



NATIONAL HIGH MAGNETIC FIELD LABORATORY REPORTS

Florida State University and Michigan State University are engaged in a collaboration to build a sweeper magnet for radioactive beam experiments.

By combining the sweeper with two other unique systems presently at MSU (coupled cyclotron facility and the S800 mass spectrometer)

MSU will provide a cutting edge platform for nuclear physics experiments along both the neutron and proton driplines.





CONTENTS

From the Director's Desk	3	Science is Without Borders	20
From the Chief Scientist's Desk:		Design and Optimization of High Sensitivity Small Volume Probes for Improved Limits of Detection in Protein NMR Experiments	21
Quantum and Environmental Effects in Single Molecule Nanomagnets	5	LANL Update	24
Attention Users:		People in the News	26
Installation of a unique resource at the NHMFL in Tallahassee for NMR Spectroscopy and Imaging	8	Education Programs	28
Actinide Research at Extremes of High Magnetic Field	11	Conference & Workshop Activity	29
Power Systems Center on the Move	13	Grants	31
James Ferner — A Man for All Seasons	14		
The NHMFL / NSCL Sweeper Magnet	15		
Florida Senator Graham Turns to NHMFL to Help Fight Terrorism	19		

Published by:

National High Magnetic Field Laboratory

1800 East Paul Dirac Drive
Tallahassee, Florida 32310-3706
Tel: 850 644-0311
Fax: 850 644-8350

Director: Jack Crow

Director, Government & Public Relations: Janet Patten

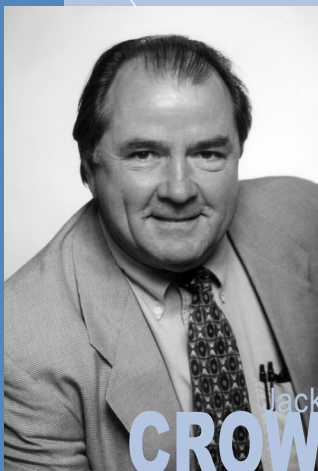
Editing and Writing: Kathy Hedick, Ceci Bell

Design and Production: Wally Thorner, Kathryn Roberts

www.magnet.fsu.edu

*This document is available in alternate formats upon request. Contact Ceci Bell for assistance.
If you would like to be added to our mailing list please write us at the address above, call 850 644-1933, or e-mail bell@magnet.fsu.edu.*

Cover designed by W.W.Thorner



from the Director's Desk

Fall at the laboratory brings with it a flurry of year-end reviews and reporting activities that prompt us to take stock. While reflection can be interesting—and fill lots of paragraphs and pages—it is most useful when it helps us focus sharply on the goals and initiatives ahead. This year's successes, including among others, the bucket test of the 900 MHz NMR magnet, the development of the sweeper magnet (see page 15), and the REU and RET summer education programs, were built on efforts in 2000 and 2001. Accomplishments during 2002 are the foundation for progress and achievements in 2003. So, what's on the horizon?

The Center for Advanced Power Systems, the brainchild of Jim Ferner and others here at the NHMFL in the late 1990s, moves into its new and permanent home across the street from the laboratory in Innovation Park, Tallahassee. In the near future, CAPS will have a test bed and state-of-the-art dynamic simulation capability for use by industry, government, and university researchers. This major center funded by the Office of Naval Research is part of a four-university consortium that includes FSU, Mississippi State University, the University of South Carolina, and the University of Texas at Austin. Read more about CAPS on page 13.

The laboratory is also involved in several R&D projects that could help in our nation's war on terrorism. Jim Brooks' group has demonstrated an integrated, hand-held sensor probe that can determine the fingerprint of a shipping container as it is lifted from the ship to the dock. Additional funding is being pursued for this very promising technology. Alan Marshall's group is preparing to use the laboratory's world-class ICR facilities to resolve and identify complex chemical compounds found in such materials as weaponized bacteria and anthrax spores. These efforts and others were presented to Florida's senior senator, Bob Graham, who visited the laboratory in August (see page 19).

continued page 4...

Research activities at NHMFL facilities at FSU, Los Alamos, and at the University of Florida continue at very strong levels and are increasingly collaborative in nature. This increase in collaborations is reflected by a recent award of \$1,800,000 for 3 years from the National Nuclear Security Administration, part of the Department of Energy. The award headed by Drs. Zachary Fisk and J. Robert Schrieffer will support collaborative research between Florida State University and Los Alamos National Laboratory.

Another strong indicator is this very newsletter. For two years now, this quarterly publication has been so brimming with articles of interdisciplinary science that we anticipate going to five issues per year in 2003. My editor tells me that in the early years of the laboratory, she had to walk the halls and cajole faculty to contribute articles. This is no longer the case, and is yet another indication of the laboratory's strength and stature.

