independent if all modes of vibration contribute equally to thermal expansion (or contraction). Fig. 1 shows γ(T) for ZrW_2O_8, which we determined by dividing the thermal contraction data in Fig. 1 with specific heat data[3]. γ(T) is of course negative at all T and its absolute value increases down to the lowest temperature probed. This indicates that low energy modes drive thermal contraction in ZrW_2O_8.

To quantify this statement we measured the phonon density of states (DOS) using inelastic neutron scattering and the result is shown in Fig. 2. The high energy modes correspond to librations of oxygen atoms. The top of the band at 140 meV lies higher than in Al_2O_3 by approximately 30 meV and this reflects the strong covalent bonding of oxygen in WO_4 tetrahedra and ZrO_6 octahedra (See inset to Fig. 2).

The low energy part of the spectrum is shown in Fig. 3. A large density of states remains down to 2.5 meV with a pronounced peak at 4 meV, which reveals low energy optical modes. Subsequent single crystal inelastic experiments have also identified several nearly dispersion-less modes around this energy.

To determine whether this DOS Peak could be important for thermal contraction we make the assumption that $\gamma(\hbar\omega) = \gamma_0 < 0$ for $E_0 < \hbar\omega < E_1$ and zero elsewhere as shown in the inset to Fig. 3. With $\gamma_0 = -14(2)$, $E_0 = 1.5(4)$ meV, and
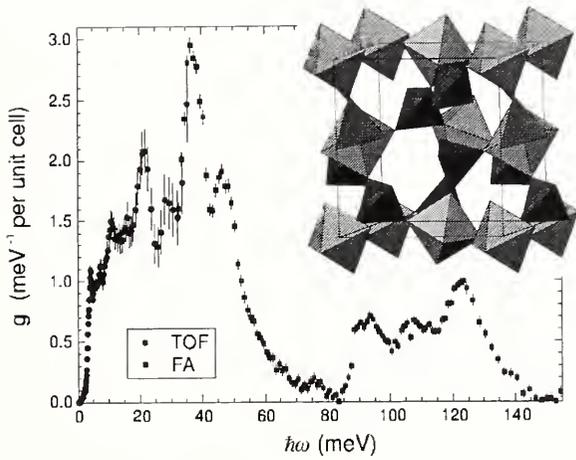
Figure 2. Density of states for ZrW_2O_8 at T=300 K measured using inelastic neutron scattering. For $0 < |\hbar\omega| < 40$ meV we used the TOF spectrometer with E_i=5 meV. For $\hbar\omega > 40$ meV we used BT4 with a polycrystalline Be filter analyser. Inset shows the structure with WO_4 tetrahedra in red and ZrO_6 octahedra in blue.

$E_1 = 9.5(2)$ meV and using the measured DOS, we obtain excellent fits to the data in Fig. 1 (solid lines). While the model is certainly not unique it establishes a range of energies for vibrations contributing to thermal contraction in ZrW_2O_8.
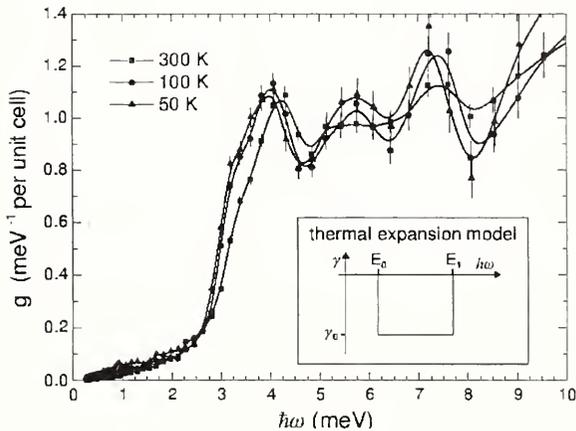
Figure 3. Low energy part of the phonon spectrum for ZrW_2O_8 and its temperature dependence. Inset shows our model for the energy dependence of the Grüneisen parameter.

An interesting aspect of these low energy modes is their temperature dependence shown in Fig. 3. There is a decrease in the frequency of the 4 meV optic mode as the temperature decreases and the unit cell volume increases. Naively this would appear to be in contradiction with a negative Grüneisen parameter because

$$\left(\partial\omega/\partial T\right)_P = -3\omega\gamma\alpha$$ must be negative. But for an anharmonic vibration the mode frequency also depends on the amplitude and we propose that this non-linear effect which is not taken into account in the Grüneisen theory is responsible for the softening of the 4 meV optical mode.

What remains is to identify the microscopic nature of these modes. Single crystal phonon data will be required to accomplish this in earnest. Nonetheless inspection of the structure shown in Fig. 2 does provide important clues. ZrW_2O_8 consists of corner-sharing WO_4 tetrahedra and ZrO_6 octahedra. The unusual low energy optic modes are likely to correspond to twisting of these units with respect to one another and this twisting leads to contraction just as a vibrating guitar string tugs on its supports. What makes ZrW_2O_8 special is the unusually low energy of these twist modes which allows them to become highly excited and pull the structure together at temperatures far below those required to excite bond-stretching modes.

References
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Spin Correlations and Impurities in a One-Dimensional Quantum Spin Liquid

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Though all solids contain electrons with spin-induced magnetic moments few materials will actually cling to your refrigerator door. The quantum theory of atoms explains that matter is generally non-magnetic because electron spins form non-magnetic (singlet-) states in the filled electronic shells of individual atoms. Here we discuss a new class of materials wherein singlet formation takes place *between* rather than *within* atoms to yield a macroscopic spin-less "molecule". We explore the magnetism of Y_2BaNiO_5, in which magnetic Ni^{2+} atoms interact antiferromagnetically (AFM) through intervening O^{2-} atoms to form spin chains.

Inelastic magnetic neutron scattering is a powerful probe of spin chains. The open circles in Fig. 1 show the low temperature equal time spin correlation function versus wave-vector transfer along the chain. In contrast to Néel AFM's that develop Bragg peaks when long range order develops at a second order phase transition, Y_2BaNiO_5 has no magnetic phase transition and our snap-shot of the spin configuration reveals short-range AFM order with a dynamic correlation length $\xi=4.3(6)$. Still this is not a thermally disordered paramagnet. The solid symbols in Fig. 1 show that at *fixed* energy transfer there are sharp peaks in the wave-vector dependence of the dynamic correlation function that allows us to put a lower limit of 50 lattice spacings on the coherence length for magnetic excitations.

Fig. 2 (a) shows another important feature of
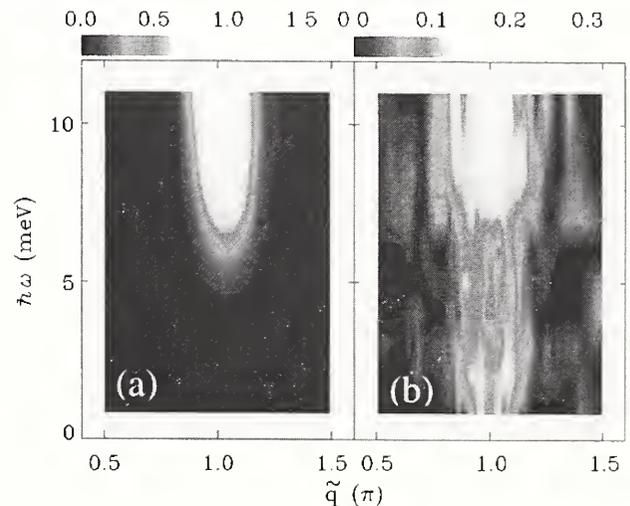
Figure 2. Contour map of low energy magnetic neutron scattering at T=10 K from (a) pure Y_2BaNiO_5 and (b) $Y_{1.905}Ca_{0.095}BaNiO_5$. The MARI spectrometer at the ISIS facility in the UK was used for (a) while BT2 and SPINS at the NIST were used for (b).

Figure 1. Neutron scattering from Y_2BaNiO_5 at T=10 K. Open symbols show energy-integrated data probing equal-time correlations. Solid symbols show a constant-$\hbar\omega$ scan at the gap energy.

the AFM spin-1 chain: There is a gap in the excitation spectrum separating the ground state from excited states. The energy gap is the cost of creating a magnetic wave packet on the spin chain.

There are interesting effects of substituting Ca^{2+} for Y^{3+}. The extra hole occupies the π-orbital on the super-exchange mediating oxygen site and leads to a ferromagnetic (FM) impurity bond in the otherwise AFM spin chain. Fig. 2 (b) shows that such doping yields new sub-gap excitations. The extra magnetic scattering takes the form of a double ridge versus energy, which indicates that we are dealing with slow fluctuations of a rigid composite object. The wave-vector dependence provides valuable but ambiguous information about the real space structure of this object. A natural first interpretation would be that the holes have ordered to yield a new incommensurate periodicity. To explore this possibility Fig. 3 shows a comparison of high statistics -integrated data for samples with Ca concentrations differing by almost 50 %. The absence of a significant shift in the peak positions rules out hole ordering.

We propose instead that the double peak in Fig. 3 is the magnetic form factor of a hole in a quantum spin liquid. Consider first the dilute and static hole
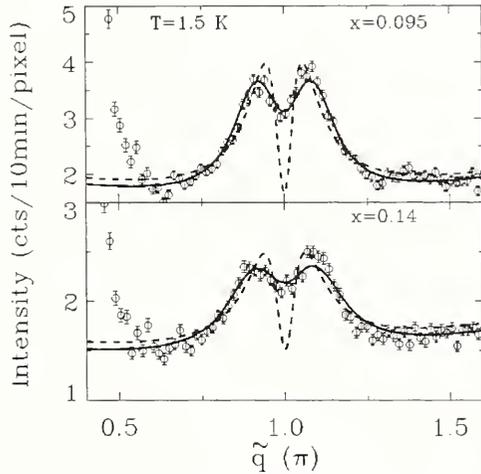
Figure 3. Q-dependence of energy integrated intensity from $Y_{2-x}Ca_xBaNiO_5$ with x=0.095(5) and x=0.14(1). The dashed line is a single impurity model. The solid line is a random impurity model.

limit of a single FM impurity bond on the spin chain. The energy of the macroscopic spin singlet has increased and a degenerate magnetizable state is now the ground state. If we assume that the spin disturbance associated with the impurity bond decays away from the impurity then we can show that the corresponding form-factor has the general features observed in the scattering data. Denote by M(q) the form factor for the spin density which develops to the right of an impurity bond.

The corresponding form-factor for the disturbance to the left of the impurity is the complex conjugate, $M^*(q)$. The form factor for the combined object becomes $F(q)=M(q)e^{iq/2}M^*(q)e^{-iq/2}$. When the chain end spin degrees of freedom are antiferromagnetically combined, corresponding to the negative sign in this equation, $|F(q)|^2$ becomes the conventional structure factor for the quantum spin liquid in Fig. 1. However when the chain ends are stitched together ferromagnetically as we should expect for FM impurity bonds we have $F_\pm(q)=2Re\{M(q)e^{iq/2}\}$. This function vanishes for $q=(2n+1)\pi$ because M(q) is real for $q=n\pi$ and the result is a notch at $q=n\pi$ as shown by the dashed lines in Fig. 3. To account for the finite intensity between the peaks we need to consider the finite density of impurity bonds. Neighboring holes arranged at random break inversion symmetry about individual holes and this brings back intensity at $q=\pi$. The solid lines in Fig. 3 correspond to an analytical expression for the scattering from a distribution of uncorrelated asymmetric impurities with exponentially decaying spin densities. The fact that the impurity scattering is distributed over a range of energies in Fig. 2 (b) indicates that the holes are moving or more likely that neighboring bound states interact.

The significance of all this is that we have directly measured the spin wave function associated with a bond reversing hole impurity in a quantum spin liquid. Because our raw data are so similar to the scattering data from doped copper oxide superconductors our results suggest that hole form-factor effects may also be important for interpreting those data.

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Deposition of Toxic Trace Elements and Heavy Metals to Lake Michigan by Size and by Source

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Atmospheric deposition by wet and dry processes is known to be an important source of several anthropogenic, particulate-bound metals in critically important waters such as the north Atlantic Ocean, the coastal mid-Atlantic waters, and the Great Lakes. Lake Michigan is especially subject to deposition of anthropogenic air pollutants as it lies in close proximity to the heavily polluted urban and industrial areas stretching from Chicago to Gary, Indiana, i.e., an area containing 20% of the US steel production.

The University of Maryland (at College Park, UMCP) aerosol chemistry group has used the NBSR reactor for instrumental neutron activation analysis to characterize atmospheric aerosol particles and gases for more than 20 years. Detailed and accurate multielement analyses are routinely achieved, nondestructively, for up to 40 elements in samples collected for periods of several hours to a few days on various types of filters and in cascade impactors which size fractionate the aerosol into as many as 10 size domains. As many as 30 elements can be determined in as little as 100 μg of a size-segregated particulate fraction, allowing the application of receptor modeling techniques to determine the sources of size segregated aerosol particles. This is extremely important in assessing dry deposition of aerosol particles and their constituents because deposition velocity is highly sensitive to particle diameter (see Figure 1). Some of the elements measured, e.g., As, Cd, and Hg, are highly toxic and are, therefore, of epidemiological interest, especially in the Chesapeake Bay, Lake Michigan, and Coastal Marine environments. Equally important is that information on elemental constituents remains a powerful, fundamental tool with which atmospheric sources, transport, and processes may be elucidated.

As a part of EPA's Great Water's project, Atmospheric Exchange Over Lakes and Oceans (AEOLOS), size segregated aerosol particulate samples were collected, simultaneously, with 10-stage cascade impactors sited in south Chicago, aboard ship at sites 20 km east of Chicago, and on the Eastern shore, about 90 km down wind (Figure 2). Sampling campaigns were conducted in spring, summer, and winter periods to observe seasonal differences in the concentrations and size distributions of inorganic elemental constituents. Several hundred size-segregated fractions were collected and analyzed by X-ray fluorescence (XRF)
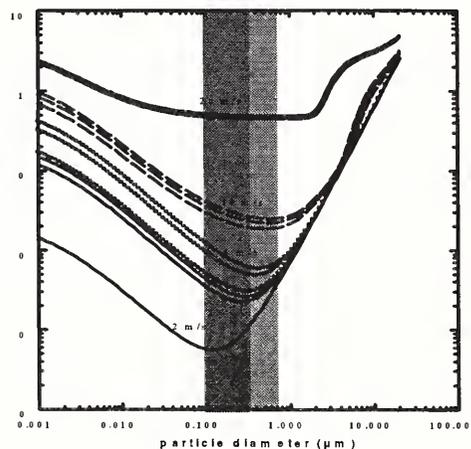
Figure1. Deposition velocity vs. aerodynamic particle diameter.

and Instrumental Neutron Activation Analysis (INAA).

A great deal of useful information about the sources of aerosol particles can be obtained from size spectra of constituent "marker" elements. In Figure 3, V, a marker of particles emitted from fuel oil combustion, is bimodal. Vanadium on
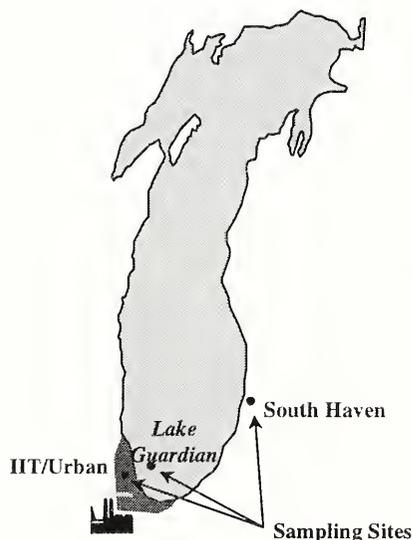
Figure2. Location of sampling sites
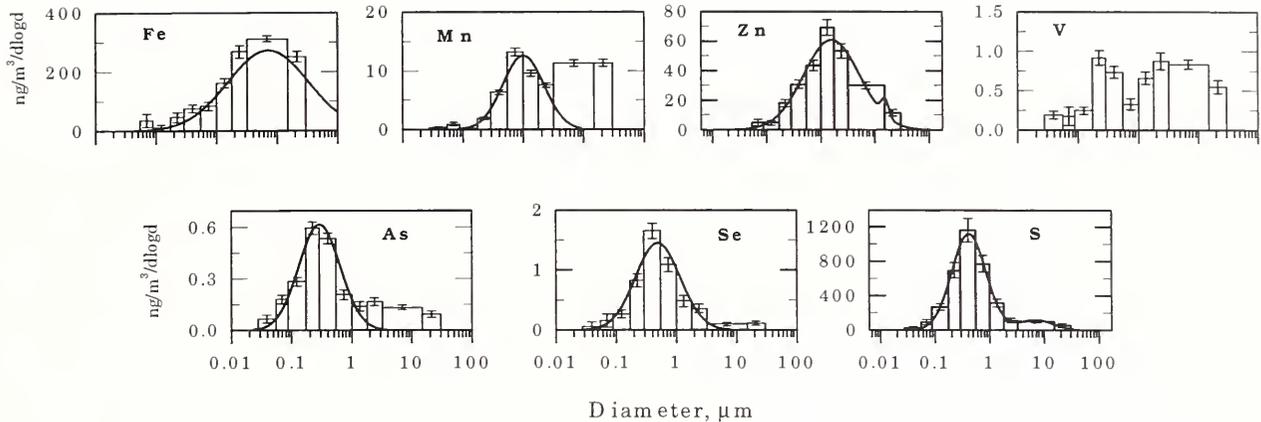
Figure 3. Concentration vs aerodynamic particle size distributions for several important "marker" elements determined from samples collected on Lake Michigan.

large (coarse) particles (i.e., those >1 μm) is associated with urban and rural dust particles. Vanadium on submic-rometer (i.e., "fine") particles was emitted from oil-fired power plants. Likewise, selenium is a marker of coal combustion particles; Zn, incineration; and As, steel mill emissions. Iron- and Mn-containing particles were also emitted from steel mills, but have substantial large particle components from this source. Manganese clearly has both a fine and coarse particle component.

Often, the size distributions of particles emitted from different sources overlap, and must be resolved by, for example, a chemical mass balance (CMB) method. The CMB involves solving a system of equations, constructed to explain the concentration of an elemental aerosol constituent at a sampling (receptor) site as a linear sum of the concentrations of elements from N number of sources for which the composition of particulate emissions is well character-ized. Results for As and Zn are shown in Figure 4. This is the first successful resolution of the contributions of toxic constituents of aerosol particles by size and source. These data, and much more like it, have been used to provide the policy makers with far more accurate estimates of the deposition fluxes of toxic substances to Lake Michigan. Similar analyses are being performed by our group for the Chesapeake Bay.

Figure 4. Distributions of As (upper) and Zn (lower) in particles sampled over Lake Michigan, by size and source.

References
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Magnetic Domains in Co-SiO$_2$ Multilayer Tunnel Junctions

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In the ongoing search for sensors for magnetic recording applications, recent research has focussed on materials that exhibit spin-dependent tunneling. These systems are comprised of metallic, ferromagnetic particles or of layers that are well separated from each other by an insulating material. Magnetoresistance (MR) from spin-dependent tunneling was first reported for granular metal/insulator films in 1972 and for Co/Ge/Fe trilayer junctions in 1975. The effect arises because the tunnel conductance is minimum when the particle or layer moments are aligned antiparallel.

From a magnetic recording perspective, the objective is to maximize the change in the resistance while minimizing the active field range. Multilayer tunnel junctions exhibit pronounced field sensitivity, but the insulating barrier layers are susceptible to pinholes that connect the ferromagnetic layers. In contrast, granular films with small ferromagnetic particles are easy to fabricate by co-deposition of a metal with an immiscible insulator. However, the saturation fields for the MR are large and the approach to saturation is gradual because the particles are magnetically isolated.

Desirable characteristics of both magnetic tunnel junctions and the granular films are combined in discontinuous metal/insulator multilayers, which represent a new class of spin tunneling devices. These hybrid systems are prepared by alternately sputtering two immiscible materials, such as Co and SiO$_2$, onto a substrate. Since the metal does not wet the insulator, the ferromagnet breaks up into nanoparticles during growth. Transmission electron microscope images and x-ray diffraction data of Co/SiO$_2$ multilayers reveal that the Co forms either individual particles with diameters of 2.5 nm or chains composed of touching particles. In contrast to granular films, the MR of these hybrid structures is maximum at a smaller magnetic field, which is useful for applications. However, the dependence of the MR on small magnetic fields is not consistent with a simple picture of the magnetic moments of individual particles changing independently. Instead it is believed that the smaller particles are magnetically coupled to form larger magnetic domains. Neutron scattering experiments characterize the magnetic structure (i.e., the magnetic correlation length) associated with the MR maximum. This correlation length is required to model the MR mechanism.

Initial neutron reflectivity studies of a [SiO$_2$(3.0 nm)|Co(2.0 nm)]$_{24.5}$ multilayer with the sharpest MR showed that the Co spins are randomly oriented along the growth direction at fields near the coercive field, H$_C$, where the magnetic hysteresis loop crosses the field axis (i.e., zero net moment). However, the average size of the magnetic domains across the sample plane is substantially larger (1 – 5 μm) than the average size of the Co particles. A multilayer with a smaller nominal Co thickness, [SiO$_2$(3.0 nm)|Co(1.6 nm)]$_{60.5}$, showed no in-plane magnetic ordering within the sensitivity of the reflectivity experiments. Small angle neutron scattering (SANS) measurements of this multilayer and a 0.5 μm thick Co(0.4)/SiO$_2$(0.6) granular
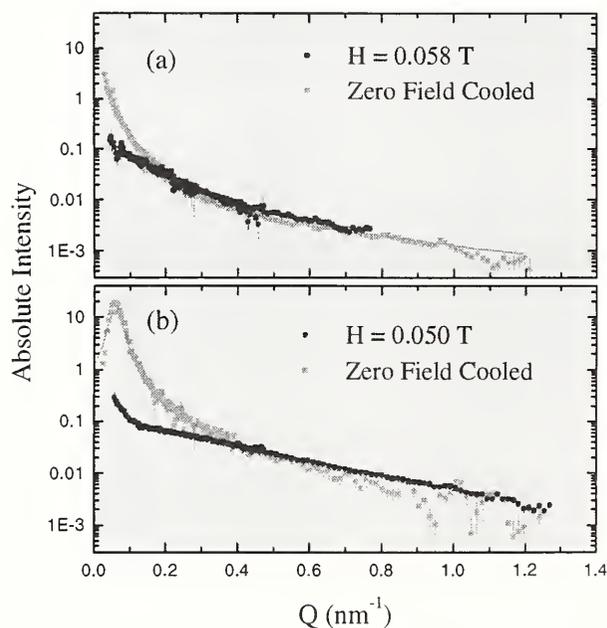
Figure 1. Circular average of SANS data for [SiO$_2$(3.0 nm)|Co(1.6 nm)]$_{60.5}$ multilayer (a) and Co(0.4)/SiO$_2$(0.6) granular film (b) at 15 K. The ZFC data for the film is a sector average at 45°. Data fits are shown as lines.

film were thus undertaken to probe smaller lengthscales. These experiments indicate that the correlation lengths at H_C are larger for the discontinuous multilayer than for the granular film. In addition, data obtained for both samples after cooling in zero field (ZFC) indicate that the Co particles have an intrinsic magnetic interaction.

With the exception of the ZFC data for the granular film (Fig. 2), all of the data were circularly symmetric and could be averaged about the center of the detector. Figure 1 (a) shows the average magnetic intensity at 15 K plotted as a function of the wavevector Q for the discontinuous multilayer at $H_C = 0.058$ T (purple circles) after saturation in a 0.5 T field. The Lorentzian fit to these data gives a magnetic correlation length of 10 ± 2 nm, which is of the order of the size of the Co nanoparticle chains.
For comparison, the coercive field data (purple circles) for the granular film are shown in Fig. 1 (b). These data fit to a linear combination of two squared Lorentzians, which is a functional form often found for scattering from disordered magnets. The dominant term gives a short correlation length of approximately 1.7 ± 0.5 nm, which is *smaller* than the 4 nm spherical particle size in the granular film. For both the granular film and the discontinuous multilayer, the static and/or dynamic magnetic domains at the coercive field appear to be limited to the individual Co particles. The dramatic contrast in the MR curves for the discontinuous multilayer and the granular film could be a consequence of the difference in the electron-scattering surface area (i.e., the granular film has smaller particles and domains and thus has more scattering surfaces).

The demagnetization process for both the film and the multilayer, however, is very sensitive to field preparation conditions. Figure 1 (a) also shows the average magnetic intensity of the discontinuous multilayer at 15 K after cooling in zero field from room temperature (green squares). These data yield a correlation length of 30 ± 1.5 nm. The act of cooling the multilayer apparently induces interparticle interactions that stabilize domains larger than a single Co nanoparticle.

Figure 2 shows the scattering pattern for the granular film after cooling to 15 K in zero field from room temperature. The intensity is asymmetric with maximum intensity along the vertical axis. These data suggest that the Co moments are preferentially aligned along the horizontal axis. However, this spin anisotropy axis is not evident from magnetization and resistivity data.

The sector average in Fig. 1 (b) further reveals that the ZFC data have a sharp peak at $Q = 0.0605$ nm^{-1}. The data fits suggest that the ZFC structure for the granular
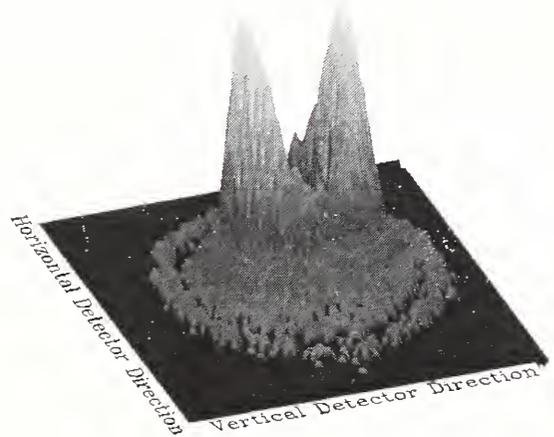
Figure 2. SANS image from a Co(0.4)/SiO$_x$(0.6) granular film after cooling from room temperature to 15 K in zero field.

film is comprised of magnetic domains separated by an average distance of 104 ± 1 nm in the film plane. Despite their small size, the Co particles interact with each other upon cooling in zero field to form a well-ordered magnetic state.

The observed difference between the magnetic domain formation in discontinuous spin-tunneling multilayers and granular films is essential to the understanding of their contrasting MR properties. Future studies will focus on the temperature and field evolution of the domains to optimize their performance as magnetic sensors.

Mechanism of Thermal Barrier Coating Failure at High Temperature

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Ceramic thermal barrier coatings (TBCs) are used in gas turbine engines and other combustion components to allow operation at increased temperatures, which increases efficiency, reduces cooling requirements, and extends component life. They are currently used in aircraft engines and are expected to be adopted for energy-generating gas turbines and diesel engines in the near future. It has been estimated that for the US power generation sector alone, a one percent increase in efficiency would lead to a savings of $140M per year.

The most common industrial TBC is yttria stabilized zirconia (YSZ), which consists of zirconia, ZrO_2 with about 8 wt % yttria, Y_2O_3 (equivalent to 8.7 mol % $YO_{1.5}$). Many factors contribute to the stability of YSZ coatings, including particle size and homogeniety of feedstock powders, coating deposition techniques, and metallic bond coat characteristics. We have been investigating the inherent stability of the crystallographic phases present in plasma-sprayed YSZ using neutron Rietveld refinement for quantitative phase analysis.

YSZ consists of three crystallographic phases: monoclinic, tetragonal, and cubic. According to the phase diagram, the tetragonal phase is predominant at about 8 wt % yttria. However, plasma spraying is a rapid solidification process that results in metastable phase mixtures of the monoclinic phase (0–6 wt % yttria), tetragonal phase (4–13 wt % yttria), and cubic phase (11–20 wt % yttria). It is thought that the coexistence of the tetragonal and cubic phases toughens the TBC through inhibition of crack propagation; however a presence of 5% or greater of the monoclinic phase results in coating instability because the monoclinic phase transforms to the tetragonal phase upon heating. Since this transformation is accompanied by a large volume change, thermal cycling generates stresses in the coatings leading to premature failure.

In order to simulate high-temperature operating conditions, we annealed plasma-sprayed YSZ coatings for periods of one to 100 hours at temperatures of 1000, 1200, and 1400 °C. These coatings were prepared from two feedstock powders with differing characteristics: feedstock **1** was prepared by a spheroidization process and feedstock **2** by fusing and crushing. High-resolution neutron powder diffraction patterns were obtained on the NCNR 32-detector powder diffractometer at BT-1 and the data were analyzed using the Rietveld refinement technique. Results of the phase analysis of the feedstock powders, as-sprayed coatings, and annealed coatings are given in Fig. 1.
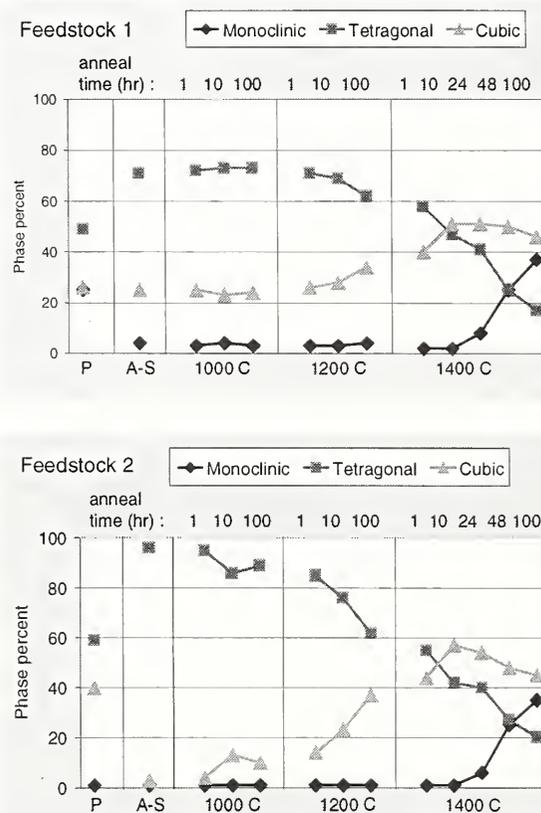
Figure 1. Change in phase composition of YSZ coatings upon annealing. P = starting feedstock powder; A-S is the as-sprayed coating.

The two feedstock powders, **1** and **2**, have quite different initial phase compositions: **1** has about 25 % of the monoclinic phase, whereas **2** has virtually none. The plasma-sprayed coatings are initially different as well, with coating **1** having 25 % cubic phase content

and coating **2** being almost totally tetragonal. The phase content of both coatings changes gradually with annealing for longer times or at higher temperature (see Fig. 1), showing a general increase in the cubic phase content and decrease in the tetragonal phase content. However, with longer annealing times at 1400 °C a significant increase in the monoclinic phase content is seen; both **1** and **2** have nearly identical phase compositions after annealing for 24, 48, and 100 hours and sufficient monoclinic phase is present to cause coating failure.

While the general phase behavior upon annealing has been known for some time from x-ray studies, the use of the neutron Rietveld technique permits us to extract more information based upon the unit cell parameters of the tetragonal and cubic phases. It is known that the lattice parameter a of the cubic phase increases linearly with yttria content, and that the c/a ratio for the tetragonal phase decreases with increasing yttria content. Earlier studies, however, either underestimated the cubic phase content or assumed equal yttria content for the tetragonal and cubic phases. We were able to use the unit cell parameters obtained from the neutron data to extract the distribution of yttria in these phases assuming that the total yttria content is constant. Results are given in Table 1. Note that the nominal composition for both samples is 8.7 mol % $YO_{1.5}$ but that sample **2** appears to be low in total yttria content.

The data given in Table 1 give an indication as to why the phase changes on annealing occur. It can be seen that even at the lower annealing temperatures the yttria is leaving the tetragonal phase and entering the cubic phase, resulting in higher yttria content of the cubic phase (coating **2**) and increased cubic phase fraction (coatings **1** and **2**). As the samples are annealed for longer periods at higher temperatures, the yttria content of the tetragonal phase drops below 3-4 mol % $YO_{1.5}$, and destructive transformation to the monoclinic phase occurs.

These results indicate that there is an inherent limit to the temperature and time of YSZ component operation. While technological improvements to YSZ coatings are possible, new materials will be needed to achieve significantly higher operating temperatures.

Table 1. Yttria content of tetragonal (T) and cubic (C) phases given in mol % $YO_{1.5}$; estimated accuracy is ± 0.2 mol % for the tetragonal phase in the annealed coatings and ±1 mol % for all other values. Yttria content of the monoclinic phase is assumed to be 3 mol % for the calculation of total yttria content.

Sample	Feedstock 1			Feedstock 2		
	T	C	total	T	C	total
Powder	7	14	8	6	7	6
As sprayed	8	15	9	8	--	8
1000 C/ 1h	6.6	14	9	7.4	--	7
10h	6.4	15	8	7.1	3	7
100h	6.2	15	8	6.9	4	7
1200 C/ 1h	6.2	15	9	7.1	5	7
10h	5.8	16	9	6.8	7	7
100h	5.0	17	9	5.3	11	7
1400 C/ 1h	5.2	14	9	5.7	8	7
10h	4.2	14	9	4.0	9	7
24h	3.8	12	8	3.5	8	6
48h	4.3	14	9	4.6	11	7
100h	6.7	14	9	7.0	10	7

A New Method to Determine Single Crystal Elastic Behavior from Polycrystals

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Modern engineering analysis techniques, used to ensure that parts in e.g. bridges, airplanes, or automobiles will survive the stresses of use, rely on understanding the proportionality bewteen stress and strain. For many applications the description of the proportionality between stress and strain in terms of isotropic, i.e. independent of direction, elastic constants is still sufficient, the knowledge of these constants for anisotropic cases becomes increasingly important for manufacturing processes, for micromechanical modeling of materials behavior, as well as for custom tailoring new composite materials. For materials which are crystalline on some length scale, anisotropy begins at the grain size level (single crystal elastic constants) and extends as far as anisotropy can be introduced into the material.

This macroscopic anisotropy is induced by two basic effects - a preferred orientation of the crystal lattice of the constituent grains and/or a preferred grain shape distribution. A preferred grain shape distribution means that grains or inclusions have a non-spherical shape on average and they are aligned to some common axis as well. This effect is not necessarily connected to the first one.

The anisotropy of elastic properties on a macroscopic scale (≈ 1 mm) can be readily measured by straining the specimen or by ultrasonic resonance. However, these methods fail in cases in which the microscopic scale is of interest. Examples are precipitations or inhomogeneities of other phases whose elastic constants are unknown but determine nonetheless the strength of the composite or alloy as a whole. The goal can therefore be formulated as the determination of the anisotropic or single crystal elastic constants on the microscopic scale. This can be achieved by diffraction which provides information about the strain and the elastic response of the crystal lattice for a particular direction [hkl].

These so called diffraction elastic constants (DEC) describe the elastic response of a particular family of lattice planes in a certain group of grains with the appropriate orientation to an applied load. Although the DEC are a feature of the polycrystal they can be readily compared to the directional dependence of the elastic constants in a single crystal (Fig. 1).
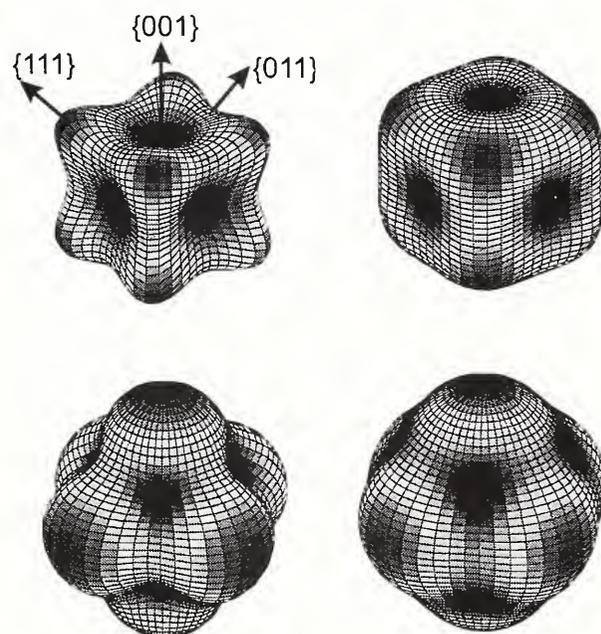
Figure 1: Dependence of Young's modulus E (top) and Poisson's ratio n (bottom) on the direction hkl in the cubic crystal lattice for Ni. The left hand side represents the case of the single crystal, whereas the right hand side shows E(hkl) and n(hkl) as they would be obtained from a set of crystallites which have been selected out of an aggregate of randomly oriented grains. The selected crystallites have in common that for a certain hkl their lattice vectors are parallel.

The smoothing effect for the 'aggregate' constant is a result of the fact that each of the grains in the polycrystal is surrounded by other, not necessarily randomly oriented grains. The elastic response of the selected grains is therefore somewhat obstructed in comparison to the single crystal.

Thus, probing the DEC can provide a wealth of information about the average local conditions on the grain size level.

Since its commissioning the residual stress diffractometer at the thermal beamline BT8 has been used for a variety of engineering-applications-related measurements as well as for basic studies of the elas-
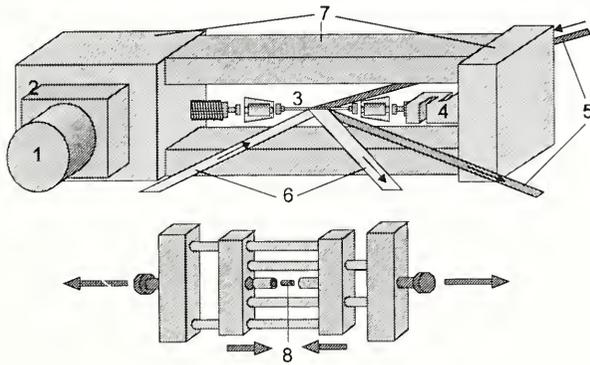
Figure 2 : Schematic of the stress rig.

tic behavior of materials. In the course of these experiments a method has been developed which allows the determination of single crystal elastic constants from measurements on polycrystals. This is done experimentally by loading a specimen in a stress rig and measuring the lattice response normal and parallel to the load direction (Fig.2 and Fig. 3).

1- stepping motor, resolution 1:360
2- gear, reduction 1:2500
3- tensile bar
4- 10 kN load cell
5- beam in transmission (Young's modulus)
6- beam in reflection (Poisson's ratio)
7- stainless steel frame
8- compression sample in compression adapter

These experimental results can be compared to models which calculate the DEC from the single crystal constants [1]. These models can be reversed in a way which considers the single crystal elastic constants as unknown parameters [2,3]. This way the problem can be expressed as a least square loop in which the single crystal elastic constants are refinable parameters.

Possible applications of the method are materials which cannot or can only under great difficulties be synthesized as sufficiently large single crystals. Examples are γ' precipitations in γ/γ' hardened superalloys or metastable phases as plasma sprayed γ-Al_2O_3.
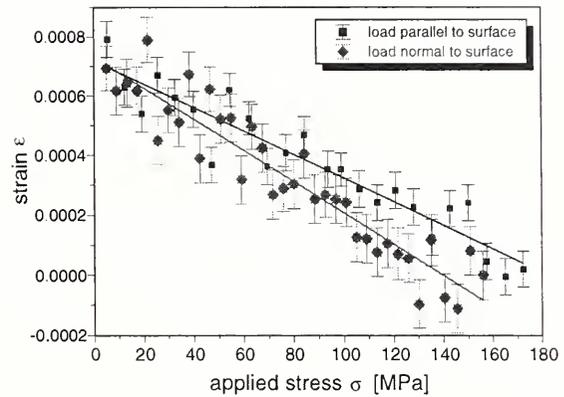
Fig. 3: Lattice strain response in a transmission-compression setup for a γ-Al_2O_3 plasma sprayed thermal barrier coating. Load experiments have been carried out normal and parallel to the coating surface. The difference in the slopes is due to the anisotropy of the sample.

γ' precipitates exist, strictly speaking, only within the equilibrium of the two phase compound, which therefore also requires the determination of their elastic constants from the composite. Thus, in these cases the method may provide the only available tool for determining their single crystal elastic constants.

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Development of Three New Standard Reference Materials

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The chemical composition of materials critically determines their uses in commerce. Chemical analysis is a large endeavor in industry, and depends on the availability of materials with well-known composition to develop and validate analytical procedures and laboratories. NIST Standard Reference Materials (SRMs) are the most important such materials in the marketplace. Nuclear analytical methods have been a crucial contributor to the certification of SRMs for thirty years, because of their high sensitivity and specificity, and their freedom from chemical interferences. In addition to the continuing production and characterization of traditional Standard Reference Materials, three new approaches are underway to satisfy critical measurement needs, using the Analytical Chemistry facilities at the NCNR.

Air particulate matter. Investigations into the amounts and composition of particulate material in air are currently carried out in virtually every country. The investigations in the United States are pointing at particularly high risk factors associated with the fine fraction (PM$_{2.5}$, which is smaller than 2.5 µm aerodynamic diameter) of aerosols. The primary techniques for trace element analysis are based on nuclear physics principles (PIXE, XRF, NAA, etc.), due to their suitability for multicomponent determinations on the small sample sizes that are represented. However, few appropriate quality assurance materials are available to support this work. To assist in effective measurement and control of PM$_{2.5}$ aerosols in an economically sustainable way, NIST is developing this new class of SRMs.

We have collected air particulate matter corresponding to the PM$_{2.5}$ fraction in Baltimore, Maryland at an established EPA monitoring site. The aerosol is removed by ultrasonication from the Teflon membrane filters and suspended in water. Individual filters are prepared by filtering aliquots of the suspension through 47 mm diameter polycarbonate filter membranes with 0.4 µm pore size to form the SRM units. Elemental concentrations in this SRM will be certified using a variety of nuclear- and non-nuclear- based analytical techniques.

Hydrogen in titanium alloy. Hydrogen causes embrittlement of many metals, and the industry-standard analytical methods need same-matrix standards to calibrate their instruments. To meet this need we are currently preparing a new SRM by direct reaction of a titanium alloy with measured amounts of hydrogen and using cold-neutron Prompt Gamma Activation Analysis to verify the doping level.

A procedure has been demonstrated for producing certified reference materials of titanium alloy (6% Al + 4% V) with a known concentration of hydrogen. In the reversible reaction Ti + H$_2$ = TiH$_2$ the equilibrium pressure is less than 10^{-13} atmospheres at room temperature, and 150 atmospheres at 900 °C. Reaction is rapid at 300 °C. This gettering reaction with hot titanium is in common use in geochemistry for separating hydrogen from oxygen and nitrogen (which react irreversibly) and from noble gases. Massive hydrides are prepared industrially by the same direct reaction process for hydrogen-based energy storage and nuclear applications.

Batches of a few grams of titanium alloy specimens have been doped with hydrogen using a simple closed gas handling system. Means are provided for pumping away air and hydrogen from samples at high temperature and for admitting a known pressure of hydrogen in a calibrated volume at room temperature, then raising the temperature of the system to carry out the reaction. The accuracy of the doping is limited by that of the pressure measurement, better than 0.5%. The amount of H in the metal samples was measured in 100-mg specimens by cold-neutron prompt-gamma activation analysis. The quantity measured by this technique and by gravimetry agreed with the volume of gas added. Eighty-gram cylinders of Ti alloy have been loaded by the same procedure, and the uniformity of doping verified elsewhere by quantitative neutron tomography.

These measurements indicate that Standard Reference Materials of hydrogen in titanium alloy can be made and certified by quantitative preparation and analysis as two independent methods, as is done with chemical solution standards at NIST. An apparatus has been constructed to dope 1-kg quantities of metal for Standard Reference Materials.

Titanium nitride films. Reference materials are a critical part of semiconductor metrology since they establish a means of comparison of data taken by different methods or between model and experiment. SEMATECH has requested a titanium nitride Standard

Reference Material as one of their highest needs. A prototype SRM has been made by ion beam sputtering onto 75-mm diameter silicon wafers that were then cut into 10-mm squares. The thickness of the TiN was about 100 nm. Four squares plus a blank were analyzed by neutron depth profiling to determine the total nitrogen concentration. The concentration was determined relative to a boron concentration standard. The relative count rates of the nitrogen and boron samples were adjusted by the ratio of the nitrogen to boron cross sections (1.819/3840). Statistical uncertainties are about 1 % (1 σ) and the overall normalization uncertainty is 2% (1 σ) due to the uncertainty of the nitrogen and boron cross sections. An approximate 3 % fall-off of the nitrogen concentration from center to edge of the original wafer was observed. A measure of

Figure 2. Proposed SRM material with expected stoichiometry. Measurements taken at different angles indicate same nitrogen distribution with differing resolution functions.

Figure 1. Three titanium samples from a previous study indicating nitrogen non-uniformity and less than a one-to-one stoichiometry.

the titanium concentration on each square was made by the technique of activation analysis. This allows a determination of the stoichiometry of the TiN.

Dimensions of Polyelectrolyte Chains with Multivalent Counterions

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Polyelectrolytes, macromolecules carrying a large number of charges, are the predominant water-soluble synthetic and natural polymers. They have wide industrial application and critical biological function. For industry, polyelectrolytes are used as stabilizers, flocculants, or surface-active agents for water treatment, paper, paints, personal care products, and pharmaceuticals. In biological systems, the binding of proteins and nucleic acids, the functioning of enzymes, and the construction of cellular components are controlled by the tensions imposed by electrostatic interactions. It is also clear that the interaction of polyelectrolytes with multivalent counterions is a critical factor in many industrial applications and biological functions. Although recent years have witnessed an impressive confluence of experiments, simulations, and theory, long-range electrostatic interactions still disrupt most traditional methods and characterization techniques. In the work described here, the method of zero-average-contrast small angle neutron scattering (SANS) is used to overcome this barrier and probe directly the most fundamental polymer property, the chain dimension, as a function of concentration and counterion valence.

For low ionic strength polyelectrolyte solutions SANS shows a maximum at finite wavevector and a steep upturn at low angles; results that are dramatically different from those of neutral polymer solutions[1]. There is no complete theory, only qualitative descriptions for these phenomena that appear for nearly all charged macromolecules. The situation is even more complicated for typical biological systems or for commercial polyelectrolyte applications because of the presence of divalent or trivalent counterions. The specificity of interactions with multivalent ions is critical to applications such as water treatment and to biological processes such as protein folding and DNA packing. Although the multivalent counterions have dramatic effects on the structure and dynamics of polyelectrolyte solutions, experimental work with scattering is both limited and difficult to interpret. A major impediment for simulations and theoretical interpretation is the lack of an adequate description for the single chain structure and dimension. The overwhelming effect of strong intramolecular and intermolecular electrostatic interactions of the unscreened charges dominates the scattering, even in dilute solution.

The method of zero-average-contrast (ZAC) in small angle neutron scattering provides a means to overcome this obstacle and measure single chain dimensions in dilute and semidilute solutions[2]. The ZAC method requires matched pairs of deuterated and hydrogenated polymers and a specific H-D solvent composition, but the charge concentration and counterions can be changed over a broad range.

Figure 1. Full contrast SANS for NaPSS (filled) and
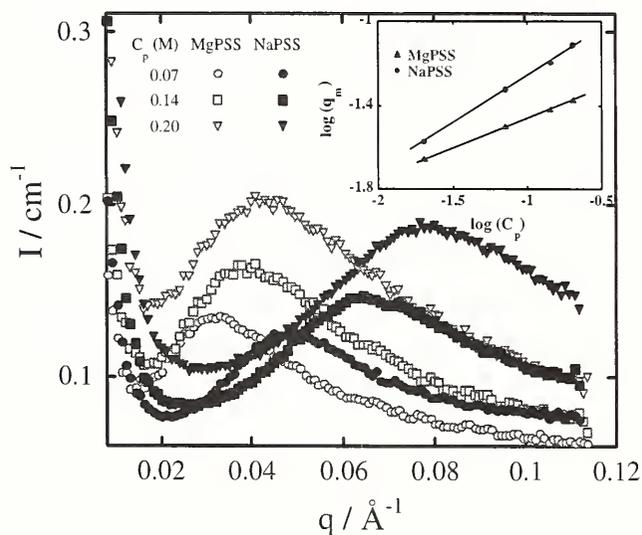
MgPSS (unfilled) in D$_2$O. Monomer concentrations: (●) 0.20 mol/L, (◆) 0.14 mol/L, and (■) 0.07 mol/L. Inset is log-log plot of peak position versus monomer concentration.