I would be remiss if I did not acknowledge and thank the new NSF Director of National Facilities, Dr. Hugh Van Horn, for his week-long visit to the NHMFL at the end of September. Dr. Van Horn started his week at NHMFL facilities at Los Alamos, meeting with LANL administrators, NHMFL program leaders, and visiting users. At mid-week, he was at the University of Florida in Gainesville touring the High B/T facility at the Microkelvin

Laboratory and the NMR/MRI facilities at the McKnight Brain Institute. In addition to discussions with university and NHMFL leaders, Dr. Van Horn met with John Eyler, who gave him an up-to-date status report on the NHMFL In-House Research Program. John is the director of the IHRP, which supports high quality science and aims to enhance NHMFL facilities and assist new faculty and research staff. Of the 31 pre-proposals submitted, 12 were selected to submit full proposals. Reviews are underway and the decisions will be announced in early November. I single out IHRP for special mention here because this program is an important vehicle for driving new instrumentation and capabilities for users at the laboratory.

At the end of the week, Dr. Van Horn was in Tallahassee for a whirlwind of informal meetings with administrators, visits with on-site users, and discussions with graduate students and user staff. The laboratory is a thriving and energetic organization with dedicated professionals and staff at all three sites, and we believe Dr. Van Horn took away a sense of this. We look forward to working with him and to continuing to work with others at the National Science Foundation as together we strive to advance science, engineering, and education.

Jack Crow



from the Chief Scientist's Desk

In this issue, Stephen Hill describes an investigation of a novel class of materials in which single molecules exhibit a large magnetic moment with weak coupling between moments. While the field of nanomagnets has been aggressively studied recently, these materials have the advantage that each magnet is identical to every other one, making precise measurements of the effective interactions possible. The key feature of the single molecule magnets is the existence of quantum tunneling between the magnetic substates of the molecule. This tunneling is induced, for example, by crystal field or dipolar interactions. The quantum tunneling can be influenced by a weak externally applied magnetic field. There is great potential for application of these materials. The unique experimental facilities of the NHMFL have been of great importance in exploring the properties of single molecule magnets.

Quantum and Environmental Effects in Single Molecule Nanomagnets

Stephen Hill, NHMFL/UF, Physics

Once the sizes of magnetic devices reach the nanoscale (≤ 100 nm), previously unimportant quantum effects will radically alter functionality. Furthermore, scalability will become a serious problem because performance will depend very sensitively on device size, shape, chemical composition, and orientation. Indeed, the discrete quantum energy level structure of magnetic devices at the nanoscale will need to be precisely controlled and understood.

Our recent research efforts have focused on nanometer scale single molecule magnets (SMMs) consisting of a core of strongly exchange-coupled transition metal ions (e.g. Mn, Fe, Ni, or Co) that collectively possess a large magnetic moment per molecule, thus far up to approximately $20\mu\text{B}$.¹ This work was recently funded by the NSF through a Nanoscale Interdisciplinary Research Team (NIRT) award, which brings together chemists and physicists from four institutions: Stephen Hill (EPR) and George Christou (materials) at UF; Naresh Dalal (NMR) at FSU; David Hendrickson (materials) at University of California-San Diego; and Andrew Kent (magnetometry) at New York University. Research in physics at the University of Florida involves the utilization of unique high-sensitivity/high-frequency (20 to 600 GHz) Electron Paramagnetic Resonance (EPR) techniques to initially probe the quantum energy level structure of SMMs and, subsequently, study the interaction between these nanomagnets and their environment.^{2,3}

SMMs offer a number of advantages over other types of magnetic nanostructures. Most importantly, they are monodisperse—each molecule in the crystal has the same spin, orientation, magnetic anisotropy, and molecular structure.¹ They thus enable fundamental studies of properties intrinsic to magnetic nanostructures that have previously been inaccessible. For example, recent studies of SMMs have revealed the quantum nature of the spin-dynamics in a nanomagnet: a metastable state of the magnetization, say “spin-up,” has been convincingly shown to decay by quantum tunneling through a magnetic anisotropy barrier to a “spin-down” state, in a process called quantum tunneling of magnetization (QTM).^{1,4} Remarkably, QTM in SMMs can be switched on and off, either via a small externally applied field or by chemically controlling local exchange interactions between pairs (dimers) of SMMs, so-called “exchange-bias.”⁵ Thus, the prospects for quantum control and quantum information processing are very exciting. In fact, there has been considerable discussion about the use of SMMs in quantum computation.⁶ While there is enormous potential for SMMs, much remains to be learned and the properties of such materials must be greatly improved and tailored for applications. In particular, the microscopic mechanism responsible for

QTM is far from understood, and the factors that affect the quantum coherence of SMMs are not known.