Poly(styrene sulfonate) (PSS) with matched degree of polymerization and degree of sulfonation were obtained as deuterated PSS and hydrogenated PSS. The sodium salt of PSS was purified by ion-exchange, dialysis, neutralization titration with NaOH or Mg(OH)$_2$, and lyophilization. Figure 1 shows typical polyelectrolyte scattering (performed on the NG1 8 m SANS instrument) without added salt. Although qualitatively the two sets are similar, including strong upturns at low q,

the concentration dependence of the broad maxima is shown in the inset with $q_{max} \propto c_p^{0.46}$ for NaPSS and $c_p^{0.29}$ for MgPSS, where c_p is the salt concentartion. Peaks for the divalent counterion polymer are also shifted to lower q.

All of these features disappear under the zero-average-contrast conditions. ZAC is achieved with an equimolar mixture of deuterated and hydrogenated polymer in a mixture of H_2O and D_2O. The fraction of D_2O in the solution is set at the value necessary to satisfy the "optical theta condition," where the scattering length densities of the hydrogenated and deuterated monomers are equal and opposite. Figure 2 displays the scattering profiles from the ZAC solutions for NaPSS and MgPSS. Each decreases monotonically with angle, as expected for the intraparticle scattering function, and each is fit adequately with a Debye function.
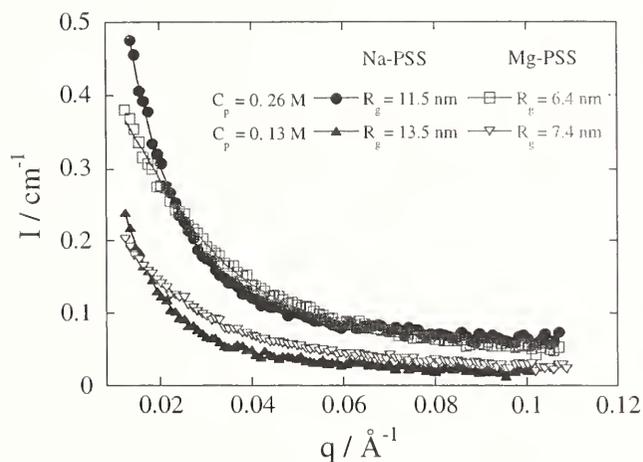
Figure 2. ZAC scattering from Na and Mg polyelectrolyte solutions under conditions of zero average contrast showing single chain scattering. Fits to Debye function.

Figure 3 shows the values of polymer chain radius of gyration as a function of concentration for NaPSS and MgPSS along with calculated estimates for the size of a single chain with degree of polymerization of 300 under random coil and rod-like configurations. For both systems, the chain dimension decreases with increasing concentration with the MgPSS chains nearly a factor of two smaller for each concentration. While the monovalent counterion chains are highly extended, they are not at the rod-like limit. At the same time, both systems are more expanded than the calcu-

lated ideal Gaussian chain value. This result implies that while the divalent counterions induce a coil contraction they do not produce a coil collapse or a coil-globule transition.
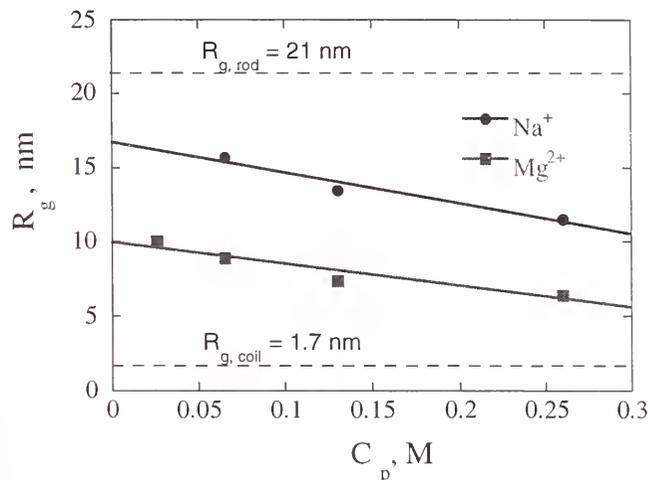
Figure 3. Polyelectrolyte chain dimensions as a function of concentration with comparison to model chain calculations.

This study demonstrates the power of the zero-average-contrast method to extract single chain information even in the presence of strong intermolecular interactions. The method, here used for dilute low ionic strength solutions, has also been applied to measure singe chain dimensions in solutions at high concentration and with arbitrary amounts of added salts as needed to explore the range of real conditions important for polyelectrolytes.

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Characterization of New Biomimetic Materials Using Neutron Reflectivity

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All cells are enclosed by a biological membrane, consisting of assemblies of lipid and protein molecules, that defines its boundaries and regulates its interactions with the environment. The lipid molecules form a continuous double layer, or bilayer, which acts as a barrier to water-soluble molecules and provides the framework for the incorporation of the protein molecules. Specialized proteins embedded in lipid bilayers participate in fusion events between cells (i.e., triggered by viruses), regulate ion transport through pores and channels (*i.e.*, neural activities), engage in enzymatic activity at membrane surfaces, and play a role in biological signaling (i.e., receptor proteins activated by hormones). Cell membranes are sufficiently complicated that they cannot be duplicated in the laboratory for study. Thus, model biological membranes, which are simpler than cell membranes but mimic their structure and function, are used to study these complicated systems. Such model membranes are known as biomimetic materials, which emulate biological function such as molecular recognition, dynamic conformational change and spontaneous self-assembly of complex arrays of molecules.

A biomimetic material which is analogous to the lipid membranes of cells and can support active membrane proteins has been made in NIST's Biotechnology Division [1]. This hybrid bilayer membrane (HBM), which is illustrated in Fig. 1, consists of two self-assembling monolayers, one which is non-biological (alkanethiol) and a second which can be found in biological cell membranes (phospholipid). This system is formed spontaneously on a planar gold surface. Since the alkanethiol monolayer is strongly bonded to the gold surface, this HBM is more rugged than a conventional supported phospholipid bilayer, which binds only weakly to a silicon or glass surface. In addition to their obvious importance as a tool for understanding and characterizing membrane protein structure and function, the biomimetic characteristics of the HBMs make them commercially significant for a number of applications including biosensors, tissue engineering, and bioelectronics and biocatalysis. The lipid and protein composition of the HBM can be readily engineered to produce structures with novel physical and chemical properties that do not occur in nature.

Phospholipid

Alkanethiol

Gold Substrate
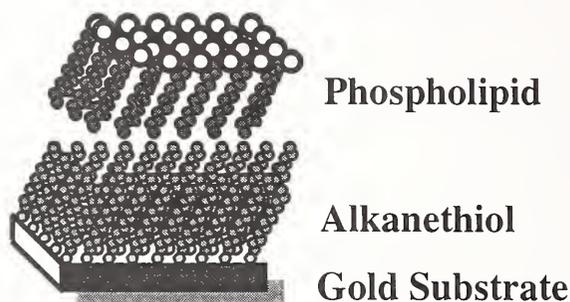
Figure 1. The alkanethiol/phospholipid hybrid bilayer membrane (HBM).

The development of measurement tools for probing the structure and function of these engineered membranes and the cell membrane components incorporated into them is essential for the optimization of their biomimetic character. To this end, the neutron reflectivity technique is being used to assist in the structural characterization of HBMs which are in contact with water. Such *in situ* measurements are only possible because neutrons interact weakly with materials, in contrast to electromagnetic probes such as light, x-rays and electrons. Thus, the planar substrate can be used as the incident medium, allowing the phospholipid side of the HBM to be in full contact with water, as it is in its native state. The neutron reflectivity measurements are being made on the NG1 reflectometer at the NCNR, shown in Fig. 2. Advancements in instrumentation, sample environment and measurement protocols now make it possible to obtain Angstrom-level information about the composition of HBMs along the axis perpendicular to the plane of the membrane.

The results from recent neutron reflectivity measurements of HBMs in water are shown in Fig. 3. The HBMs were formed on single crystal silicon substrates, which had been coated with ~50Å of gold on a ~15Å chromium adhesion layer, and were measured in contact with water. The neutron scattering length density (SLD) profile shown in Fig. 3 was obtained by fitting the reflectivity data using the model-independent fitting program, PBS (2). Since the neutron scattering length density of each element in the bilayer depends upon its chemical composition, the SLD profile is essentially a

Figure 2. Members of the experimental group at the NG1 reflectometer at the NCNR. Clockwise from bottom: S. Krueger, A. L. Plant, C. W. Meuse, N. F. Berk and C. F. Majkrzak.

corporation of transmembrane proteins. However, the neutron reflectivity measurements provided **direct** evidence that the ethyleneoxide region contains no water. Furthermore, the reflectivity measurements confirmed that melittin does not alter the membrane structure in a way that would allow water into this region. These important results have led to the development of new HBMs which more closely mimic biological membranes and are capable of supporting transmembrane proteins.
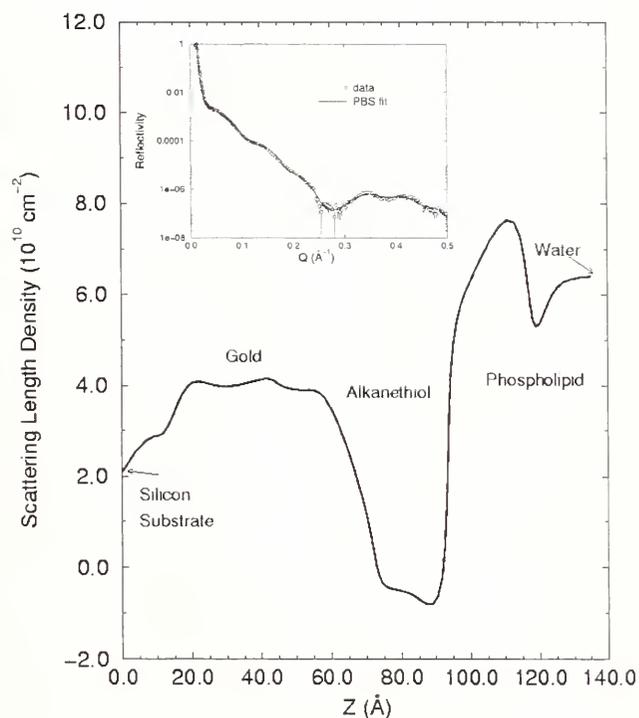
Figure 3. A representative neutron scattering length density profile for a hybrid bilayer membrane. The location of the silicon substrate is defined as Z=0. The corresponding neutron reflectivity data are shown in the inset.

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map of the bilayer structure in the plane perpendicular to that of the membrane, generally defined as the Z direction. The silicon substrate is at Z=0 by definition. The locations of the gold layer, the alkanethiol monolayer and the phospholipid monolayer relative to the substrate can be easily distinguished in the SLD profile.

Neutron reflectivity measurements have also been made, for the first time, on HBMs in the presence of the membrane protein, melittin, a relatively small peptide toxin that is found in bee venom. Although melittin is an important model compound for pore-forming peptides such as antibiotics, its exact location in the membrane is not known. The structure of HBMs in the absence and presence of melittin now can be directly compared and questions about how deeply melittin penetrates into the bilayer, and whether melittin forms pores that allow water into the bilayer, can be addressed.

Most recently, neutron reflectivity has been used to study the structure of a novel HBM matrix consisting of an ethyleneoxide-containing alkanethiol monolayer and a phospholipid monolayer. The ethyleneoxide moiety tethered to the gold surface was intended to act as a loosely-packed "spacer", allowing water to penetrate into the region near the gold surface, thus providing a suitable environment for the in-

25

The Dynamics of Hydrogen in Solid C_{60}

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Carbon is the most studied element in the entire periodic table. For decades it was believed that pure carbon existed in two forms, diamond and graphite. Thus it was quite surprising when a third form of

Figure 2. A Fourier difference map of the 100 crystallographic plane which shows the locations of the C_{60} molecules using dashed white lines and the location of the deuterium molecules by the red and yellow contours at the octahedral position.

Figure 1. Schematic diagram of the interstitial spaces in a C_{60} lattice. The gray balls indicate the positions of the C_{60} molecules while the red ball resides in the larger octahedral site and the blue ball sits on one of the tetrahedral sites. The hydrogen molecules must go into one of these spaces between the "buckyballs".

pure carbon, called fullerenes, was discovered in the mid 1980's. The most well-known of this new-class molecular materials is the one consisting of 60 carbon atoms which takes the shape of an atomic-scale soccer ball. These beautifully symmetric molecules are commonly called "buckyballs".

In the solid state C_{60} molecules form a structure with large interstitial spaces between the molecules. (Figure 1) These spaces are easily large enough to accommodate a wide variety of atomic and molecular

species, which can significantly influence the properties of the resulting compound. Most notable are the alkali doped C_{60} compounds, which display superconductivity at reasonably high temperatures. However it has also been shown that various gases including hydrogen, nitrogen, carbon monoxide, and oxygen can be absorbed into the spaces between C_{60} molecules. This suggests that solid C_{60} might be useful as a medium for the safe storage of hydrogen or as a molecular sieve to separate these gases. In spite of this, relatively little effort has been made to understand the interactions which govern these potentially useful properties namely, the interaction of the trapped species with the C_{60} host. Hydrogen in C_{60} is also of fundamental interest because it is a nearly perfect example of a simple quantum object (hydrogen) trapped in a classical matrix (C_{60}). Neutron spectroscopy is a direct way of probing the bonding in materials and it is a particularly powerful tool with which to study the dynamics of hydrogen because of the large incoherent

scattering cross-section of hydrogen. Inelastic scattering spectra obtained using the Fermi Chopper Spectrometer (Figure 3) show well-defined peaks, which
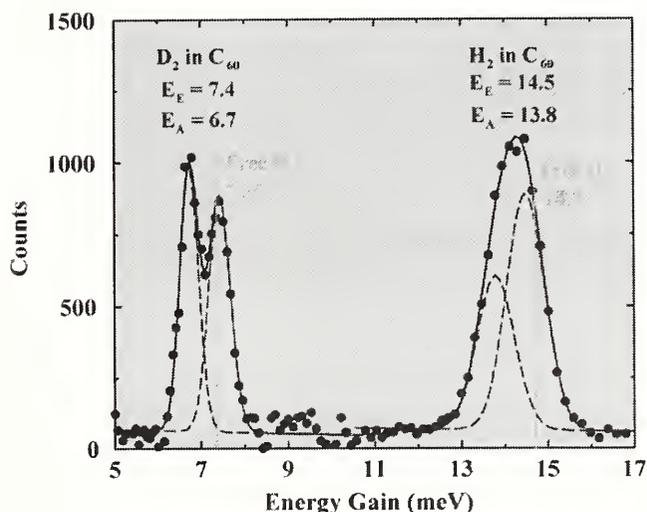
Figure 3. Neutron spectra showing the rotational transitions for hydrogen and deuterium absorbed in solid C_{60}. Note that the transition is a doublet in both cases with a splitting of 0.7 meV. The center of the doublet is slightly shifted from the value expected for the free molecules, which is indicated by the green arrow.

can be attributed to the quantized rotational levels of the hydrogen and deuterium molecules.

These peaks are only slightly shifted from the positions expected for the free rotations of these molecules. The simplicity of this behavior allows us to probe the effects of relatively weak interactions with the host lattice, which lead to the small departure from the free rotor case.

To explore this more quantitatively we have performed model calculations using a simple Born-Meyer type of potential. The rotational potentials felt by hydrogen and deuterium molecules within this model are shown in Fig. 4. The panel on the left shows the calculated potential for the case of complete orientational disorder of the C_{60} molecules while that on the right shows the potential for ordered C_{60}. The difference in energy between the red and blue regions is only ~1 meV, in agreement with the experimental observation that the rotations are nearly free. The diagrams below the calculated potentials show the change in the quantum energy levels as the strength of the orientational potential is varied. For the disordered case, no change is seen over this limited range of po-

tential, whereas for the ordered C_{60} case, the level at ~14.7 meV splits into 2 states, as is observed experimentally. Thus the degree of splitting is extremely sensitive to the symmetry and the strength of the interactions.
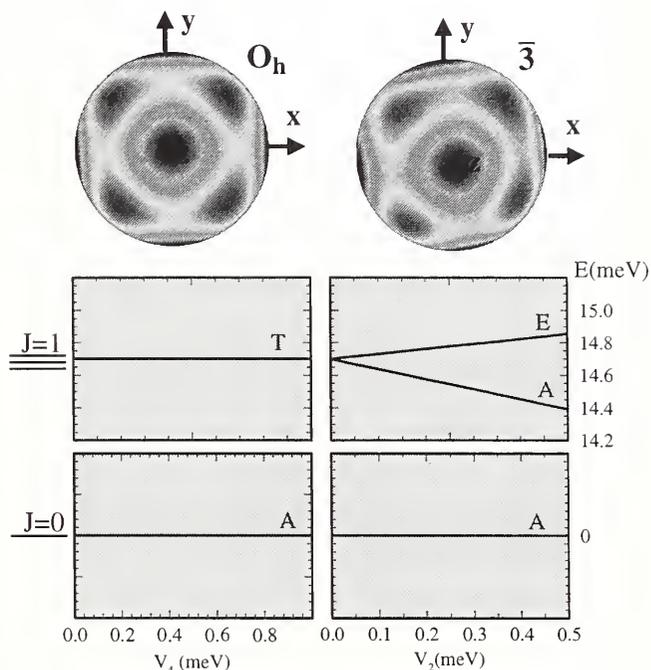
Figure 4. The top diagrams show contour plots of the orientational potential felt by a hydrogen molecule when C_{60} molecules are orientationally disordered (left) and orientationally ordered (right). The total variation in the potential (from red to blue) is about 1 meV indicating that the rotation is only weakly hindered. The bottom diagrams show the quantum rotational levels as a function of the orientational potential when C_{60} molecules are orientationally disordered (left) and orientationally ordered (right).

Neutron scattering combined with self-consistent phonon calculations demonstrates that the symmetry of the interstitial site is bar-3. Furthermore, the magnitude of the splitting (0.7 meV0 is comparable to the size of the rotational barrier arising from the intermolecular interactions between the hydrogen and the C_{60} molecules. Additional studies are underway which will probe how these interactions are changed by the application of pressure and the co-intercalation of charged species into the C_{60} host.

Polarons in Colossal Magnetoresistive Materials

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The magnetic properties of the lanthanum manganese oxide class of materials have attracted tremendous interest recently because of the dramatic increase in conductivity these systems exhibit when the magnetic moments order ferromagnetically, either by lowering the temperature or by applying a magnetic field. This huge increase in the carrier mobility, which has been given the name "colossal magnetoresistance" (CMR), is both of scientific and technological interest. In particular, it is anticipated that these materials may provide the next generation of read/write heads for the magnetic data storage industry, while the "half-metallic" behavior provides fully spin polarized electrons for use in magneto-electronics applications, and for sensors in a variety of applications such as in the automotive industry.

CMR can be strongly enhanced in systems with reduced dimensionality and so there has been considerable interest in the two-layer Ruddlesden-Popper compounds, $La_{2-2x}Sr_{1+2x}Mn_2O_7$. The reduced dimensionality leads to significant extension of the temperature range over which magnetic correlations are important, and thereby allows a detailed examination of the link between local spin correlations and the resulting magnetotransport. We have therefore investigated the magnetic correlations in $La_{1.2}Sr_{1.8}Mn_2O_7$ using neutron scattering. Over a large temperature range above $T_c = 112$ K, we found evidence for two-dimensional magnetic correlations which peak in intensity at the transition. Although the in-plane correlations are predominantly ferromagnetic, a canting of spins in neighboring planes within the bilayers, at an angle that is dependent both on temperature and magnetic field, was observed [1,2].

One of the central questions in the field of manganites concerns the lattice involvement in the mechanism of CMR. While the relation between ferromagnetism and conductivity was explained in terms of double exchange, it is now clear that a full understanding of these materials must include the lattice degrees
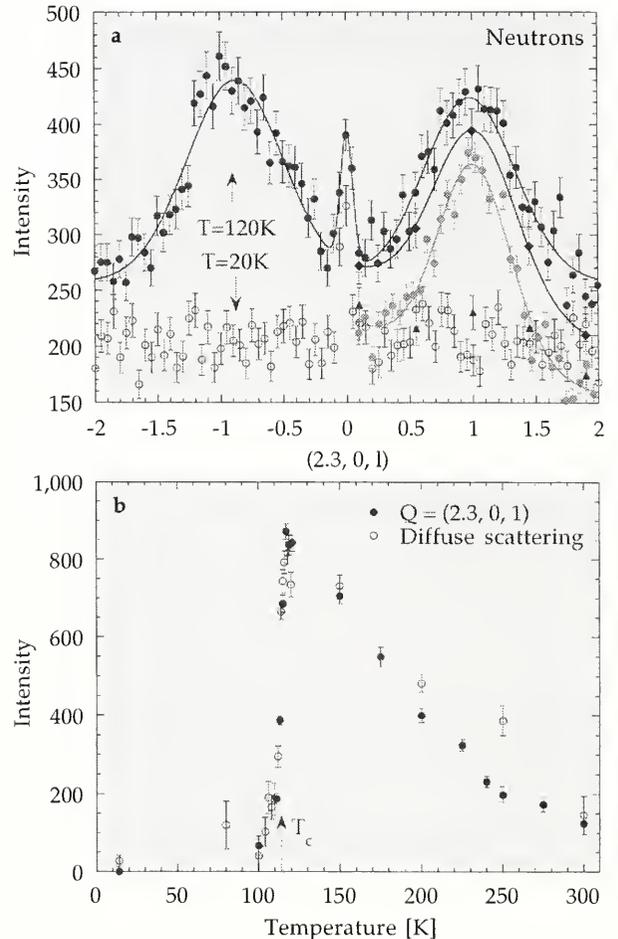
FIG. 1 (a) *l*-scans through the charge ordering peaks at (2.3, 0, 1) at T=120 K: energy-integrated (red), elastic (orange), non-spin-flip scattering measured with polarized neutrons (green diamonds), spin-flip scattering (green triangles). The orange and green data points have been scaled by appropriate factors. The *l*-scan at T=20 K (open purple circles) shows that the charge peaks have vanished. (b) Temperature-dependence of the intensity of the superlattice peak (2.3, 0, 1) (red), and of the diffuse scattering after correction for the phonon scattering (blue), showing that the charge order and lattice polarons collapse at the Curie temperature.

of freedom. In particular, the formation of lattice polarons above the Curie temperature has been inferred from a variety of measurements, but direct evidence has been lacking.

Neutron measurements carried out at NIST, and X-ray measurements at the Advanced Photon Source, have revealed charge localization in the paramagnetic-insulating phase of the layered $La_{1.2}Sr_{1.8}Mn_2O_7$ CMR material, with the associated diffuse polaron scattering that originates from the lattice distortions around the localized charges. Figure 1(a) shows two of the observed incommensurate superlattice peaks associated with the charge ordering, characterized by the wave vector (0.3, 0, 1). Polarized neutron scattering has shown that the incommensurate superlattice peaks are pure structural reflections, originating most likely from Mn^{3+}-Mn^{4+} charge correlations. These correlations are quasi-static on a time scale ps set by the energy resolution of the instrument. The superlattice peaks are broader than the q resolution in both h and l directions, showing that both the in-plane and out-of-plane charge correlations remain short range at all temperatures. The charge order melts as the insulator-to-metal transition is traversed and long-range ferromagnetic order is established [3], as shown in Fig. 1 (b). By similarity with the 3D perovskite manganites and with the cuprates, this scattering may originate from a charge-ordered stripe phase above T_c, which is destroyed when the double exchange mechanism drives the system metallic. The lattice strain induced by the localized charges gives rise to a four-fold, lobe-shaped pattern of diffuse scattering around the Bragg peaks. The upper panel in Fig. 2 shows a contour plot of the diffuse X-ray scattering in the [h, 0, l] plane around the (2, 0, 0) reflection. Only the $l > 0$ half is shown, but the pattern is symmetric with respect to $l = 0$, as proved by the neutron l-scans in the lower panel of Fig. 2. The sharp rod of scattering along the [0, 0, l] direction is resolution limited in the [h, k, 0] plane and is associated with stacking faults. Part of the lobe-shaped diffuse scattering is due to conventional acoustic phonons, while the temperature dependence of the additional, polaron scattering (blue open circles in Fig. 1(b)), arises from static or quasi-static atomic displacements as revealed by elastic neutron scattering (see Fig. 2 (bottom)). The lattice strain caused by the polarons relaxes when the short-range charge order melts at the Curie temperature, providing compelling evidence of the role of polarons in the origin of CMR. Further work is now in progress to determine if the charge melting can be controlled by the application of magnetic or electric fields, which would open up completely new avenues for applications.
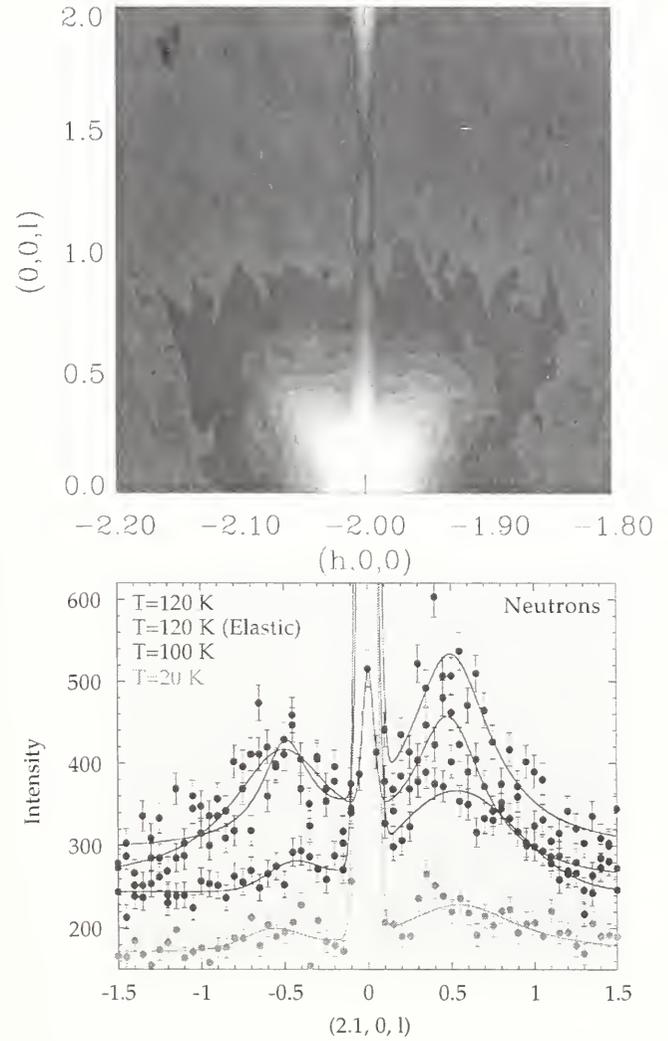
FIG. 2 (Top) Contour plot showing the lobe-shaped pattern of diffuse scattering around (2, 0, 0). (Bottom) Neutron energy-integrated l-scans across the diffuse scattering in the upper panel, for T=120, 100, and 20 K. The scan at T=120 K (red circles) is an elastic scan, and has been scaled by an appropriate factor.

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Neutron Interferometry and Optics Facility (NIOF)

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A neutron interferometer (NI) is analogous to a classical Mach-Zehnder type optical interferometer and it is the only device that allows direct measurement of the phase of a neutron wave. The first neutron interferometer was operated over two decades ago in Vienna, Austria. In the USA, a very successful group has been operating at the University of Missouri-Columbia for the last two decades. Gravitationally induced quantum interference of neutron waves, 4π spinor rotation of neutrons in a magnetic field, and observation of the Aharonov-Casher effect (neutron analog of the Aharonov-Bohm effect for electrons) are among the seminal experiments that were carried out during this period. By measuring the phase shift of the neutrons that pass through a sample it is possible to accurately determine the neutron refractive index, n, of the material. The NI method of determination of n is, for the most part, independent of the microscopic details of the sample and perhaps the most accurate method that is available today. The refractive index, n, of many solids (e.g. uranium, chromium, vanadium) and gases (hydrogen, helium etc.) that are important to condensed matter and solid state physics have been measured and are being measured today.

The NIST Neutron Interferometry and Optics Facility (NIOF) is one of the premier facilities for neutron optics research. Located in the NCNR guide hall, it uses single crystal neutron interferometers (perhaps the best in the world today) with exceptional phase stability and fringe visibility that are crucial for the success of experiments in both fundamental and applied research. This exceptional performance is in part attributed to the state-of-the-art thermal, acoustical and vibration isolation system that has been successfully designed and built during the past few years.

During the past year the NIST NIOF has provided unique research opportunities for both applied and fundamental research and a diverse selection of experiments have been successfully carried out. Two Ph.D. dissertation research were carried during this period and six articles have been written for publications. Research collaborations have been established with the University of Missouri-Columbia, the Hahn-Meitner-Institute and the University of Innsbruck and EXXON.
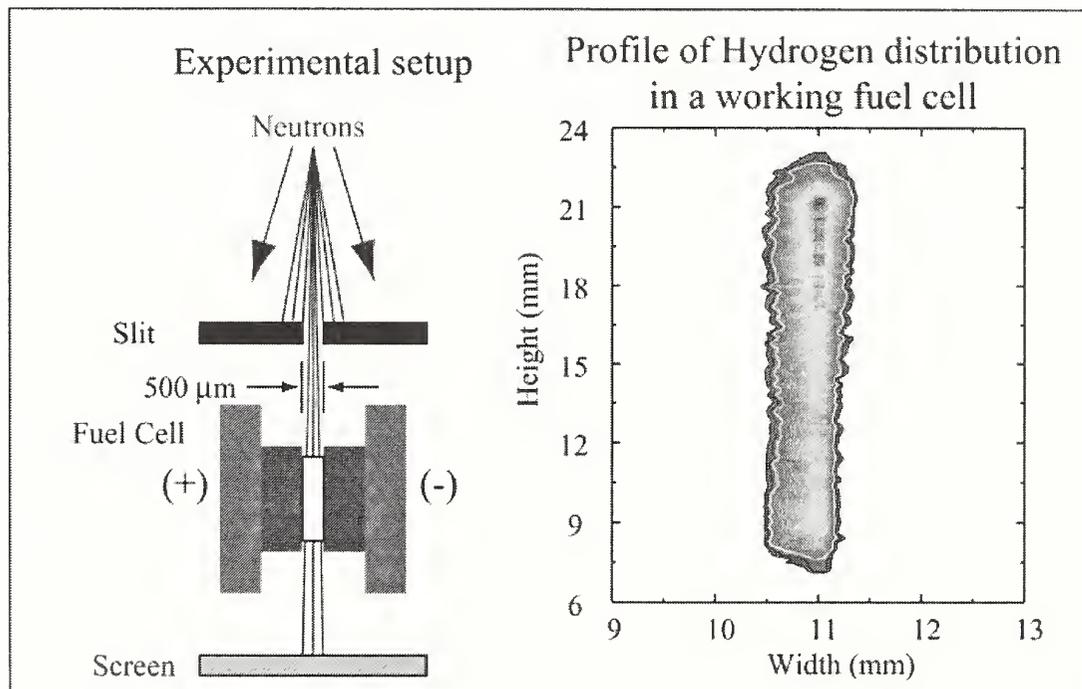
Figure 1. Neutron image of the water gradient inside a fuel cell.

Special effort has been made to apply neutron-imaging techniques for industrial research. The NIOF is equipped with a high resolution CCD type 2-D position sensitive neutron detector to perform high-resolution neutron radiography of samples using a mono- or a poly-energetic energetic neutron beam. Early performance tests of a neutron tomography station have been successfully carried out. In addition to radiography, many other types of diffraction imaging experiments may be performed at the NIOF. Researchers from EXXON have exploited the convenience of this facility for both hydrogen fuel cell research and for studying hydrocarbons. For the first time the water gradient inside a working fuel cell has been successfully imaged (fig.1). Results from these experiments have allowed verification of theoretical predictions of water transport mechanism in a working fuel cell [1]. Researchers from the University of Innsbruck, Austria, have also used this facility to study the diffraction of neutrons (λ=0.235 nm) from macroscopic objects ~0.1 mm in size. Finally, a semi-finalist in the 57th Westinghouse Science Talent Search has demonstrated the Neutron Phase Contrast Imaging technique.
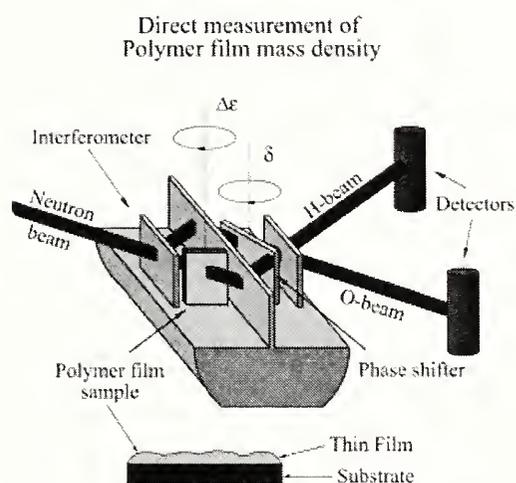
Figure 2. Schematic of the polymer thin film measurement setup.

The first successful neutron interferometric measurements of scattering length density in polymer thin films (1<μm) have been carried out in collaboration with the NIST Polymers Division (fig. 2). This technique is independent of calibration standards and complex mathematical modeling of the physical process of interaction. This measurement has opened the possibility of using NI as an important tool for establishing well defined densities of thin films that is critical in many analysis techniques in surface physics research

[2].

An important experiment has been carried out to verify the recent predictions of quantum entanglement of the nuclear states in a mixture of fluids. The existence of such entanglement would suggests that that the refractive index, 'n', of a mixture cannot be calculated only from the knowledge of fractional abundance and n of the constituent elements. If this weretrue, the implications would be profound for many neutron scattering techniques. A NIOF experiment measured scattering length density, Nb, for various mixtures of H_2O and D_2O. It had been proposed that for these mixtures a 5-10% deviation from the traditional theory might occur because of quantum entanglement of H and D at room temperature. However, the experimental data agreed with the traditional theory within the statistical fluctuation of the data, which was of order 0.4% and within this limit no deviation from standard theory has been observed [3].

The capability of the facility has been augmented by the addition of a transmission neutron polarizer and RF gradient flipper. Neutron polarization in excess of 98% has been obtained with thermal neutrons. This new capability was exploited in an experiment which observed the 4π spin rotation symmetry of the neutron wave function. This experiment was unique in that the neutron guide field was gently rotated by 180° allowing the neutron spin direction to adiabatically follow the field. This experiment provides the first *direct* observation of 4π spin rotation symmetry of neutrons under space rotation.

New experiments such as the measurement of the internal charge structure of a neutron, measurement of mass densities of thin films as a function of thickness and scattering length of samples (such as D_2 gas) that important for many body calculations are being planned. Future plans also include constructing large separated-section interferometers. Such interferometers are crucial for phase transition studies in samples and fundamental physics experiments with at least an order of magnitude more sensitivity than what is possible today.

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Protein Conformations and Interactions in Biochemical Regulation

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Small-angle neutron scattering, with contrast variation, has provided key insights into the regulation of protein activities. Life functions at the molecular level via a large number of highly regulated molecular networks through which messages are communicated so that cells can maintain vital ongoing functions and also can respond as needed to external stimuli. Proteins are the work-horses of life carrying out all the functions required for survival, growth and reproduction. They are responsible for motility, transport, signal transduction, catalysis, protein synthesis and degradation, energy capture, transport and conversion, damage recognition and repair, replication and transcription, etc. These activities all must be strictly coordinated, and there are a variety of mechanisms for regulating protein function that are key to healthy function. One of the most common regulatory mechanisms of protein activity is the addition, or removal, of phosphate groups from hydroxyl groups on proteins. Protein phosphorylation reactions are catalyzed by a family of enzymes called the protein kinases of which several hundred have been identified to date. Protein kinase activities themselves are frequently regulated by "second messengers" that are released into the cellular cytoplasm in response to a "first messenger" signal, such as a hormone binding to a cell surface receptor. Two commonly used second messengers are divalent calcium ions and cyclic nucleotides. These messengers modulate kinase activities generally by binding to intermediary regulatory proteins that then either bind to or modulate their interaction with the kinase such that the kinase activity is switched on or off.

Small-angle scattering from proteins in solution gives information on their overall shapes and is particularly sensitive to domain movements as well as protein-protein associations. In the case of neutron scattering, the differences in the scattering properties of hydrogen and deuterium allow one to use specific deuterium labeling with contrast variation to extract structural data on individual components within complexes. We have used neutron scattering with contrast variation to characterize the conformational transitions and associations in the activation mechanism of two model kinases; the Ca^{2+}/calmodulin-dependent kinase myosin light chain kinase (MLCK), and the cyclic nucleotide (cAMP)-dependent protein kinase.

In our neutron scattering studies of the Ca^{2+}/calmodulin/MLCK activation mechanism we have determined the conformational transitions undergone by both the kinase and calmodulin upon complex formation [2], and the effects of substrate binding on the complex [3]. These experiments were performed using samples prepared with the MLCK enzyme complexed with deuterated calmodulin. Data were measured for the complex in solvents having a range of D_2O levels. The basic scattering functions for calmodulin and MLCK within the complex, as well as the cross term, were extracted from these neutron data. Uniform two-ellipsoid models were used to aid in the interpretation of the scattering data. Figure 1 shows the conformations of calmodulin and MLCK in the complex with and without substrate as determined by the neutron scattering experiment. By fitting the high resolution crystal or NMR structures available on the components of these complexes into our ellipsoid models we have been able to gain new insights into the molecular basis for the kinase regulation. Figure 2 summarizes the information derived from the solution scattering studies concerning the activation mechanism.

Our more recent solution scattering studies of the cAMP-dependent protein kinase [4] have revealed the quaternary structure of this kinase which has two identical catalytic and two identical regulatory subunits that bind the cAMP second messenger. This binding results in the dissociation and activation of the catalytic subunits. Again by fitting the high resolution structures into the molecular envelops defined by the neutron data, we have been able to compare and contrast the different regulatory mechanisms for the highly conserved catalytic core of the two kinases we have studied thus far.

Our neutron contrast variation studies provide critical information about the dynamic conformational transitions underlying the regulatory mechanisms we are studying. The ability to study the global shapes of the component structures within complexes in which

MLCK

catalytic cleft

calmodulin   MLCK-I

No substrates   Plus substrates
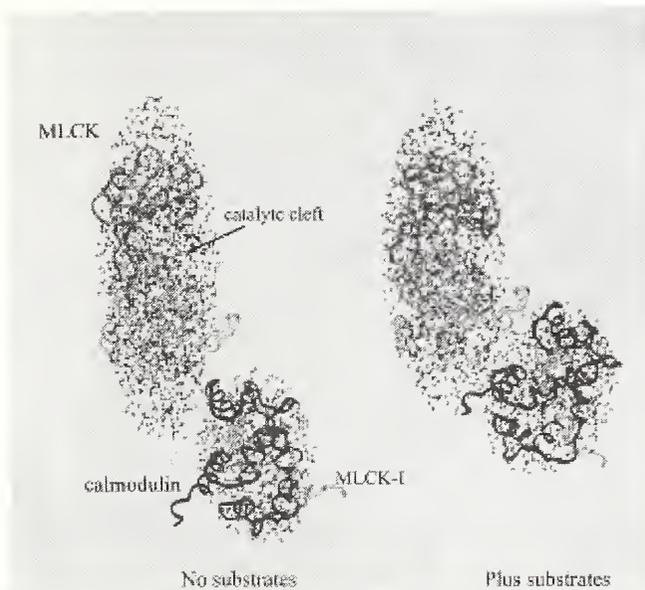
Figure 1. Ellipsoid models derived from the neutron scattering data for 4Ca2+•calmodulin•MLCK complexes with (right) and without (left) substrates. Superimposed within the ellipsoids are the known structures for the upper (orange ribbon) and lower (yellow ribbon) lobes of the MLCK catalytic core. Within the smaller ellipsoid Calmodulin is represented as a red ribbon, with the MLCK calmodulin-binding domain (MLCK-I) in yellow. Upon substrate binding there is movement of the calmodulin closer to the catalytic cleft. At the same time the catalytic cleft of MLCK closes, presumably about its substrate.

there is inherent flexibility provides a critical framework into which higher resolution structural data on the individual components can be fit. These types of problems cannot be studied by high resolution crystallography when flexibility inhibits crystallization. Neither can they be studied by NMR when the structures are larger than ~ 40 kDa. Thus neutron small-angle scattering and contrast variation fills an important niche that helps to assemble the molecular jigsaw puzzles that we need to solve in order to understand the way in which molecular networks operate. This understanding is key to medical and biotechnology applications that utilize biomolecules and their unique properties.

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Calmodulin

MLCK

CaM binding domain

open catalytic cleft

autoinhibitory sequence

+ Ca^{2+}

Substrates: AMP-PNP LC peptide
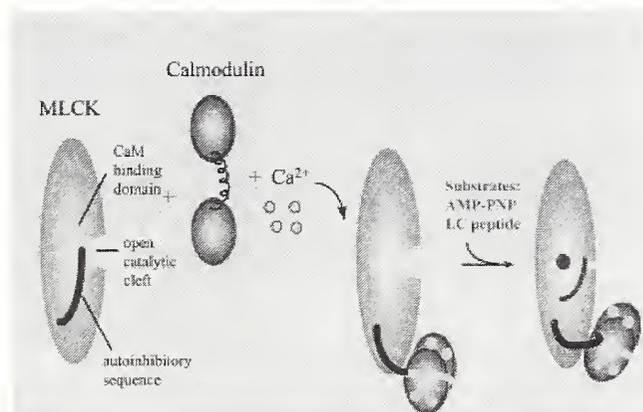
Figure 2. Schematic summarizing the sequential conformational transitions for calmodulin activation of MLCK. In its inactive conformation, MLCK maintains an open catalytic. Upon binding 4Ca2+, calmodulin undergoes a conformational collapse as it interacts with hydrophobic residues at each end of the calmodulin-binding sequence that forms a helix. Substrate binding induces closure of the kinase catalytic cleft. Thus the fully activated complex is formed.

press, 1998

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Microstructure Transformation During Microemulsion and Micellar Polymerizations

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Emulsion polymerization is the most widely used process to prepare polymer colloids (latexes) of sizes 100 to 10,000 nm, finding use in applications such as paints and adhesives. Microemulsion systems contain larger amounts of surfactant relative to the monomer and produce much smaller polymer particles of 20 to 50 nm diameter. The surfactant molecules themselves can be functionalized and polymerized producing even smaller structures of 3 to 5 nm, still retaining a well-defined shape. The reduced size and increased surface area of these structures allows for a variety of new applications beyond conventional emulsion latexes, such as adsorbents and receptor binders for biomedical compounds [1].

In all of these reaction systems there is a definite need to understand the details of the underlying mechanisms in order to control the final product. A number of models for free-radical polymerization kinetics have been proposed, and all depend on the location of monomer relative to the growing polymer chain. This partitioning of monomer determines the overall rate of reaction as well as the dominant free-radical termination events. The widely different initial microstructure of emulsion, microemulsion, and micellar systems leads to important differences in the localization of monomer and polymer. Typical experiments attempt to correlate the overall rate of reaction with the initial and final properties of the microemulsion and latex respectively, with little information about the specifics of the compartmentalized monomer and polymer. In order to elucidate the mechanistic details, polymerization reactions can be performed on-line, using Small-Angle Neutron Scattering (SANS) to provide microstructural information as a function of conversion (or time). SANS is well suited to investigate polymerization reactions, non-invasively probing appropriate length scales in as short as one-minute intervals.

A microemulsion polymerization of hexyl methacrylate was performed on-line using SANS while simultaneously measuring the conversion [2]. Representative SANS spectra at increasing conversion are shown in Figure 2. As the reaction proceeds, the diminishing peak in the spectra shows the smooth decrease in the size of the monomer-swollen microemulsion droplets. Simultaneously, the increase in the low-q scattering indicates a steady growth of latex particles.

Quantitative modeling shows that the average diameter of the latex particles remains nearly constant, simply increasing in number with time. These results support a model of polymerization in which the propagation reaction occurs in a monomer-rich shell surrounding a growing polymer particle that is not swollen with monomer. It also provides insight into the behavior of monomers with different partition coefficients.

Micelle polymerization should behave even less like an emulsion polymerization than a microemulsion. There is now no monomer to partition, since the surfactant is the monomer and is constrained to a specific location in the aggregate. If there is no transfer of monomer between aggregates during the polymerization, the process can be thought of as a "zippering" of the individual micelles.

Unlike most microemulsions, micellar aggre-
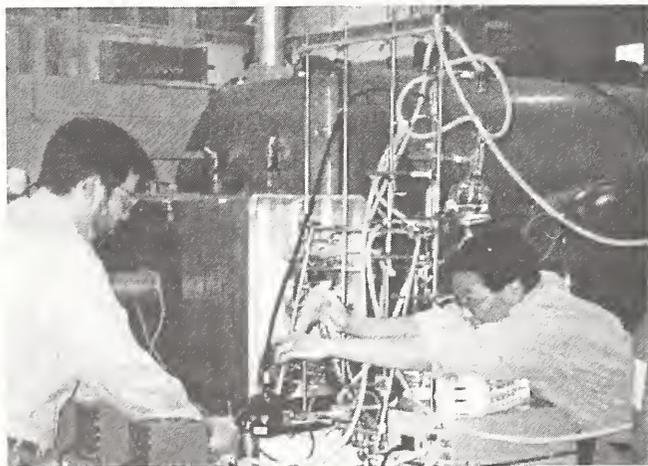
Figure 1. Prof. Kaler (L) and graduate student Carlos Co (R) withdraw a polymerization sample for SANS measurement.
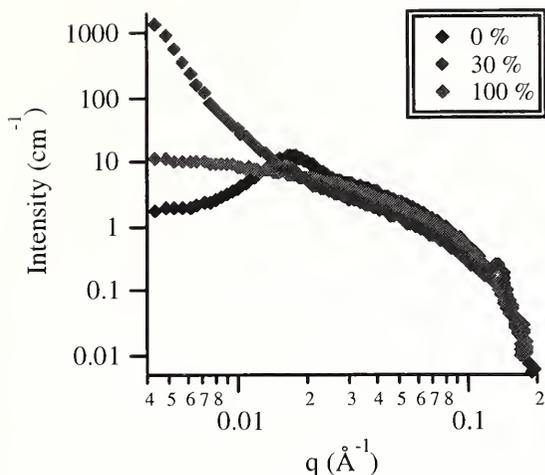
Figure 2. SANS spectra of the polymerizing hexyl meth-acrylate microemulsion as a function of monomer conversion.

inders 4 nm x 80 nm [3]. This novel ordering behavior is not fully understood, but is in sharp contrast to the smooth structural changes seen in microemulsion polymerization. On-line polymerization SANS measurements provide a visualization of the evolving microstructure that cannot be provided by other methods, permitting validation of polymerization mechanisms.

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gates are not limited to globular structures. In particular, cylindrical surfactant structures can be polymerized. The surfactant cetyltrimethylammonium 4-vinylbenzoate forms viscoelastic solutions in water containing cylindrical micelles of 4 nm diameter and thousands of nanometers long. The SANS curves in Figure 3 show the evolution of structures from the initial charged micelles to the final polymerized cylinders. At intermediate (20 - 70%) conversion the reacting system passes through a highly turbid and ordered phase, with a sharp peak indicating a well-defined spacing of 5 nm. The ordered phase abruptly disappears, resulting in a stable dispersion of discrete, polymerized cyl-
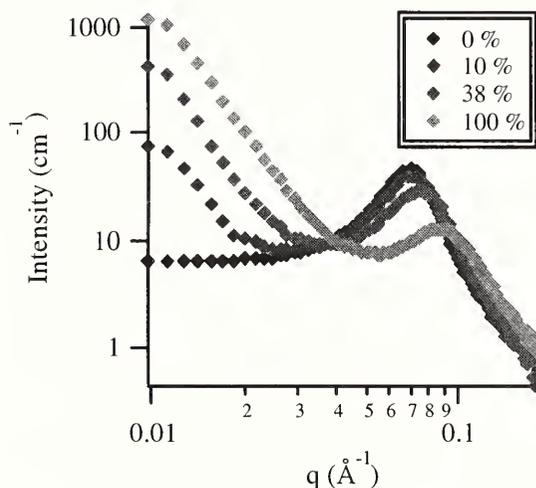
Figure 3: SANS spectra of polymerizing cetyltrimethylammonium 4-vinylbenzoate micelles as a function of time (increasing conversion).

Arborescent Graft Polymers

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Arborescent graft polymers (AGP) are a new class of polymer molecules with potential for use as drug delivery systems, monomolecular micelles for catalyst dispersions, waste water treatment and flow modifiers. AGP's are highly branched (i.e. treelike or arborescent) macromolecules synthesized by successive generations of functionalization and grafting reactions [1]. These molecules fall into a class of controlled architecture polymers that have generated considerable research interest in recent years and include dendrimers, arborescent, and hyperbranched polymers [2]. The applications envisaged for these types of polymers are based on exploiting the highly branched architecture of the polymers and require an understanding of the size and shape of the molecules in solutions and mixtures with other polymers. Small-angle neutron scattering (SANS) has been used to provide the foundation for understanding the shape-property relationships in these systems.

The chain architecture of AGP's is shown schematically in figure 1. The synthesis goal is to provide methods for producing polymers with controllable size, shape and functionality for use in such applications as coatings, membranes, drug release systems and flow modifiers. By synthesizing molecules with an outside shell of a hydrophilic polymer and an inner core of a hydrophobic polymer these molecules can act as water dispersible monomolecular micelles which can absorb organic molecules from waste water or help to disperse water insoluble catalyst systems. In order to design APG's for specific applications it is necessary to have detailed information on the intermolecular density profile, molecular size and shape in solutions and in mixtures with other polymers. We have been using small angle neutron scattering (SANS) to measure the size and shape of APG's under a range of different conditions.

SANS curves for a series of polystyrene AGP's as a function of generation in deuterated cyclohexane at 30°C is shown in figure 2. The radii of gyration (R_g) of the polymers were measured and are plotted as a function of generation in figure 3.

For generations 0 and 1 the size of the molecules is essentially equivalent under all measured con-
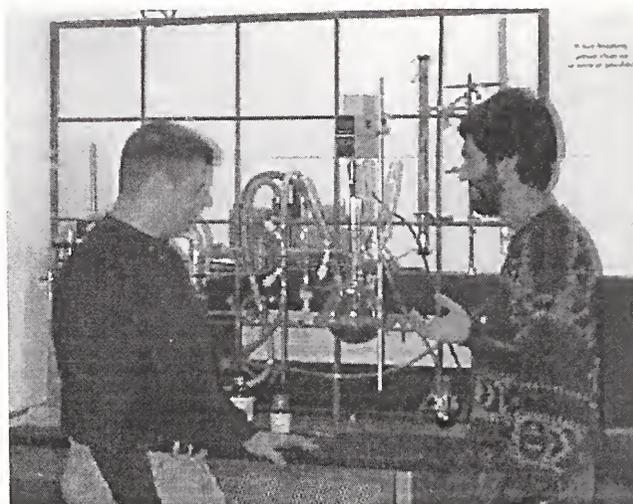
Andy Kee (left) and Mario Gauthier (right) discussing the synthesis of arborescent polymers.

ditions while for generations 2 and 3 the molecules vary in size significantly (particularly for generation 3) depending on the solvent or matrix polymer. The generation 3 molecules show the largest expansion in (deuterated) toluene which has the highest solvent power of the various systems studied. The most compact structure for the generation 3 molecule occurs in linear (deuterated) polystyrene. For comparison the R_g of a
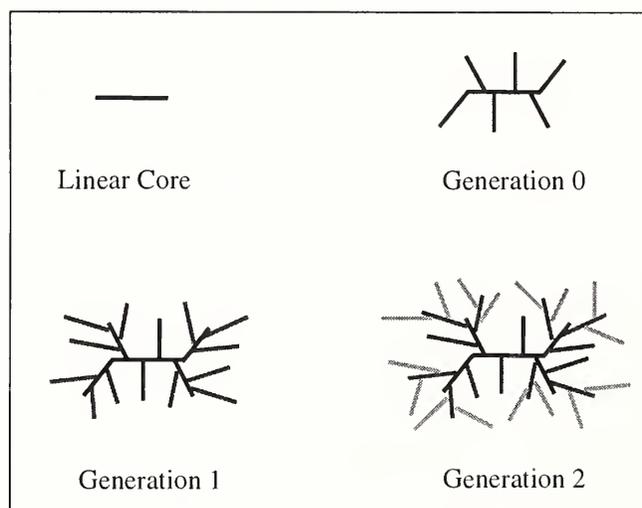
Figure 1. Schematic representation of arborescent graft polymer chain architecture.
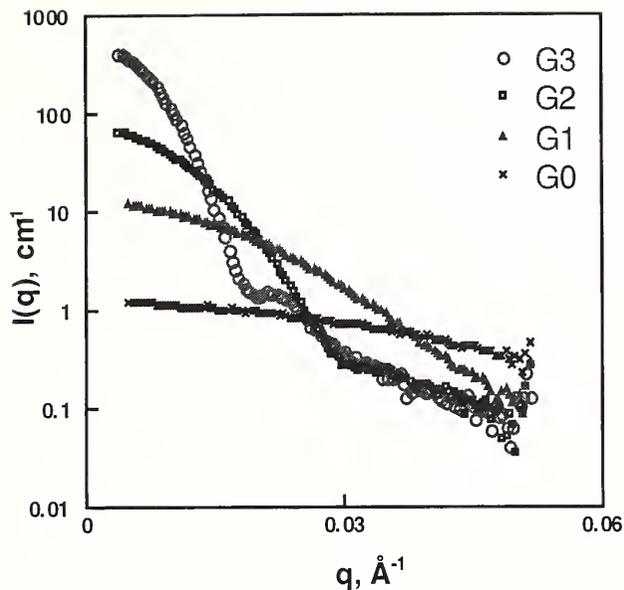
Figure 2. SANS data for all generations of polystyrene

mating the solvating power of these systems for use as monomolecular micelles and for understanding the role of entanglements in determining their flow properties.

The SANS data for generation 3 arborescent graft polymers in deuterated cyclohexane showed a clear Guinier region and a second interference peak at
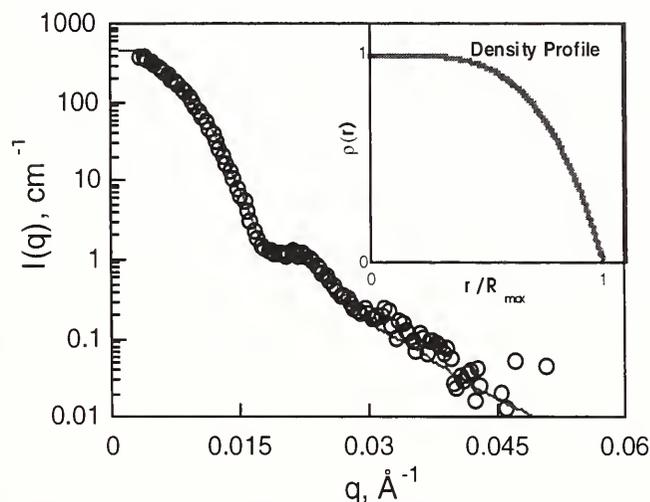
Figure 4. Scattering function calculated (solid line) compared with SANS data.

sphere was calculated assuming the generation 3 molecule was collapsed to bulk density. The R_g obtained was 170 Å which is close to the R_g of the generation 3 polymer in linear (deuterated) polystyrene. This indicates that the generation 3 molecules should be essentially non-interpenetrating and the linear polystyrene matrix chains are largely excluded from the arborescent graft molecules. This data is important for esti-

higher q which can be attributed to the single particle form factor (figure 4). A power law function was used to estimate the intermolecular density profile and calculate the scattering for comparison with experiment (see $\rho(r)$ inset in figure 4).

Our neutron scattering work indicates that for the largest molecules studied (generation 3) the shape of the molecules is quite compact, and in mixtures with linear polymer chains there is relatively little interpenetration of the arborescent molecules by the linear chains. These results will help guide chemists in synthesizing new types and variations of arborescent graft polymers to exploit the unique possibilities of shape-tailored molecules for a range of applications.

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Figure 3. Radius of gyration of polystyrene AGP's in solutions and blends for all generations.

The Vibrational Isocoordinate Rule in Se-As-Ge Glasses

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Inorganic glasses are among the most widely used classes of materials, yet they remain poorly understood at the atomic level, because the lack of long-range atomic order makes it difficult to obtain detailed information. Drawing unifying concepts from data on many materials, and identifying exceptional cases that can have potential value to technology, are the goals of a neutron scattering program at the NCNR.

Chalcogens (S, Se or Te) combined with Column IVB or VB elements form a large variety of covalent systems which readily form glasses when quenched from the melt [1]. They offer a wide range of optical and electronic applications. For example, transmission bands in the infrared region of the spectrum permit applications such as fibers for IR laser surgery, cutting and welding, night-vision devices, etc. which are based on selecting materials to optimize transmission in a particularly useful IR band. Chalcogenide glasses are also used in extremely fast switching devices, in X-ray imaging, and in imagers for video cameras. In terms of basic physics, these materials present a fertile testing ground for studying the effect of network topology on glass properties.

In the Se-As-Ge system, Se atoms are almost always covalently bonded to two other atoms, while As and Ge are respectively almost always 3- and 4-coordinated. An isocoordinate rule is one that identifies a property of a multicomponent covalent network glass system that stays constant for all compositions which have the same average coordination number, $<r>$. There are several of these evident in ternary Se-based glass alloys. Examples are the glass transition temperature, softening temperature, elastic constants, measures of hardness, and Se-H spectral hole-burning relaxation. Most of these rules cover behavior that is nearly static and on a macroscopic length scale. Our neutron scattering experiments extend the range of times involved in these rules by many orders of magnitude. We have identified a simple feature in the *dynamics* of chalcogenide glasses, the vibrational isocoordinate rule (VIR), which states that *up to some frequency the vibrational density of states (VDOS) is the same for alloys having the same $<r>$ [2].* This observation extends the time scale for the operation of such rules to the picosecond regime and the length scale to a few bondlengths.

Fig. 1 shows the Generalized Vibrational Density of States (GVDOS) measured by neutron TOF inelastic scattering for several Se-As-Ge glasses. Some data sets were measured at NIST-CNR using the Fermi Chopper Spectrometer (FCS) and some at the IN4 TOF spectrometer at ILL. There are two or three curves for each value of $<r>$ which correspond to the compo-
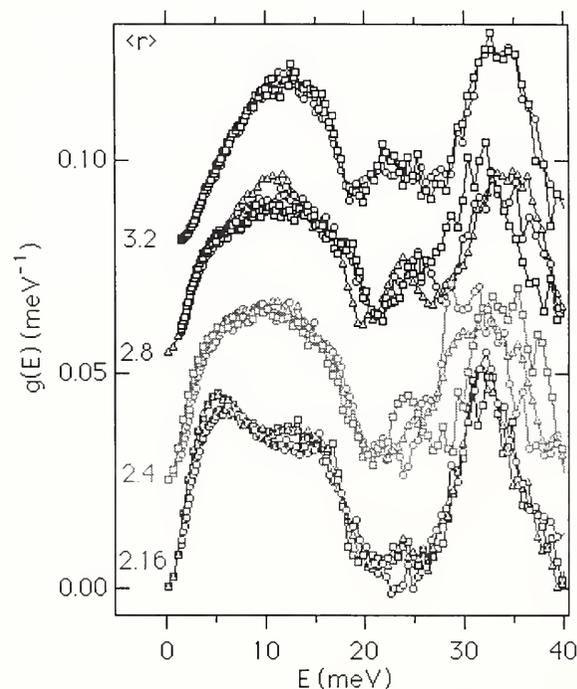
Figure 1. The VIR is best shown by plotting GVDOS of isocoordinated alloys on top of each other. $<r> = 2.16$: ? $Se_{92}Ge_{08}$ (IN4), [a]$Se_{89}As_{06}Ge_{05}$ (IN4), o $Se_{84}As_{16}$ (FCS); $<r> = 2.4$ including the binary alloys terminating the isocoordinate line are shown: [a] Se_8Ge_2 (IN4), ? $Se_{675}As_{250}Ge_{075}$ (IN4), o Se_3As_2 (FCS). $<2> = 2.8$: [a]$Se_{51}As_{18}Ge_{31}$ (IN4), o $Se_4As_4Ge_2$ (FCS), ? $Se_3As_6Ge_1$ (FCS); $<r> = 3.2$: o $Se_{25}As_{30}Ge_{45}$ (FCS), ? $Se_{175}As_{450}Ge_{375}$ (FCS). Starting from the bottom, successive data curves are shifted up by 0.025 units on the vertical scale.

sitions indicated in the figure caption. The data at $<r>$ = 2.4 are particularly remarkable in that they include As_2Se_3 having a nearly 2-D network and Ge_2Se_8 which has a network closer to 3-D in character. The energy bands below 20 meV are nearly identical. Near 25 meV the VIR breaks down since the tetrahedral breathing mode appears in the Ge glass but not in the As one, i.e. the short range order of the network matters for this mode. Apparently the VIR holds when *network connectivity and not short-range order* is important.

A clear departure from the VIR for $<r>$ = 2.6 is shown in Fig. 2. The GVDOS of the lower curve, which clearly follows the trend of Fig. 1, is for $Se_{55}As_{30}Ge_{15}$. The upper curve displaying several sharp features is for glassy As_3Se_2. Surprisingly, these features are not evident in Raman scans in this glass. The origin of these features is not yet certain, but it is probable that they arise from a nanoscopic phase separation of isolated molecules within the glass that retain their well-defined molecular vibrational modes. Evidence supporting this view is that one can make several As_xSe_{1-x} glasses for $x > 0.5$ which display sharp features at the *same* frequencies, thus pointing to the

the exception of a small region near the composition As_6Se_4. (2) Highly unusual behavior is observed for As_6Se_4 indicating the formation of molecular clusters or small structural units. The combination of (1) and (2) is intriguing, and may be relevant to unusual photocontractive effects that recently have been observed in As-Se thin films. Better understanding of the structural properties of the Se-As-Ge forms an improved basis for potential applications.

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Figure 2. The bottom curve: ? $Se_{55}As_{30}Ge_{15}$ (FCS) follows the VIR. The top curve: o As_3Se_2 (FCS) is an exception to the VIR. Both datasets are for $<r>$ = 2.6. Starting from the bottom, successive data curves are shifted up by 0.030 units on the vertical scale.

same molecular species.

The conclusions of this research are twofold: (1) The VIR is followed closely across the entire glass-forming region of the Se-As-Ge phase diagram, with

Membrane Mediated Polymer Interdiffusion

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Understanding the interdiffusion of polymer chains at interfaces is critical to many applications such as coatings, adhesion, composite lamination and fracture strength development. Neutron reflectivity has proven to be a very powerful technique for studying polymer interdiffusion at polymer-polymer interfaces [1]. These studies have examined the role of temperature and molecular weight on interdiffusion between hydrogenated and deuterated polymer bilayers. More recently, the sensitivity of the neutron reflectivity technique has allowed the analysis of thickness dependent diffusion when the film thickness approaches the radius of gyration of the polymer.

The present study probes how the introduction of ultra-thin barrier layers between the interdiffusing polymers affects their dynamics. The study of interdiffusion through barrier membranes is of significant importance in many areas of material science, including metallurgy, biology and polymer science. As an example, consider a system where the barrier is in fact an oxidized layer brought about by degradation of one of the materials. This is an important aspect in materials science where the effects of oxide layers on the interdiffusion in metallic systems have received considerable attention [2]. For polymeric systems one can create an ultra-thin barrier membrane composed of a crosslinked polymer. The crosslinking makes the barrier insoluble in the surrounding polymers while still allowing the interdiffusion of polymers through the membrane.

The geometry of a model system designed for this study is shown in Fig. 1. It is a trilayer system, containing two polystyrene (PS) layers separated by a membrane. One of the polymer layers (either the top or bottom layer) is hydrogenated while the other is deuterated. Molecular weights of both the hydrogenated and deuterated polymer layers were closely matched ($hPS: M_w = 40$ kg·mol^{-1}; $dPS: M_w = 39$ kg·mol^{-1}).

The sample was prepared in three stages. First, a polymer layer was spin coated on a silicon substrate covered with a uniform oxide layer (~10Å). The barrier membrane itself consisted of a blend of isopentylcellulose cinnamate (IPCC) and PS (34 wt%). It was transferred on top of the bottom polymer layer
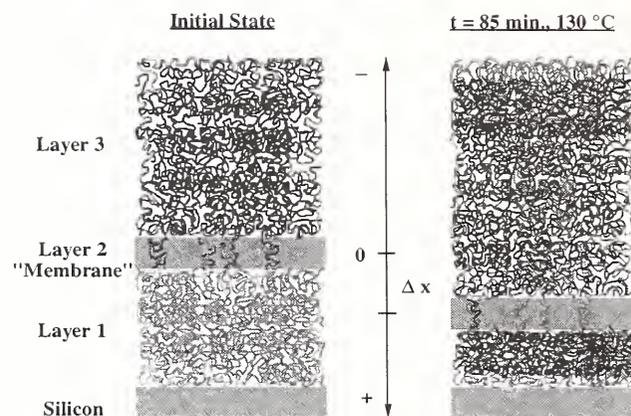
Figure 1: Schematic drawing of the sample geometry for Air//hPS/IPCC(34 wt% PS)/dPS//SiO/Si. Red (dPS) and blue (hPS) are used to distinguish between isotopically different polymer chains. The membrane (green) is displaced by Δx from its original position as hPS and dPS mix during annealing.

by the Langmuir-Blodgett technique. The IPCC/PS layers can be transferred in increments of 10Å. Using a blend of IPCC and PS as a membrane material allows for the control of the membrane's porosity as the PS component is free to leave the barrier layer during the experiment thereby creating holes and channels in the membrane's network which facilitate PS transport across the membrane. In the present case the IPCC (34 wt%PS) membrane is 60 Å (6 layers) thick. After transfer the IPCC in the film was cross-linked for 15 min. by UV irradiation under a nitrogen atmosphere. The third and final PS layer was floated on top of the sample. The trilayer system was dried under vacuum at 70 °C to remove residual solvents from the polymer. The thickness and roughness of the trilayer system was characterized at each stage by x-ray reflectivity.

A neutron reflectivity curve from the as prepared sample

Air // hPS/IPCC(34 wt% PS)/dPS // SiO$_2$/Si

is shown in Fig. 2. The orange curve is a fitted reflectivity profile based on the corresponding scattering length density profile (sld) shown in the inset (also orange). The position of the three films, dPS (~500 Å), IPCC(34 wt% PS) membrane (~60 Å), and hPS (~800 Å) can be accurately determined by neutron

reflectivity. After annealing the sample at 130 °C for 80 minutes, changes in the thicknesses and compositions of the PS layers as well as the location of the membrane can be obtained by fitting the reflectivity data (brown). The inset shows the corresponding sld profile (also brown) for the annealed sample revealing an excess of dPS at both the air and SiO interfaces as has been observed in blank experiments[2] with bilayers of dPS and hPS without the membrane. It takes about 10 times longer to achieve this final state with the membrane present (80 min) than the corresponding time without a membrane (8 min).

More important, we see a movement of the membrane, Δx, relative to its initial position as measured from the Si interface. Neutron reflectivity measurements are very sensitive to the location of the membrane in this trilayer system and its position can be very accurately tracked as a function of annealing time which is shown for this sample in the upper half of Fig. 3. At later annealing times (80 min), the membrane has moved by ~120 Å from its original position in the
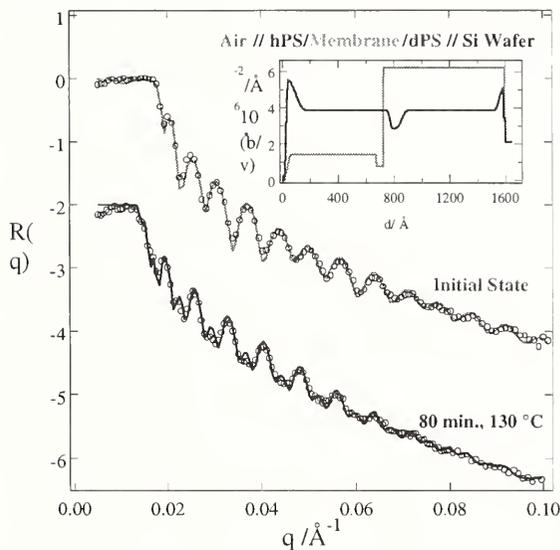
Figure 2: Neutron reflectivity data for initial and final state of the sample Air//hPS/IPCC(34wt% PS)/dPS// SiO$_2$/Si. The lines are the best fit to the data.

film relative to Si.

An interesting result is observed in a sample where the position of the dPS and hPS layers have been switched. The bottom panel of Fig. 3 shows the relative movement of the membrane in a sample

Air // dPS/IPCC(34 wt% PS)/hPS // SiO$_2$/Si

as a function of annealing time. It is obvious that the two different geometries result in a reversal of the travel direction of the membrane. In both cases, the membrane moves towards the dPS rich side of the membrane indicating a higher mobility of dPS through the membrane as compared to hPS.

In bilayer interdiffusion studies the influence of unmatched molecular weights has been investigated where the movement of the diffusion boundary has been tracked by observing the movement of gold marker particles (3). Those results show a movement of the interdiffusion boundary towards the direction of the lower molecular weight component. In the present study, the molecular weights of the hPS and the dPS were closely matched, therefore the observed movement of the membrane can be connected to slightly different interactions between the membrane's material (IPCC) and the two isotopically different polymers hPS and dPS leading to a higher permeability of dPS through the barrier.

This result opens up the possibility of a number of new experiments in this area. These include the
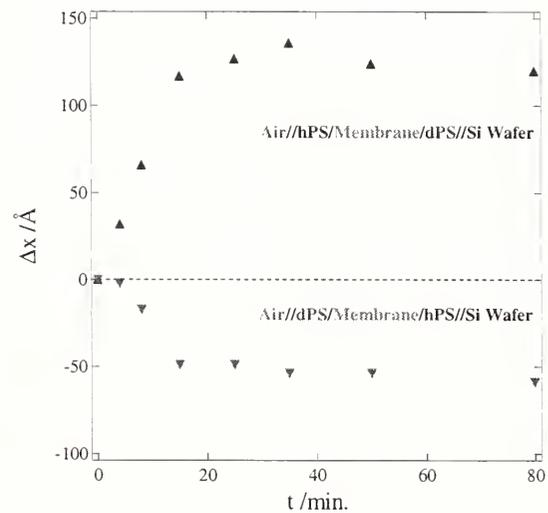
Figure 3: Displacement of the membrane relative to Si

effects on the mobility of polymers through membranes as a function of: 1) the molecular weight of the polymer, 2) the degree of crosslinking of the barrier layer, 3) the wt% of PS in the membrane (porosity), and 4) the thickness of the barrier. Besides providing valuable insight into the transport properties of ultra-thin membranes, this project serves as a stepping stone for designing future reflectivity experiments to probe transport properties in biological membranes.

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Interactions

A User Facility: Neutrons for the U.S. Research Community

The NCNR is a national resource, providing state-of-the-art neutron beam instrumentation for industry, government, and university research programs. User activity has increased rapidly as the number and capability of the instruments has risen. As shown in Fig.1, user participation has tripled since the start of operations in the NCNR guide hall in 1990.

In FY98:
37 Government Agencies
57 Industrial Organizations
96 U.S. Universities

Cold Source Upgrade
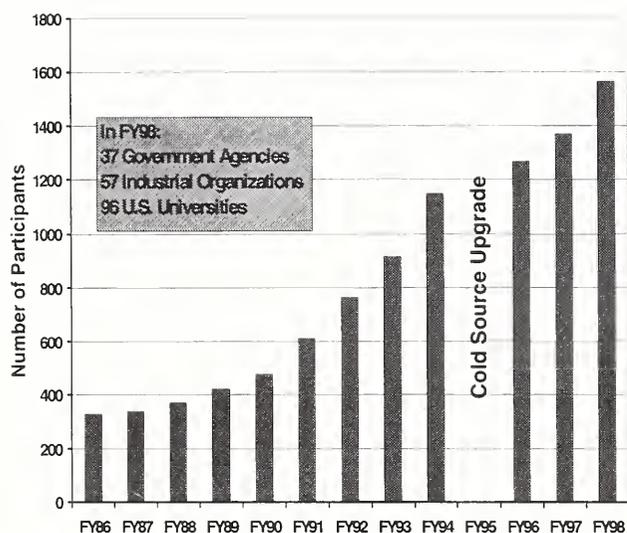
Fig. 1. Research participants at the NCNR.

The bar at far right in Fig. 1 represents participants from 96 universities, 37 government institutions, 57 U.S. industrial laboratories, and 168 foreign institutions. Participants include those who were at the NCNR at least once for an experiment or collaborated in other ways, such as sample preparation or co-authoring a publication. NIST researchers comprise a small fraction of the total user population, but are naturally a critical factor, often enabling other users to perform the best measurements possible.

The NCNR has always striven to enable researchers to obtain access through procedures that are appropriate for their needs, without excessive delay or bureaucracy. In practice, that has meant allowing several different modes of access through formal proposals, informal collaborations, and Participating Research Teams. In some cases, industrial R&D of a proprietary nature is carried out at the NCNR, provided that appropriate beam-time charges are paid on a full-cost-recovery basis to the U.S. government.

Formal User Program

The Program Advisory Committee (PAC) is the body primarily responsible for proposal review and user policies. The PAC advises the NCNR Director on these and other aspects of the NCNR operation. Its current (1997-1998) membership includes Jill Trewhella (chair, Los Alamos National Laboratory), William Graessley (Princeton University), Sanat Kumar (Penn State University), Gabrielle Long (NIST), Laurence Passell (Brookhaven National Laboratory), Sunil Sinha (Argonne National Laboratory), Thomas Russell (University of Massachusetts), and Emile Schweikert (Texas A&M University). The PAC membership represents a wide range of expertise in neutron beam research, and advises NIST on many aspects of the research activities and instrumentation at the NCNR, especially those concerning user interaction.

The most direct area of involvement for the PAC lies in the formal research proposal system, which is based on a submission deadline and subsequent review at six- to eight-month intervals. After each deadline, proposals are peer-reviewed by mail or electronic mail by experts in the research area specific to each proposal. The PAC then meets to consider the proposals with their reviews, together with technical and safety reviews provided by NCNR staff, and makes recommendations for approval or rejection and allocation of specific amounts of beam time for each proposal.

The PAC met twice at NIST during FY 1998, first on November 21, 1997, and again on July 13-14, 1998. 130 proposals were reviewed on the first occasion, and 162 proposals requesting 1563 instrument-days on the second. The review was confined to proposals for small-angle neutron scattering (SANS), reflectometry, cold-neutron triple-axis spectrometry, and time-of-flight spectroscopy. Other categories of proposals, such as powder diffractometry and chemical analysis, are reviewed on a continuing basis rather than at the regular PAC meetings. Both the number of proposals and the number of requested instrument-days show a continuing growth. For comparison, the call for proposals in August 1995 stimulated 100 proposals requesting 549 instrument-days.

The two 30-m SANS diffractometers still account for the largest category of proposals (67 during the last proposal round), but proposals for the two reflectometers have risen to a comparable number (58 during the last round). The demand for SANS is now rising relatively slowly, while that for reflectometry still shows strong growth. The oversubscription in number of instrument-days (i.e., days requested divided by days available) was approximately 3 for reflectometry, and approximately 2 for SANS and inelastic scattering. The oversubscription for the reflectometers was high at both PAC meetings in FY 1998, despite the provision of more instrument-days for users at the second meeting. There are plans to construct another reflectometer in the near future to accommodate the increasing demand, especially in the area of biology, where experiments can require large blocks of beam time.

The demand for high-resolution inelastic neutron scattering is also increasing. The number of proposals for the SPINS spectrometer (cold-neutron triple-axis with polarized beam option) was 15 in Nov. 1997, and 24 in July 1998. In the last instance, the oversubscription in instrument-days was 2.9. Requests for the Fermi-chopper time-of-flight spectrometer also showed growth, with 9 proposals in 1996, 13 proposals in Nov. 1997, and 15 proposals in July 1998, with an oversubscription of 1.4 at the last PAC meeting. The three new inelastic scattering instruments about to come into operation will stimulate further demand, so that this proposal category should show a substantial increase in the near future. The next call for proposals will offer the backscattering spectrometer, which is now operational, to users on a limited basis. The disk-chopper time-of-flight spectrometer and the spin-echo spectrometer are nearing completion and will be offered to users in the near future.

In addition, time on the 32-detector powder diffraction instrument at BT-1 is also available for users through proposals. For the present, sufficient time is available for all proposals received, and time is directly scheduled by the NCNR staff when proposals are received. During the past year, approximately 80 proposals were granted time on this instrument, approximately half of which were from outside users.

Some users devote a substantial part of their research effort to neutron scattering measurements at the NCNR. At the most recent PAC meeting, it was felt that these users would make best use of their instrument time if they could be assured of access to beam time distributed over an extended period of about two years. The PAC therefore recommended that a new proposal category be instituted, called program proposals. The latter would be longer and more detailed than a regular proposal, describing a course of measurement rather than a single experiment. NCNR management agreed to implement program proposals on a trial basis.

Collaborations

Direct collaborations remain a common way to access the instruments at the NCNR, accounting for approximately 60% of the number of instrument-days. The thermal-neutron triple-axis spectrometers are mainly scheduled in this way. Most of the time reserved for NIST researchers on other instruments is also devoted to experiments that are collaborations with non-NIST personnel.

Participating Research Teams

Another mode of access to NCNR instrumentation takes place through Participating Research Teams (PRT). In this case, groups of researchers join together to build and operate an instrument, using additional funding derived outside of NIST (although NIST does participate in some PRTs). Three-quarters of the time on such instruments is reserved for the PRT, and the balance is allocated to general user proposals. Several instruments have been developed in this way, and others are under consideration. One particular version of this is the Center for High Resolution Neutron Scattering (**CHRNS**), which is funded by the National Science Foundation (NSF) and NIST. The instruments include a 30 m SANS machine, a Spin Polarized Inelastic Neutron Spectrometer (SPINS), and a perfect crystal very low angle SANS now under development at BT-5. In CHRNS, all of the NSF time is returned to the general user community for allocation by the PAC. A detailed description of the activities of CHRNS is prepared as an annual report to the NSF, and is available on request.

Feedback from Users

Users are encouraged to offer their comments concerning the instrumentation, operations, and policies at the NCNR. Their input is being obtained in several ways. First, the NCNR local contact personnel interact directly with each research group using the facility. This informal method typically identifies concerns about a specific instrument. Responsibility for

action then resides with the cognizant NCNR instrument scientist. Users may also offer comments on a form provided on the facility Web pages. The NCNR Researcher's Group, an independent body currently chaired by Professor Anne Mayes of MIT, is in the process of obtaining further information through a survey of its membership.

Other communication with users

For the past several years, the primary means of communication with the NCNR user community has been through electronic mail and the facility Web pages at http://rrdjazz.nist.gov. For almost all the major neutron scattering instruments, beam time requests that are not formal proposals must be submitted through a Web page form. Most formal proposals for beam time are submitted using the same form, accounting for approximately 80% of proposals received in response to the last call. The current hit rate for the NCNR web page is 1 M/year. Electronic submission has many advantages, facilitating the compilation of a comprehensive database on investigators, proposals, referees, and experiments. This is extremely useful in the increasingly complicated task of assigning and scheduling beam time and equipment, and in making administrative decisions concerning NCNR operations.

Independent Programs

The **Polymers Division** of the Materials Science and Engineering Laboratory has two major program elements at the NCNR. For the first, the objectives are to help the U.S. microelectronics and supporting infrastructure industries by addressing their most pressing materials measurement and standards issues. In today's ICs and packages the feature size is ever shrinking, e.g., on the chip level the feature size is approaching 250 nm while the size of a polymer molecule is typically 5-10 nm. As feature size shrinks the structure and properties of interfaces play an increasingly important role controlling the properties of the polymer layers used in interconnects and packages. In this program both neutron reflectivity and neutron scattering have played an essential role for characterizing polymer/metal interfaces including local chain mobility, moisture absorption, glass transition temperature and crystalline structure. For the second, the objective is to understand the underlying principles of phase behavior and phase separation kinetics in the bulk and on surfaces of polymer blends in order to facilitate morphology/structure control during processing. SANS and reflectivity measurements in equilibrium, in transient, and under external field provide essential information for general understanding as well as for specific application of polymer blend/alloy systems. Customers include material producers and users, ranging from chemical, rubber, tire, and automotive companies, to small molding and compounding companies. The focus of research on polymeric materials includes commodity, engineering and specialty plastic resins, elastomers, coatings, adhesives, films, foams, fibers, and non-woven's.

The **Exxon Research and Engineering Company** is a member of the Participating Research Team (PRT) that operates, maintains, and conducts neutron-related research activities at the NCNR's NG7-30M SANS and NG5-Neutron Spin Echo Spectrometer (to be dedicated soon) instruments. The mission is to use those instruments, as well as other neutron scattering techniques, to conduct scientific research that complements the research activities at Exxon's main laboratories as well as at its affiliates' laboratories throughout the world. The aim of these research activities is to deepen knowledge of the nature of the products and processes of the business so as to better serve customers and to improve the return on shareholders' investment. In line with that, and taking full advantage of the unique properties of neutrons, most of the experiments use SANS or other neutron techniques to study the structure and dynamics of hydrocarbon materials, especially in the fields of polymers, complex fluids, and petroleum mixtures. Exxon views its participation in the NCNR and collaborations with NIST and other PRT members as an excellent investment for the company and a good way to contribute to the scientific health of the nation.

The **Nuclear Methods Group** (Analytical Chemistry Division, Chemical Science and Technology Laboratory) has as its principal goals the development and application of nuclear analytical techniques for the determination of elemental compositions with greater accuracy, higher sensitivity and better selectivity. A high level of competence has been developed in both instrumental and radiochemical neutron activation analysis (INAA and RNAA). In addition, the group has pioneered the use of cold neutron beams as analytical probes with both prompt gamma activation analysis (PGAA) and neutron depth profiling (NDP). PGAA

measures the total amount of a particular analyte present throughout a sample by the analysis of the prompt gamma-rays emitted during neutron capture. NDP, on the other hand, determines concentrations of several important elements (isotopes) as a function of depth within the first few micrometers of a surface by energy analysis of the prompt charged-particles emitted during neutron bombardment. These techniques (INAA, RNAA, PGAA, and NDP) provide a powerful combination of complementary tools to address a wide variety of analytical problems of great importance in science and technology, and are used to help certify a large number of NIST Standard Reference Materials. During the past several years, a large part of the Group's efforts has been directed towards the exploitation of the analytical applications of the guided cold-neutron beams available at the NIST Center for Neutron Research. The Group's involvement has been to design and construct state-of-the-art cold neutron instruments for both PGAA and NDP and provide facilities and measurements for outside users, while retaining and utilizing our existing expertise in INAA and RNAA.

The **Center for Food Safety and Applied Nutrition**, U. S. Food and Drug Administration (FDA), directs and maintains a neutron activation analysis (NAA) facility at the NCNR. This facility provides agency-wide analytical support for special investigations and applications research, complementing other analytical techniques used at FDA with instrumental (INAA), neutron-capture prompt-gamma (PGAA), and radiochemical Neutron Activation Analysis (NAA) procedures, radioisotope X-ray fluorescence spectrometry (RXRFS), and low-level gamma-ray detection. This combination of analytical techniques enables diverse multi-element and radiological information to be obtained for foods and related materials. The NAA facility supports agency quality assurance programs by developing in-house reference materials, by characterizing food-related reference materials with NIST and other agencies, and by verifying analyses for FDA's Total Diet Study Program annually. Other studies include the development of RXRFS methods for screening foodware for the presence of Pb, Cd and other potentially toxic elements, use of INAA to investigate bromate residues in bread products, and use of PGAA to investigate boron nutrition and its relation to bone strength. FDA's NAA laboratory personnel frequently provide intra-agency technical assistance, the most recent example being participation in the production of the document "Accidental Radioactive Contamination of Human Food and Animal Feeds: Recommendations for State and Local Agencies" by the Center for Devices and Radiological Health.

The Neutron Interactions and Dosimetry Group (Physics Laboratory) provides measurement services, standards, and fundamental research in support of NIST's mission as it relates to neutron technology and neutron physics. The national and industrial interests served include scientific instrument calibration, electric power production, radiation protection, defense nuclear energy systems, radiation therapy, neutron radiography, and magnetic resonance imaging. The Group's activities may be represented as three major activities. The first is Fundamental Neutron Physics - including operation of a neutron interferometry and optics facility, development of neutron spin filters based on laser polarization of ^{3}He, measurement of the beta decay lifetime of the neutron, and investigations of other coupling constants and symmetries of the weak interaction. This project involves a large number of collaborators from universities and national laboratories. The second is Standard Neutron Fields and Applications - utilizing both thermal and fast neutron fields for materials dosimetry in nuclear reactor applications and for personnel dosimetry in radiation protection. These neutron fields include thermal neutron beams, "white" and monochromatic cold neutron beams, a thermal-neutron-induced ^{235}U fission neutron field, and ^{252}Cf fission neutron fields, both moderated and unmoderated. The third is Neutron Cross Section Standards - including experimental advancement of the accuracy of neutron cross section standards, as well as evaluation, compilation and dissemination of these standards.

Several universities have also established long term programs at the NCNR. The **University of Maryland** is heavily involved in the use of the NCNR, and maintains several researchers at the facility. **Johns Hopkins University** participates in research programs in solid state physics and in instrument development at the NCNR. The **University of Pennsylvania** is working to help develop biological applications of neutron scattering. It is also, along with the University of California, Santa Barbara, duPont, Hughes, and Allied Signal participating in development of a new filter analyzer neutron spectrometer. The **University of Minnesota** participates in two PRTs; the **University of Massachusetts** participates in one.

Reactor Operations and Engineering

Reactor Operations and Engineering Group after award of Department of Commerce award for outstanding service.

Reactor on-line time for the year was 67% of real time, which is excellent, compared to the maximum achievable of 73%. The reason for the slightly lower on-line time than last year's 70% is two fold. There was a one-week shutdown for shipment of spent fuel and a three-week shutdown for licensing of new personnel and requalifying of current operators. This time was also used to perform maintenance on the guide tubes and refurbish the cooling tower. In addition, towards the end of the year, a very small leak, on the order of 0.01 liter per hour was discovered in the vicinity of the thermal column. As a result, it was decided to shut down the reactor and search for the leak. After an exhaustive search and testing, the source of the leak was not found and the leak had not returned. The situation will continue to be monitored.

Three new operators received their senior operator license following comprehensive written, oral, and operating examinations by the Nuclear Regulatory Commission. They passed their examinations and qualified with distinction achieving near perfect scores in all categories. All 17 currently licensed personnel passed their requalification examinations.

For the first time in ten years, three shipments of spent fuel were made to the DOE facilities at Savannah River, South Carolina. The shipments consisted of 126 elements equivalent to about 5 years of 20 MW operation. This has greatly relieved storage space in the spent fuel pool. Two more shipments are scheduled for the latter part of 1999.

Plans are underway for comprehensive review of all major reactor systems for upgrade or improvement. An outage of 3 – 5 months is scheduled for early 2000 to replace the control rods and the heavy water and to perform other maintenance items. Plans are also being made, if time permits, to replace the existing cooling tower with a larger wet-dry tower of new design and to replace the existing cold source with an advanced version that will double the flux.

An updated safety analysis report is in the final stages of review. It will be submitted to the Nuclear Regulatory Commission next year as the first step in the relicensing of the reactor.

Instrumentation Developments

High-flux Backscattering Spectrometer Commissioned

The first vanadium spectrum from the NCNR high flux backscattering spectrometer (HFBS) was obtained in June of 1998 after a design and construction effort lasting more than six years. The measured energy resolution of $0.9\ \mu eV$ is a factor of 50 better than that routinely obtained using any other spectrometer currently in operation at the NCNR (Figure 1). This exceptional energy resolution will enable the investigation of many types of dynamical processes in materials, including molecular reorientations, diffusion, dynamics of liquids, glasses and polymers, and critical scattering near phase transitions.
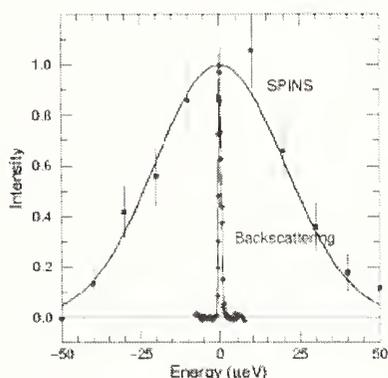
Figure 1. Comparison of resolution of HFBS to SPINS (Cold Neutron Triple Axis spectrometer).

A backscattering spectrometer can be viewed most simply as a limiting case of a triple-axis spectrometer where the scattering angles of the neutrons from both the monochromator and analyzer crystals are 180 degrees[1]. This geometry decouples the beam divergence from the energy resolution allowing the instrument to achieve an ultimate energy resolution defined by the properties of the crystals. The HFBS uses the (111) reflection from bent silicon crystals to both monochromate and analyze the neutron energies. The final energy, defined by the Bragg condition from the silicon analyzers, is 2.08meV corresponding to a neutron wavelength of 6.27Å. The incident energy is varied by shaking the monochromator using a cam-operated drive system thereby Doppler shifting the incident neutron energy. To date, this device has been
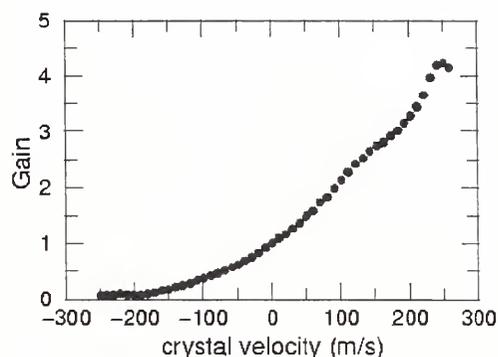
Figure 2. Measured gain from use of phase space transform chopper.

used to obtain energy transfers of +/- $45\mu eV$. The ultimate overall energy transfer range measured by this instrument will exceed $50\mu eV$.

The primary design goal of this instrument was to maximize the count rate for a given experiment while maintaining an energy resolution of better than $1\mu eV$ full width at half maximum (FWHM). This has been achieved by matching the divergence of the front-end of the instrument with the divergence of the secondary spectrometer, utilizing a phase-space transform (PST) chopper and by maximizing the area of coverage for the analyzer and monochromator crystals. The HFBS design incorporates a 4m long converging guide which increases the incoming beam divergence and results in
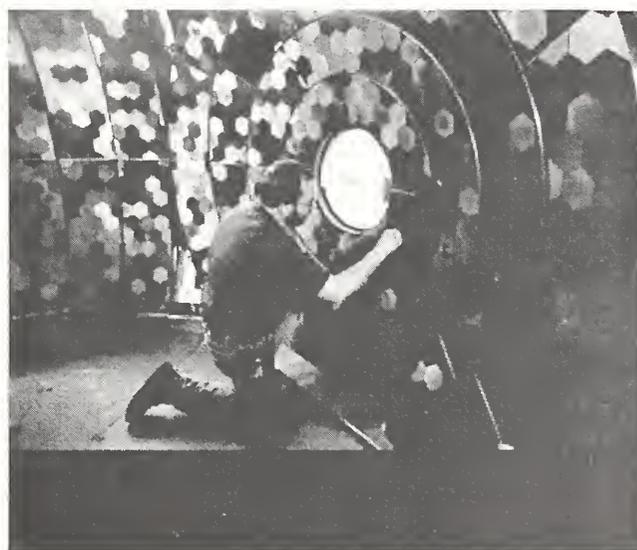
Figure 3. Scott Slifer adjusting the analyzer assembly on the HFBS.

47

3.9 times more flux at the end of the guide. The PST is a novel device, conceived originally by Schelten and Alefeld[2], which acts as a premonochromator for the instrument: reflecting the beam of neutrons towards the monochromator while focussing their energy distribution towards the narrow value required by the backscattering monochromator crystal. Measurements carried out at the HFBS have demonstrated for the first time that this device increases the neutron flux from the monochromator by more than a factor of four from that obtained with a stationary crystal (Figure 2). The spherically focussed monochromator and analyzer crystals cover very large areas (the analyzer subtends 20% of the total solid angle) and make the instrument very efficient in its use of the available neutrons (Figure 3).

Monte Carlo simulation of neutron beam lines

Monte Carlo simulation of cold neutron beam tube performance is a powerful tool for predicting neutron fluxes and developing optimized neutron scattering instrumentation. A Monte Carlo program has been developed at the NCNR which makes use of modeled reflectivity curves and parameterized neutron cross-sections to simulate the neutron beam delivery system. The neutron beam system may consist of any combination of straight, bent, focusing and channeled guide sections, circular and rectangular diaphragms, neutron collimators, neutron velocity selectors and variety of commonly-used cooled and room temperature crystal filters. The program can also allow for non-ideal configurations such as random Gaussian

These flux enhancing devices together with the flux available from the NG-2 guide have resulted in a measured flux at the sample position of 1.4×10^5 cm^{-2}-sec^{-1} in good agreement with calculations. This flux makes the HFBS competitive with any instrument of its kind in the world.

References

[1] P. M. Gehring and D. A. Neumann, Physica B **64**, 241-243 (1998).

[2] J. Schelten and B. Alefeld, in Proc. Of a Workshop on Neutron Scattering Instrumentation for SNQ, ed. R. Scherm and H. H. Stiller, Report Jul-1954, (1984)

guide section misalignments. Modeled guide coatings include natural Ni, ^{58}Ni, multilayer and supermirror. Using reference neutron spectrum data, gold foil activation data and measured reflectivity data obtained from two of the NCNR cold neutron beam tubes, the Monte Carlo program has been used to characterize the liquid hydrogen cold neutron source brightness. In turn, this brightness model has been incorporated into simulations of all the neutron beam tubes (NG-0-NG-7) installed on the NCNR cold source. Table 1 shows that the agreement of the simulated and measured capture fluxes is remarkably good. The program has been used extensively to predict and optimize the performance of projected future reconfigurations of the NCNR beam tubes as well as to characterize neutron fluxes per unit wavelength at locations where flux measurements are not yet available.

Guide system	ϕ_c^{meas} (cm^{-2}s^{-1})	ϕ_c^{sim} (cm^{-2}s^{-1})	ϕ_{int}^{sim} (cm^{-2}s^{-1})	$<\lambda>$ (Å)
NG-0 before NDP chamber	2.56×10^9	2.336×10^9	6.020×10^8	6.976
NG-1 at reflectometer monochromator	3.1×10^9	3.376×10^9	1.023×10^9	5.93
NG-2 before filter	3.5×10^9	3.498×10^9	1.055×10^9	5.96
NG-2 at HFBS shutter	2.15×10^8	2.094×10^8	6.08×10^7	6.20
NG-2 at HFBS (after converging guide)	8.29×10^8	7.75×10^8	2.25×10^8	6.20
NG-3 before SANS filter	1.7×10^9	1.725×10^9	5.30×10^8	5.85
NG-4 at DCS shutter	2.7×10^9	2.62×10^9	7.94×10^8	5.93
NG-4 at DCS sample (Choppers removed)	9.92×10^8	9.96×10^8	3.39×10^8	5.28
NG-5 at Guide Hall entrance	2.3×10^9	2.148×10^9	6.42×10^8	6.02
NG-6 at Guide Hall entrance	2.3×10^9	2.197×10^9	6.66×10^8	5.93
NG-6 at end of guide	1.37×10^9	1.387×10^9	4.37×10^8	5.71
NG-7 at reflectometer monochromator	1.9×10^9	1.948×10^9	5.90×10^8	5.93
NG-7 before SANS filter	1.56×10^9	1.639×10^9	5.12×10^8	5.75

Table 1. A comparison of measured and simulated capture fluxes for various locations on the NCNR cold neutron beam tubes. The table also gives simulated integrated fluxes ($\phi_{int}^{sim} = \int (d\phi/d\lambda) d\lambda$) and average wavelengths ($\langle\lambda\rangle = 1.8 \phi_c^{sim}/\phi_{int}^{sim}$) in the guide at the reference positions.

New capabilities for sample environment and preparation

This year the NCNR added several new sample environment capabilities. The obtainable temperature equivalent magnetic field energy per Bohr magneton was increased from 0.4 Kelvin to 0.52 Kelvin by the procurement of a 9 Tesla vertical field superconducting magnet. In order to reach sample temperatures comparable with this field energy range, a pumped helium-3 refrigerator with a base temperature of 0.29 Kelvin is incorporated into the 9 Tesla magnet system. These low temperatures and high fields are critical for the NCNR's ongoing program of research on low dimensional magnetism. The new superconducting magnet system is top-loading which facilitates quick turn around for studies involving multiple samples. The horizontal field magnet, shown in Fig. 1, was recently returned to service.

A new 2000 K variable temperature vacuum furnace was acquired this year providing new capability for neutron scattering experiments at high tempera-
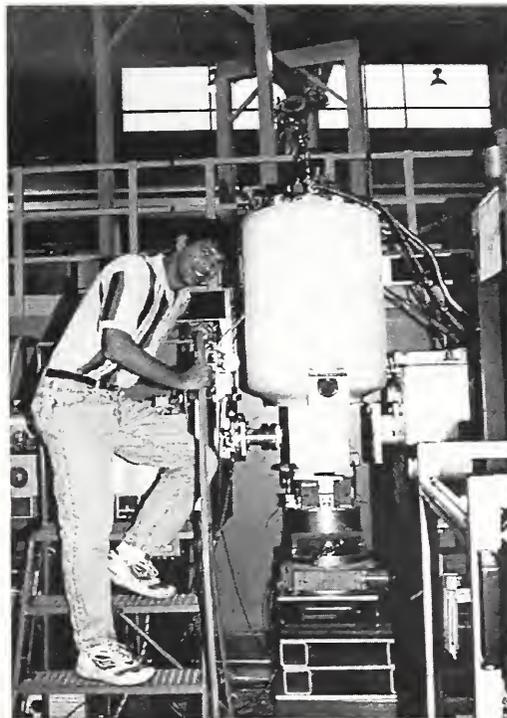
Figure1. John Barker sets up the recently repaired superconducting horizontal field magnet on the NG-7 SANS.

Detector Electronics for the HFBS

The recently commissioned High Flux Backscattering Spectrometer provided a unique design challenge for the ^{3}He neutron detector electronics. The combination of a large evacuated flight path together with close packing of the half inch diameter detectors meant that the traditional preamplifier/amplifier/discriminator (PAD) modules could only be utilized outside of the vacuum chamber. This option would have resulted in an unacceptable noise susceptibility for the weak detector signals being transmitted over long cables and through vacuum feedthrough devices. The HFBS project opted, instead, to design a small form-factor, fully vacuum rated PAD module that could be located within the vacuum flight chamber and then route the robust digital discriminator outputs to the outside data acquisition electronics.

The NCNR design is based on two commercially available hybrid circuits: a preamplifier/shaping amplifier, and an amplifier/discriminator. Both parts dissipate power at the milliwatt level and are fully vacuum (space) rated. The output stage uses a CMOS dual inverting/non-inverting driver which also exhibits very low power dissipation, even when driving large loads. The balanced output is used to provide ECL level logic output with excellent common mode rejection for the signal transmitted out of the flight chamber to the data acquisition electronics. Careful component selection and package design resulted in a small form-factor, flat-package design with a thickness of less than 0.45 inches consistent with the detector spacing requirements. Additional features in the NCNR design include: a robust input protection network to protect the preamplifier, on-board regulation of the discriminator level reference voltage, separate high and low level discriminator settings, and convenient on-board connections for daisy chaining high voltage and test pulse inputs to adjacent PAD modules.

Data Acquisition Electronics for the DCS Time-of-flight Spectrometer

The Disk Chopper Time-of-flight Spectrometer (DCS) presents unique requirements for its data acquisition system. The choppers of the DCS instrument (see Figure 1) periodically illuminate the sample with pulses of neutrons which are then scattered towards the detectors. Each period the chopper system produces a signal synchronous with the incoming neutron pulse that starts a free-running clock which is used to time the neutron flight. When a neutron event occurs, the front-end data acquisition electronics create a 30-bit binary event word which encodes which detector, and at what time, registered a scattered neutron. The rest of the data acquisition system is responsible for reading out the event words, decoding the data event words, and histogramming the data. The user workstation processes the stored histograms from the measurement.

Both the large number of detectors (nearly 1000) and the high-energy resolution characterize the NIST DCS instrument. This requires that the time-of-flight measurement to be resolved to better than 100 nanoseconds over a timing interval which can exceed 50 milliseconds (a timing dynamic range of over 10^6). To meet these requirements the detectors must be interrogated at a raw rate exceeding 10^{10} s^{-1}. The actual worst-case neutron event rate (all neutrons in a pulse scattered into one time channel) is under 10^7 s^{-1}, while the time-averaged data rate at which the histogram must be updated is only on the order of 10^5 s^{-1}. Bridging these drastically different data rates is the primary function of the data acquisition electronics. The general approach adopted in the NIST design is to process data hierarchically, in a tree-like structure, which mirrors the data bandwidth requirements. In this concept, multiple front-end elements operate in parallel at high speed, passing valid events to the next level where they are multiplexed and then passed on to be histogrammed into memory.

The DCS data acquisition electronics were successfully tested under test-bench conditions and under "live" conditions during a recent reactor cycle. The NCNR design uses two types of single width, 6U-sized VME modules to process incoming events and multiplex the events for VME readout to the crate controller computer where the events are histogrammed. The input modules are capable of processing events from 30 detectors creating the appropri-
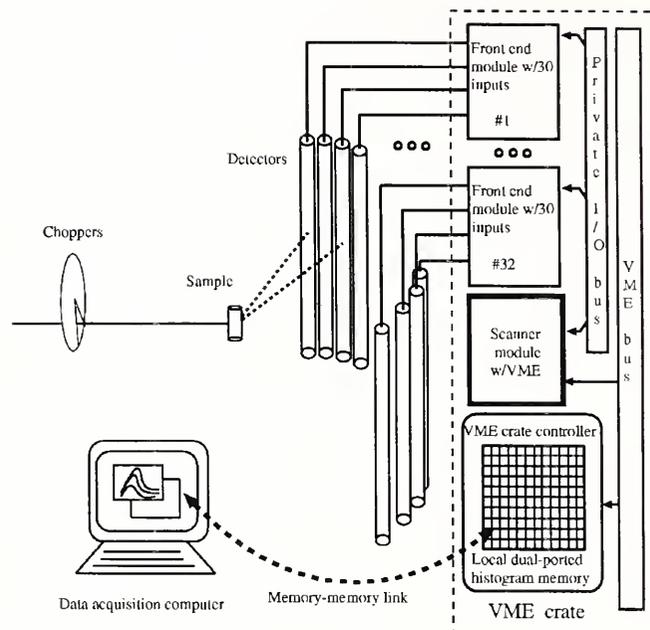
Figure 1. Schematic diagram of DCS Data Acquisition system.

ate time-stamped data words and storing the events in a 64 deep FIFO memory for readout. The DCS instrument requires 31 input modules to handle all of the 913 detectors in the current configuration. A scanner module polls all of the 31 input modules over a private bus to see if they have valid events ready for readout. If data is available, the scanner module reads the valid events from the input modules and stores the data for readout over the VME bus to the VME crate controller. The crate controller computer reads the events from the scanner module, filters valid events, processes the timing information, and histograms events by detector and time channel into a block of memory accessible to the user workstation computer.

50

Research Topics

The topics listed here represent research undertaken during the year. For further details on any area, please contact the authors directly, or write to Linda Clutter, 100 Bureau Drive Stop 8562, Gaithersburg, MD 20899-8562

Materials Science

A New Phase of Silver Fluoride?
R. Harlow[39]

A Ring/Plug Reference Specimen for Residual Stress Measurements
T. Gnäupel-Herold[188], P. C. Brand[98], D. Balzor[105], A. V. Clark[105] and H. J. Prask[98]

Acid Sites in Zeolite ZSM-5
A. Peters[36], R.-H. Hu[212], S. Purnell[212], B. H. Toby[98], R. Senesi[142], D. A. Neumann[98] and D. H. Olson[199]

Aerogels Investigated by SANS with Contrast Masking Solutions
C. Merzbacher[95], M. Anderson[95] and J. Barker[98]

Amorphous Content Determination Methodology
J. K. Stalick[98], R. Senesi[142] and B. Toby[98]

A Structural Sudy of the Ruddlesden-Popper Calcium Manganate $Ca_4Mn_3O_{10}$
M. Greenblatt[135] and I. Fawcett[135]

Ceramic Mixed Conducting Membrane Materials
H. Prask[98] and E. Drescher-Krasicka[106]

Characterization of Microcracking in Iron Titanate by SANS
A. Allen[102] and E. Fuller[102]

Characterization of Standard Reference Specimens for Residual Stress Measurements as Part of VAMAS
T. Gnäupel-Herold[188], P. C. Brand[98], H. J. Prask[98] and G. A. Webster[57]

Charge, Orbital and Magnetic Ordering in the Manganate Perovskites
P. Woodward[20] and T. Vogt[20]

Chemical Ordering in Ni-Mn-Ga Heusler Alloys
R. Overholser[188], M. Wuttig[188] and D. A. Neumann[98]

SANS from Oil Bearing Sedimentary Rocks
A. Radlinski[13] and G. Wignall[115]

Comparison of Residual Stress Measurement Techniques
T. Gnäupel-Herold[188], P. C. Brand[98], H. J. Prask[98], S. Spooner[115], B. Pardue[153], D. Nelson[141] and S. Foss[71]

Complex Oxide Structures
A. Sleight[119], I. Radosavljevic[119] and T. Amos[119]

'CONV' and 'STRESS': New Codes for Data Reduction in Neutron Diffraction Residual Stress Measurements
P. C. Brand[98] and T. Gnäupel-Herold[188]

CPD Round Robin on Quantitative Phase Analysis
J. K. Stalick[98]

Crystal Chemistry of Protonic Centers in Zeolites
D. H. Olson[199] and Brian Toby[98]

Determination of Residual Stresses in an Al plate for Helicopter Applications
P. C. Brand[98], H. J. Prask[98], T. Gnäupel-Herold[188] and D. Ludin[19]

Effect of Annealing on ZrO_2 Phase Composition
J. K. Stalick[98] and J. Ilavsky[34]

Fast Ion Conductors
J. K. Stalick[98], B. Wuensch[81] and E. Ku[81]

Grazing Incidence SANS from Plasma Sprayed Coatings
A. Allen[102] and H. Boukari[102]

Hydrogen-Induced Lattice Migration in Palladium/Nickel Alloys
T. Flanagan[210] and J. Barker[98]

Hydrogen Location in Graphite Nano-Fibers
S. F. Trevino[98, 11] and P. Anderson[112]

Identification Of A Hydrogen-Induced Tetragonal Phase In $Ti_{48}Al_2Nb_2Cr$ Alloys.
M. DeGraef[23] and B. Mollosseau[23]

Influence of Thermal Treatment on Void Morphology in Polyethylene-Carbon Black Composites
D. Marr[30], J. Oakey[30], K. Schwartz[129] and M. Wartenberg[129]

Investigation of the Zr_9Pt_{11} Structure Type
J. K. Stalick[98] and R. Waterstrat[98]

Kinetics of Gellation of Silica under Shear
C. Muzny[111], H. Hanley[111] and G. Straty[111]

Low Temperature Crystal Structure Study of DZSM-5·4D_2O (Si: Al=26)
D. H. Olson[199]

Magnetic Structure of Layered Perovskites as a Function of Temperature
A. K. Cheetham[177] and B. J. Campbell[177]

Measurement and Modeling of Residual Stresses in Multi-pass Weldments
T. Gnäupel-Herold[188], H. J. Prask[98], P. C. Brand[98], R. Lloyd[55] and W. Reuter[55]

Measurement of Diffraction Elastic Constants of γ-Alumina and Zirconia Plasma Sprayed Coatings
T. Gnäupel-Herold[188], J. Matejicek[142] and H. J. Prask[98]

Micro-Porosity in Amorphous Carbons and Li-Carbons
J. E. Fischer[199], P. Zhou[199], Y. Sorek[199], A. Claye[199] and W. Kamitakahara[98]

Microstructure of Permeable Hydrogel Lens Materials
J. S. Huang[44], J. Li[44] and P. Vilant[16]

Microstructure of Silica-Aerogel Sensor Materials
R. Reidy[131] and A. Allen[102]

Morphological and Kinetic Study of Early Calcium-Silicate-Hydrate Gel Development during the Hydration of Cement and Tricalcium Silicate
H. M. Jennings[112], J. J. Thomas[112] and A. J. Allen[102]

Neutron Diffraction Data of Beta-PtO_2
B. Chamberland[9] and M. O'Keeffe[9]

Neutron Diffraction Measurements of Nanostruc-tured, Non-Equilibrium Spinel Ferrites
V. G. Harris[95]

Neutron Diffraction Studies of AlFeMn Solid Solutions
V. G. Harris[95] and Q. Huang[98, 188]

Neutron Diffraction Studies of the Zeolites Cancrinite and (Ba,K)G-L
A. Burton[181] M. Feuerstein[181] and R. Lobo[181]

Neutron Diffraction Validation of Scanning Acoustic Imaging Residual Stress Measurements
T. Gnäupel-Herold[188], H. J. Prask[98] and E. Drescher-Krasicka[106]

Order-Disorder in CoFe/Carbon Composites
J. H. Scott[110], M. E. McHenry[23], Z. Turgut[23] and M. Storch[23]

Polymerized Fullerenes
S. F. Trevino[98, 11], N. Beck-Tan[11] and L. Balogh[86]

Pore Size Distribution Analysis of Activated Carbons
P. Pendleton[201] and C. Howard[14]

Radiation-Induced Microstructure in Reactor Pressure Vessel Steels
G. R. Odette[177], B. Wirth[177] and D. Klingensmith[177]

Residual Stresses around Weldments in Various Steel-Plate Configurations
T. Gnäupel-Herold[188], P. C. Brand[98], I. Varhol[24] and H. J. Prask[98]

Residual Stresses in a Failed Steel Structural Member
P. C. Brand[98], H. J. Prask[98], T. Gnäupel-Herold[188], E. Drescher-Krasicka[106] and C. Ostertag[172]

Residual Stresses in a Powder Metallurgy Gear
T. Gnäupel-Herold[188], H. J. Prask[98], B. Chelluri[53]

Residual Stresses in Powder Metallurgy Test Specimens
T. Gnäupel-Herold[188], H. J. Prask[98], M.-J. Yang[123] and R. German[123]

Residual Stresses in a Shrink-Fit Ti/SiC Ring
T. Gnäupel-Herold[188] and S. F. Trevino[98, 11]

Residual Stresses in Thermally-Sprayed Coatings
J. Matejicek[142], T. Gnäupel-Herold[188], P. C. Brand[98], H. J. Prask[98], S. Sampath[142] and H. Herman[13]

Residual Stresses in Ti Rib Implants for Children
T. Gnäupel-Herold[188], H. J. Prask[98] and R. Roberts[5]

Residual Stress Measurements on Railroad Rails
T. Gnäupel-Herold[188], P. C. Brand[98], J. Gordon[160], J. Magiera[33], J.

Polymers

Complex Fluids

S. Trevino[98, 11] and N. Beck-Tan[11]

Static and Flowing Microstructure of Drilling Muds

M. Paquette[37], N. Moll[37] and C. Glinka[98]

Structure of PEO-PPO-PEO Tri-Block Copolymer Micelles

I. Goldmints[81] and P. Huibers[81]

Temperature and Concentration Dependence of Polymer (PEO) –Surfactant (SDS) Complexes in Aqueous Solutions

K. Chari[42] and M. Lin[44]

Condensed Matter Physics

A Bond-Valence Analysis of the Structure of $Ba_{0.875}Sr_{0.125}RuO_3$

A. Santoro[98], I. Natali Sora[98, 167] and Q. Huang[98, 188]

A Bond-Valence Analysis of the Structure of $YBa_2Fe_3O_8$

I. Natali Sora[98, 167] and A. Santoro[98]

Anisotropic Spin Hamiltonians Due to Spin-Orbit and Coulomb Exchange-Interactions

T. Yildirim[98], A. B. Harris[199], A. Aharony[173] and O. Entin-Wohlman[173]

Antiferromagnetic Ordering of $La_{0.33}Ca_{0.67}MnO_3$ Thin Films

Y. Ijiri[98], J. A. Borchers[98], J. W. Lynn[98], R. W. Erwin[98], M. Rajeswari[188], M. C. Robson[188], R. Ramesh[188] and V. Venkatesan[188]

Antiferromagnetic Spin Ordering in $FeMn/Ni_{80}Fe_{20}$ Superlattices

Y. Ijiri[98], J. A. Borchers[98], D. Dender[98,188] and R. W. Erwin[98], J.-C. A. Huang[89] and C-H Lee[94]

Characterization of the Antiferromagnetic Order in Exchange-biased $Ni_{80}Fe_{20}/CoO$ Bilayers

N. Gokemeijer[70], C. L. Chien[70], Y. Ijiri[98], J. A. Borchers[98] and R. W. Erwin[98]

Characterization of the Crystal and Magnetic Structures of Dicyanamide Complexes by Neutron Powder Diffraction

C. R. Kmety-Stevenson[116], J. L. Manson[209], Q. Huang[98, 188]

Charge and Magnetic Ordering in $La_{1/2}Ca_{1/2}MnO_3$

Q. Huang[98,188], J. W. Lynn[98], V. Smolyaninova[188], K. Ghosh[188] and R. L. Greene[188], D. Dander[98] and R. W. Erwin[98]

Critical Magnetic Scattering in $LaCaMnO_3$

L. Vasiliu-Doloc[98, 188] and J. W. Lynn[98]

Crystal and Magnetic Structures in $Co_{2.25}Ru_{0.75}O_4$ and $Co_{2.25}Sn_{0.25}Ru_{0.50}O_4$

Q. Huang[98, 188], J. W. Lynn[98], R. W. Erwin[98], M. Crawford[39], R. L. Harlow[39] and E. M. McCarron[39]

Crystal and Magnetic Structures of NiF_3

L. Chacon[172], N. Rosov[98] and J. W. Lynn[98]

Structural Change and Charge Ordering in Bilayered $La_{2-2x}Sr_{1+2x}Mn_2O_7$

W.-H. Li[88], S. Y. Wu[88], nd H. D. Yang[92]

Crystal Structure and Magnetic Ordering in $CoMoO_3$

Q. Huang[98,188], J. W. Lynn[98], R. W. Erwin[98] and M. Crawford[39]

Crystal Structure and Magnetic Order in the Nd-based CMR Compounds

W.-H. Li[88], K. C. Lee[88], R. S. Liu[93], C. Y. Huang[98,188] and J. W. Lynn[98]

Crystal Structure of the Ca-Doped $(La/Sr)_3Mn_2O_7$

W.-H. Li[88], S. Y. Wu[88] and H. D. Yang[92]

Determination of the Crystal Structure of Conducting Polymer FeOCl and Aniline FeOCl

W.-H. Li[88], S. Y. Wu[88] and C.-G. Wu[88],

Determination of the Spin Hamiltonian for a Spin-1/2 Antiferromagnetic with a Spin Gap

M. Stone[72], J. Rittner[72], D. H. Reich[72] and C. Broholm[72, 98]

Effect of Si-Doping on the Spin-Peierls Phase of $CuGeO_3$

S.-H. Lee[98,188], P. M. Gehring[98], K. Hirota[156], G. Shirane[20], T. Masuda[205], K. Uchinokura[205] and M. Hase[62]

Effect of Superconductivity on the Lattice Dynamics of $Ba_{0.6}K_{0.4}BiO_3$

C. P. Adams[98, 188], J. W. Lynn[98] and S. N. Barilo[17]

Effect of Zn Substitution on the Magnetic Resonance Peak in $YBa_2Cu_3O_7$

H. F. Fong[127], B. Keimer[127] and R. W. Erwin[98]

Effects of Field Cycling on Co/Cu and Co/Ag Multilayers

J. A. Borchers[98], J. A. Dura[98] and C. F. Majkrzak[98], S. Y. Hsu[87], R. Loloee[87], W. P. Pratt, Jr.[87] and J. Bass[87]

Effects of H on Magnetic Coupling in FeV Superlattices

B. Horvarsson[132], G. Andersson[132], J. A. Dura[98], T. Udovic[98], C. F

Majkrzak[98]

Effects of Si-Doping on Magnetic Excitations in the Spin-Peierls System, $CuGeO_3$

S.-H. Lee[98,188], G. Shirane[20], P. M. Gehring[98] and K. Hirota[156]

Flux Lattice Structure in Nb and $BaKBiO_3$

D. Dender[98,188], C. Adams[98,188] and J. Lynn[98]

Ground-State Selection in FCC and FCT Antiferromagnets Due to Quantum Disorder

T. Yildirim[98], A. B. Harris[199] and E. F. Shender[172]

Incommensurate and Commensurate Magnetic Structures in the Magnetoresistive $R_2Ni_3Si_5$ Materials

F. Bourdarot[31], S. Skanthakumar[8], J. W. Lynn[98] and L. C. Gupta[146]

Incommensurate Spin Fluctuations and Structural Transitions in Excess Oxygen-doped La_2CuO_{4+y}

R. J. Birgeneau[81], Y. S. Lee[81], R. J. Christianson[81], M. A. Kastner[81] and R. W. Erwin[98]

Influence of Interface Structure on the Magnetic Polarizability of a Pd-Co Alloy Overlayer in Close Proximity to $CoPt_3$

M. Fitzsimmons[78], F. Hellman[175], B. Maran[175], A. Shapiro[175]

Interfacial Spin States in Magnetic Tunnel Junction Multilayers

C. Platt[175], A. E. Berkowitz[175], J. A. Borchers[98], J. A. Dura[98] and C. F. Majkrzak[98]

Interlayer Spin Coupling in FeMn-based Spin Valves

J. A. Borchers[98], C. F. Majkrzak[98], A. Reilly[87], W. P. Pratt, Jr.[87] and J. Bass[87]

Lattice Dynamics of a Material with Negative Thermal Expansion, ZrW_2O_8

G. Ernst[80], C. Broholm[72,98], A. P. Ramirez[80], G. Kovac[80] and G. Gasparovic[72]

Low-Temperature Neutron Diffraction Studies of $Pr_3(Fe,Co)_{27.5}Ti_{1.5}$ Permanent Magnets

V. G. Harris[95] and Q. Huang[98,188]

Magnetic and Crystal Structure Phase Transitions in $R_{1-x}Ba_xCoO_{3-y}$ (R=Nd,Gd)

I. O. Troyanchuk[17], D. D. Khalyavin[17], T. K. Solovykh[17], H. Szymczak[17], Q. Huang[98,188] and J. W. Lynn[98]

Magnetic Correlations and Lattice Distortions in the Bilayer Manganite $La_{1.2}Sr_{1.8}Mn_2O_7$

L. Vasiliu-Doloc[98, 188], S. Rosenbranz[8], R. Osborn[8], S. K. Sinha[8], J. W. Lynn[98] and J. F. Mitchell[8]

Magnetic Correlations in Discontinuous $Co-SiO_2$ Thin Films and Multilayers

S. Sankar[188], A. E. Berkowitz[175], D. Dender[98,188], J. A. Borchers[98], R. W. Erwin[98], S. R. Kline[98], J. A. Dura[98] and C. F. Majkrzak[98]

Magnetic Depth Profile of CMR Perovskite Films and Spin Valves

Y. Ijiri[98], J. A. Borchers[98], J. W. Lynn[98], R. W. Erwin[98], C. F. Majkrzak[98], M. Robeson[188], R. Ramesh[188], V. Venkatesan[188] and R. Greene[188]

Magnetic Domains in Co/Cu Multilayers

J. A. Borchers[98], J. A. Dura[98], C. F. Majkrzak[98], J. Unguris[103], D. Tulchinsky[103], M. H. Kelley[103], R. Celotta[103], S. Y. Hsu[87], R. Loloee[87], W. P. Pratt, Jr.[87] and J. Bass[87]

Magnetic Domain Structure in CoPt Thin Films

C. Glinka[98] and M. Toney[54]

Magnetic Domain Structure of Thermally Treated Nanocrystalline Ni_3Fe

H. Frase[21] and L. Robertson[115]

Magnetic Ordering in the Spin-Ladder Compound $CaCu_2O_3$

V. Kiryukhin[81], Y.-J. Kim[81], R. Erwin[98], R. J. Birgeneau[81]

Magnetic Ordering in the System $La_{1-x}Pr_xBaCuFeO_5$

W. Mombru[162], F. Araujo-Moreira[188] L. Suescun[208]

Magnetic Structure and Site Occupancies in $YFe_{11-x}Co_xTi$ for x=1,3,7, and 9

J. K. Liang[59], Q. Huang[98, 188] and A. Santoro[98]

Magnetic Field Effects on Antiferromagnetic Ordering in a Fe/FeF$_2$ Bilayer

Y. Ijiri[98], J. A. Borchers[98], R. W. Erwin[98], M.–C. Cyrille[175], I. K. Schuller[175], J. Nogues[163] and D. Lederman[218]

Magnetic Order and Crystal Field Effects in RNiBC

F. Bourdarot[26, 98], J. W. Lynn[98], Q. Huang[98, 188], D. R. Sanchez[28], M. B. Fontes[28], J. C. Trochez[28] and E. Baggio-Saitovitch[28]

Magnetic Order and Fluctuations in a Zig-Zag Spin-1/2 Chain

I. A. Zaliznyak[72, 98], C. Broholm[72, 98], M. Kibune[205] and H. Takagi[205]

Magnetic Order in Pr-Containing Cuprate Superconductors

W.-H. Li[88], K. C. Lee[88], H. C. Ku[94] and J. W. Lynn[98]

55

Biomolecular Science

Chemical Physics of Materials

Instrumentation

ment, Texture Determination and Single Crystal Diffraction
   P. C. Brand[98], H. J. Prask[98] and T. Gnäupel-Herold[188]
Development and Installation of a Leak-tight, Top-loading, Horizontal Field Superconducting Magnet
   D. Dender[98,188] and R. Erwin[98]
Development and Installation of a Remote Controlled Monochromator Changer for the BT-9 Thermal Triple Axis Spectrometer
   K. T. Forstner[98], P. Brand[98], A. Clarkson[98] and T. Thai[98]
Development of a Radially-Focussed Polarizing Supermirror Analyzer Array
   M. Murbach[188], P. Brand[98], and N. Rosov[98]
Development of a Robust Static Thermal Switch for Fixed Sample Environment Temperatures from 15-650K
   L. Santodonato[98]
Development of Synthetic Mica Monochromators
   K. T. Forstner[98] and L. Passell[20]
Development and Testing of Fe/Ni Supermirror Plates for the NSE Analyzer
   N. Rosov[98], S. Rathgeber[61], C. F. Majkrzak[98] and J. Wood[120]
Development of a VME-Based Data Acquisition System for the HFBS
   P. D. Gallagher[98], N. C. Maliszewskyj[98] and M. Kirsch[143]
Development and Testing of the Doppler Drive System for the HFBS
   R. Christman[98], P. Brand[98] and C. Karmonik[98,188]
Development of a Vacuum Rated Preamplifier/Amplifier/-Discriminator for He Neutron Detectors
   J. Ziegler[98]
Design of a Cable and Hose Management System for the NSE Spectrometer
   D. Fulford[98]
Design and Development of the Filter Analyzer Spectrometer
   D. J. Pierce[98], R. Christman[98], J. Kenney[98] and D. A. Neumann[98]
The High Flux Backscattering Spectrometer (HFBS)
   P. M. Gehring[98], D. A. Neumann[98], C. Karmonik[98,188] and A. Meyer[98].
The Disk Chopper Time-of-Flight (DCS)
   J. R. D. Copley[98], J. C. Cook[188,98] and F. B. Altofer[98]
Design and Fabrication of the Voltage and Signal Distribution System for the DCS Detectors
   H. Layer[98], J. Raebiger[61], M. Garland[98], D. Kulp[98], P. Tobin[98] and T. Thai[98]
Design and Installation of the Sample Chamber, Flight Chamber and Detector Assembly for the DCS
   C. Brocker[98], M. Rinehart[98], G. M. Baltic[98] and Slifer[98]
Design and Performance Testing of the DCS Data Acquisition System Electronics
   H. Layer[98], J. Raebiger[61], P. Klosowski[98] and N. C. Maliszewskyj[98]
Evaluation of New Neutron Area-Detectors
   Y. T. Cheng[99,97]
Evaluation of a Beryllium Single Crystal as a Monochromator for"DARTS"
   P. C. Brand[98] and T. Gnäupel-Herold[188]
The Filter Analyzer Spectrometer
   D. A. Neumann[98], P. Papanek[199], J. E. Fischer[199], J. J. Rush[98], M. L. Klein[199] and A. C. Cheetham[177]

Hydrogen Cold Source Development
   R. E. Williams[98], P. A. Kopetka[98] and J. M. Rowe[98]
Installation and Alighment of the Spherically Focussed Si(111) Analyzer Assembly for the HFBS
   C. H. Appel[120], R. Wise[120], G. M. Baltic[98] M. Rinehart[98] and S. Slifer[98]
Installation and Testing of the New Thermal Beam Tube Shutter Design Using a Remote Actuated Cast System
   J. Moyer[98], C. Wrenn[98], P. Brand[98], A. Clarkson[98], G. M. Baltic[98], D. Clem[98], M. Rinehart[98] and S. Slifer[98]
Laue Focussing and Its Applications
   V. K. Kvardakov[75], V. A. Somenkov[75], S. Shilstein[75], J. W. Lynn[98], D. R. Mildner[99] and H. Chen[99]
MBE Chamber for In-Situ Neutron Scattering: Instrument Development
   J. A. Dura[98]
Mica and Ge Reflectivity
   K. T. Forstner[98] and C. F Majkrzak[98]
Monte Carlo Methods for Nuclear Applications

R. E. Williams[98]
Monte Carlo Simulation of the NIST Cold Neutron Beamlines
   J. C. Cook[188,98]
Neutron Powder Diffraction Study of the Crystal Structure of $Ba_{0.78}Sr_{0.22}RuO_3$
   I. Natali Sora[98,171]
The NIST Neutron Spin Echo Spectrometer (NSE)
   N. Rosov[98], S. Rathgeber[61] and M. Monokenbusch[61]
Osmic and Mica Supermirror Tests
   K. T. Forstner[98] and C. F. Majkrzak[98]
The Perfect Crystal SANS Diffractometer
   J. G. Barker[98], C. J. Glinka[98], A. Drews[98] and M. Agamalian[115], and J.Moyer[98]
Performance Tests of the Optical Filter and Chopper System for the DCS, Including Crystal Filter Options
   J. R. D. Copley[98], J. C.. Cook[188,98], N. C. Maliszewskyj[98] and D. J. Pierce[98]
Performance Tests of the Phase Space Transform Chopper on NG-2
   P. M. Gehring[98], D. A. Neumann[98] and C. Karmonik[98,188]
Spin Echo Supermirror Development
   N. Rosov[98] and C. F. Majkrzak[98]
Supermirror Reflectivity Measurements
   C. F. Majkrzak[98]
Testing and Optimization of a Rise-Time Encoding 2-D Neutron Detector for the NSE
   S. Rathgeber[61] and J. Ziegler[98]

Neutron Physics

Accurate Determination of Neutron Capture Flux
   M. S. Dewey[104], M. Arif[104], D. Gilliam[104], G. L. Greene[78], W.M. Snow[58], J. Pauwels[64], and R. Scott[82]
Benchmark Measurements and Calculations of Neutron Transport
   D. Gilliam[104], M. S. Dewey[104], J. Nico[104], C. Eisenhauer[104], J. Grundl[104], and H. Gerstenberg[10]
Certified Neutron Fluence Standards from the Cavity Fission Source
   J. Adams[104] and J. Grundl[104]
Defined-Geometry Alpha Counting
   D. Gilliam[104] and J. Nico[104]
Determination of the Neutron Lifetime
   M. S. Dewey[104], J. Nico[104], D. Gilliam[104], W.M. Snow[58], G. L. Greene[78] and X. Fei[58]
Highly Accurate Neutron Wavelength Mea-surements
   M. S. Dewey[104], K. Coakley[109], W. M. Snow[58], and M. Arif[104]
Intercomparison of NIST and PNL Calibration Facilities
   A.   Thompson[104], R. Schwartz[104], J. McDonald[15], and M. Murphy[15]
LASER Polarization of ^{3}He for Neutron Spin Filters and Medical MRI
   A. Thompson[104], T. Gentile[104], M. S. Dewey[104], G. L. Jones[104,58], F. Wietfeldt[104,52], W. M. Snow[58], and R. Rizi[199]
Neutron Calorimetry
   W. M. Snow[58], Z. Chowdhuri[58], X. Fei[58], and M. S. Dewey[104]
Neutron Fluence Rate Measurements
   D. Gilliam[104], J. Nico[104], and J. Adams[104]
Neutron Interferometry and Optics
   M. Arif[104], D. Jacobson[104], R. Clothier[18], A. Thompson[104], S. Werner[192], A. Ioffe[192, 104], A. Zeilinger[186], K. Raum[194], B. Schillinger[194], C. Rausch[194], andW. Richards[82]
Neutron Radiography/Tomography
   T. Gentile[104], M. Arif[104], and D. Jacobson[104]
Parity Non-Conserving Neutron Spin Rotation
   B. Heckel[212], D. Markoff[212], E. Adelberger[212], S. Penn[212], and F. Wietfeldt[104,52]
Quality Assurance Checks on Masses and Impurities in Neutron Dosimeters for NRC Reactor Pressure Vessel Embrittlement Surveillance
   J. Adams[104], D.Gilliam[104], and J. Grundl[104]
Response of Albedo Dosimeters Versus Distance from a Neutron Source
   R. Schwartz[104] and A. Thompson[104]
Response of Albedo Neutron Dosimeters as a Function of Angle
   R. Schwartz[104]
Study of Time Reversal Invariance in Neutron Beta Decay

J. Wilkerson[217], E. Wasserman[172], J. Nico[104], R. G. H. Robertson[172], S. Freedman[172], A. Garcia[196], T. Chupp[14], K. Coulter[14], M. S. Dewey[104], G. L. Greene[78], A. Thompson[104], B. Fujikawa[172], G. L. Jones [104,58], J. Adams[104], F. Wietfeldt[104,52], L. Lising[172], S. Hwang[14] and T. Steiger[212]

Trapping of Ultra Cold Neutrons

J. Doyle[52], S. Lamoreaux, R. Golub[51], G. L. Greene[78], M. S. Dewey[104], P. Huffman[52], C. Brome[52], C. Mattoni[52], J. Butterworth[52], and D. McKinsey[52]

Utilization of the Materials Dosimetry Reference Facility-Tests of New IRMM ^{237}Np and ^{238}U Fast Neutron Dosimeters

J. Adams[104], J. Grundl[104], C. Eisenhauer[104], D. Gilliam[104], and P. Simpson[14]

Materials Analysis

A Bender-Focuser for Prompt Gamma Activation Analysis

E. A. Mackey[99], H. H. Chen-Mayer[99], R. M. Lindstrom[99], D. F. R. Mildner[99], R. L. Paul[99], Q.-F. Xiao[211] and V. A. Sharov[220]

Analytical Applications of Cold Neutrons

H. H. Chen-Mayer[99], R. Demiralp[99], R. R. Greenberg[99], G. P. Lamaze[99], J. K. Langland[99], R. M. Lindstrom[99], E. A. Mackey[99], D. F. R. Mildner[99], R. L. Paul[99] and V. A. Sharov[220]

Applications of Neutron Laue Diffraction Focusing Methods

H. H. Chen-Mayer[99], V. V. Kvardakov[123], J. W. Lynn[98], D. F. R. Mildner[99] and V. A. Sharov[220]

Application of Radioisotopc-Induced X-Ray Emission to the Identification of Lead and Other Elements in Ceramic Glazes and Housewares

D. L. Anderson[47] and W. C. Cunningham[47]

Archeological Applications of NAA

R. Bishop[139], M. J. Blackman[99] and J. E. Myers[99]

Bromation in Breadmaking

W. C. Cunningham[47] and C. R. Warner[47]

Bio-Analytical and Specimen Bank Research

K. A. Fitzpatrick[99], R. R. Greenberg[99], G. V. Iyengar[108], J. K. Langland[99], E. A. Mackey[99], B. J. Porter[99] and R. Zeisler[99]

Certification of Standard Reference Materials by Neutron Activation Analysis

D. A. Becker[99], R. Demiralp[99], R. R. Greenberg[99], R. M. Lindstrom[99], E. A. Mackey[99] and R. Zeisler[99]

Characterization of Sources and Fluxes of Particulate Pollutants Depositing to Great Waters

P. F. Caffrey[188], A. E. Suarez[188] and J. M. Ondov[188]

Characterization of Submicrometer Aerosol Particles

J. M. Ondov[188], S. F. Heller-Zeisler[188] and R. Zeisler[99]

Determination of Hydrogen by PGAA

R. R. Greenberg[99], R. M. Lindstrom[99], E. A. Mackey[99] and R. L. Paul[99]

Determination of Phosphorus via RNAA with Beta Counting

R. L. Paul[99]

Development of a Position-Sensitive Video Radiation Detector

H. H. Chen-Mayer[99] and C. J. Zeissler[110]

Development of Radiochemical Separation for NAA

D. A. Becker[99], R. R. Greenberg[99] and E. A. Mackey[99]

Elemental Characterization of High Temperature Superconductors

D. A. Becker[99], R. R. Greenberg[99], R. M. Lindstrom[99] and R. L. Paul[99]

Evaluation of Accuracy and Precision in INAA of Botanical Materials

D. A. Becker[99]

Evaluation of Errors and Interferences in NAA

D. A. Becker[99], M. J. Blackman[139], R. R. Greenberg[99], R. M. Lindstrom[99] and R. Zeisler[99]

Focusing Methods for Radiography and Topography

H. H. Chen-Mayer[99], D. F. R. Mildner[99], K. M. Podurets[75] V. A. Sharov[220] and S. Shilstein[75]

High Sensitivity Gamma-Ray Spectrometry

R. M. Lindstrom[99]

Homogeneity and Composition of Small Solid Samples

R. Zeisler[99]

Hydrogen Detection in Industrial Materials by Incoherent Neutron Scattering

H. H. Chen-Mayer[99], V. V. Kvardakov[75] D. F. R. Mildner[99] and V. A. Somenkov[75]

Improvements to INAA Methodology

D. A. Becker[99], R. Demiralp[99], R. R. Greenberg[99], R. M. Lindstrom[99], E. A. Mackey[99] and R. Zeisler[99]

Improvements to PGAA Methodology

D. L. Anderson[47], R. M. Lindstrom[99], E. A. Mackey[99] and R. L. Paul[99]

Lithium Migration in Electrochromic Thin Films

G. P. Lamaze[99], H. H. Chen-Mayer[99], M. Badding[136], A. Gerouk[159] and R. Goldner[159]

Multielement Analysis of Foods and Related Materials by NAA

D. L. Anderson[47] and W. C. Cunningham[47]

Neutron Absorption Measurements Using Converging Beams

H. H. Chen-Mayer[99], E. A. Mackey[99], D. F. R. Mildner[99] and R. L. Paul[99]

Neutron Autoradiography of Paintings

Y.-T. Cheng[97,99] and J. Olin[118]

Neutron Beam Spatial Distributions Using Imaging Plate Technology

H. J. Bahre[48], H. H. Chen-Mayer[99], Y.-T. Cheng[97,99], D. F. R. Mildner[99] and V. A. Sharov[220]

Neutron Depth Profiling of AlN Thin Films

H. H. Chen-Mayer[99], G. P. Lamaze[99] and S. McGuire[32]

Neutron Depth Profiling of c-BN

H. H. Chen-Mayer[99], G. P. Lamaze[99] and L. Pilione[15]

Nitrogen Profiling of Thin Titanium Nitride Films

G. P. Lamaze[99], H. H. Chen-Mayer[99], N. Cox[69] and E. B. Steel[110]

Neutron Focusing for Analytical Chemistry

H. Chen-Mayer[99], G. P. Lamaze[99], J. K. Langland[99], R. M. Lindstrom[99], E. A. Mackey[99], D. F. R. Mildner[99], V. A. Sharov[220] and J. R. Swider[110]

Neutron Distribution Measurements by Neutron Induced Autoradiography

Z. En[211], J. S. Brenizer[211] and D. A. Becker[99]

Neutron Dosimetry for Instrument Development

R. M. Lindstrom[99]

Neutron Scattering Effects on PGAA

R. R. Greenberg[99], R. M. Lindstrom[99], E. A. Mackey[99] and R. L. Paul[99]

Neutron Transmission through Tapered Capillaries

H. H. Chen-Mayer[99], D. F. R. Mildner[99] and V. A. Sharov[220]

New Developments in Monitor Activation Analysis

G. P. Lamaze[99], R. M. Lindstrom[99], E. A. Mackey[99] and R. L. Paul[99]

New Developments in NDP

H. H. Chen-Mayer[99], G. P. Lamaze[99] and J. K. Langland[99]

Quality Assurance Improvements for NAA

D. A. Becker[99], R. Demiralp[99], R. R. Greenberg[99], R. M. Lindstrom[99], E. A. Mackey[99] and R. Zeisler[99]

Quality Assurance Programs

D. L. Anderson[47] and W. C. Cunningham[47]

Reactor Characterization for NAA

D. A. Becker[99]

Radionuclides in Foods

D. L. Anderson[47] and W. C. Cunningham[47]

Revalidation of Food SRMs

D. L. Anderson[47] and W. C. Cunningham[47]

Size Distribution and Deposition of Toxic Elements to Lake Michigan, by Size and by Source.

P. F. Caffrey[188] and J. M. Ondov[188]

Studies in Elemental Speciation

D. A. Becker[99], E. A. Mackey[99] and R. Zeisler[99]

Test of a Novel High Sensitivity Neutron Detector

B. Feller[113], H. H. Chen-Mayer[99] and G. . Lamaze[99]

Trace Elemental Characterization of Silicon Semiconductor Materials

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Mattoni, C. E. H.
Schwartz, R. B.
Steiger, T.*
Wietfeldt, F.

NUCLEAR METHODS GROUP-(839)
Greenberg, R. R., Leader
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Becker, D. A.
Chen-Mayer, H. H.
Demiralp, R.
Fitzpatrick, K. A.
Iyengar, V.
Lamaze, G. P.
Langland, J. K.
Lindstrom, R. M.
Mackey, E. A.
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Paul, R. L.
Porter, B. J.
Zeisler, R. L.

Guest Researchers
Bishop, R. L.
Blackman, M. J.

HEALTH PHYSICS - Div. 354
Slaback, L. A., Leader
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Deardorff, G. E.
Fink, L. E.
Mengers, T. F.
Shubiak, J. J.

*left during fiscal year

Research and Engineering Staff

J. G. Barker	SANS instrumentation and research Microstructure of materials
N. F. Berk	Condensed matter theory Scattering theory for microstructure analysis Computer software for graphics and data analysis
N. A. Bickford	Reactor operations Reactor irradiations Reactor utilization
J. A. Borchers	Thin-film analysis Artificially modulated materials Magnetism
D. E. Brady	Electrical/electronic engineering Nuclear reactor instrumentation NDE diffraction methods
P. C. Brand	Materials engineering Neutron residual stress measurements Engineering physics
J. M. Boyd	Electrical/electronic engineering Nuclear reactor instrumentation
J. R. D. Copley	Time-of-flight spectrometer development Neutron instrumentation conceptual design Condensed matter physics
W. E. Dickerson	Neutron scattering instrumentation Microcomputer interfacing

J. A. Dura	Nuclear and engineering physics
	Combined molecular beam epitaxy and neutron reflectivity
	Instrumentation
	Surface, interfacial, and epitaxial physics
R. W. Erwin	Magnetic materials
	Phase transformations
	Cryogenics
S. A. FitzGerald	Neutron and optical spectroscopy
	Condensed matter physics
	Fullerenes and cements
K. T. Forstner	Instrumentation
	Monochromator development
D. B. Fulford	Mechanical engineering
P. D. Gallagher	Neutron instrumentation
	Interfacial phenomena in polymer systems and complex fluids
	Phase transitions and critical phenomena
P. M. Gehring	Neutron backscattering instrumentation
	Magnetic and structural phase transitions in disordered systems
	Dynamics of high T_c materials
C. J. Glinka	SANS microstructure of metals and porous media
	CHRNS project director
	Cold neutron instrument development
G. C. Greene	System and user software for cold neutron instrumentation
	Spectrometer and data acquisition systems interfaces
B. Hammouda	SANS from polymers, liquid crystals, and colloids
	Dynamics of polymers in solution
	Scattering from sheared fluids
A. E. Heald	Design engineering
	Neutron instrumentation
	Shielding
Y. Ijiri	Condensed matter physics
	Thin films and multilayers
	Magnetism
W. A. Kamitakahara	Dynamics of disordered solids
	Condensed matter physics
	The NCNR guest researcher program
V. L. Karen	Crystallographic database development
	Theory of lattices and symmetry
	Neutron and x-ray diffraction
S. R. Kline	Microstructure of colloids and microemulsions
	Novel surfactant systems
	SANS instrumentation

P. Klosowski	Scientific data visualization Numerical computer modeling Data acquisition software and hardware
P. A. Kopetka	Mechanical engineering Cold source design Electro-mechanical systems
S. T. Krueger	Structure of biological materials SANS and neutron reflectometry methods Computer software development
J. G. LaRock	Mechanical engineering Neutron instrumentation design
H. P. Layer	Electronics and data processing Advanced instrumentation Fundamental physics
P. J. Liposky	Design engineering Nuclear systems and components
J. W. Lynn	Condensed matter physics Magnetic and superconducting materials Neutron scattering methods
C. F. Majkrzak	Condensed matter physics Polarized neutron scattering and instrumentation development Neutron reflectivity measurements
N. C. Maliszewskyj	Computer software development Time-of-flight instrumentation Condensed matter physics
T. J. Myers	Reactor operations Safety analysis
D. A. Neumann	Molecular and layered materials Condensed matter physics Neutron and x-ray scattering instrumentation
D. J. Pierce	Mechanical engineering Neutron instrumentation design
H. J. Prask	Residual stress measurement methodology Neutron NDE applications Neutron NDE instrumentation
T. M. Raby	Reactor operations and standards Nuclear engineering Nuclear systems and components
G. D. Reilly	Design engineering Nuclear systems and components
N. Rosov	Spin echo techniques Phase transformations

	Magnetic materials
J. M. Rowe	Orientationally disordered solids
	Cold source development
	Cold neutron research and instrumentation
J. J. Rush	Catalysts and molecular materials
	Hydrogen in metals
	Inelastic scattering methods
L. Santodonato	Condensed matter physics
	Cryogenics
A. Santoro	Structure of electronic and structured ceramics
	Theory of crystal lattices
	Powder diffraction methods
S. K. Satija	Low-dimensional molecular systems
	Fractal aspects of microporous media
	Neutron reflectometry
I. G. Schrēder	Cold neutron instrumentation development
	Nuclear and engineering physics
	Optical devices for neutron transport
T. M. Slawecki	SANS and reflectometry from polymers
	Complex fluid microstructure
	SANS instrumentation
J. K. Stalick	Neutron and x-ray diffraction
	Inorganic chemistry
	Crystal database development
M. A. Suthar	Design engineering
	Nuclear systems and components
B. H. Toby	Neutron and synchrotron diffraction
	Zeolite crystallography
	Structure determination methods
J. F. Torrence	Reactor supervision
	Reactor maintenance
	Nuclear engineering
T. J. Udovic	Neutron time-of-flight instrumentation
	Properties of catalysts and adsorbates
	Hydrogen in metals
R. E. Williams	Cold neutron source development
	Nuclear engineering
	Reactor physics simulations