All of the SMMs of interest possess a dominant uniaxial magnetocrystalline anisotropy and, to lowest order, the effective spin Hamiltonian may be written

$$\hat{H} = D\hat{S}_z^2 + g\mu_B\vec{B}\cdot\hat{S} + \hat{H}', \quad (1)$$

where D (< 0) is the uniaxial anisotropy constant, the second term represents the Zeeman interaction with an applied field, B , and \hat{H}' includes higher order terms in the crystal field, as well as environmental couplings such as intermolecular dipolar interactions. This Ising-type anisotropy is responsible for the energy barrier to magnetization reversal and the resulting magnetic bistability—factors that lead to magnetic hysteresis at sufficiently low temperatures. Unlike bulk magnets, this hysteresis is intrinsic to each individual molecule—hence the term SMM. Tunneling in zero-field is caused by interactions in \hat{H}' which lower the symmetry of the molecule from strictly axial, thereby mixing otherwise degenerate pure “spin-up” and “spin-down” states. Tunnel rates depend on the degree of symmetry breaking, which is something that can be determined very precisely via single crystal EPR measurements. Fig. 1 shows EPR spectra obtained for the $[\text{Ni}(\text{hmp})(\text{tBuEtOH})\text{Cl}]_4$ SMM. The symmetry of this approximately cubic molecule is rather high (S_4); the data obtained for field rotations about its easy axis reveal a pronounced four-fold pattern (lower panel of Fig. 1), consistent with a weak crystal field term of the form $(\hat{S}_+^4 + \hat{S}_-^4)$ in \hat{H}' . Tunnel rates deduced on the basis of these findings are in good agreement with magnetic relaxation experiments. Indeed, this represents one of the most clear cut determinations of the tunneling mechanism in a SMM, because $(\hat{S}_+^4 + \hat{S}_-^4)$ causes strong mixing of the $M_s = \pm 4$ zero-field ground states.

The multitude of EPR peaks seen in Fig. 1 is partly due to the large spin of the molecule ($S = 4$), and also due to the transverse applied field, which leads to allowed double quantum transitions (these are seen at fields below 2 T). All of the main peaks may be explained according to Eq. 1. The splittings of some of the peaks (e.g., the 5.5 T peak), however, was unexpected; artifacts such as crystal twinning have been ruled out. A systematic investigation of a series of Ni_4 SMMs, where the intermolecular Cl–Cl contact distances can be varied, reveal that the splitting scales

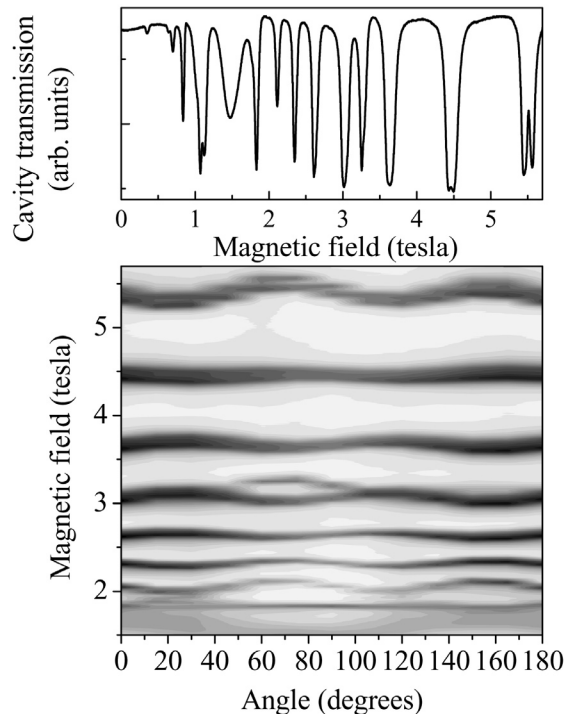


Figure 1. Top panel: a typical EPR spectrum obtained for $[\text{Ni}(\text{hmp})(\text{tBuEtOH})\text{Cl}]_4$ at a frequency of 101.2 GHz and a temperature of 10 K; the many dips in cavity transmission correspond to EPR transitions.⁷ Lower panel: a gray scale map of the EPR absorption intensity versus magnetic field and field orientation within the hard magnetic plane of the sample; the data clearly reveal a four-fold rotation pattern in the positions of the absorptions. The spectrum in the upper panel was obtained at an angle corresponding to 75° in the lower panel.

with the expected strength of intermolecular exchange interactions, which are known to be particularly strong for this family of SMMs.⁷ While detrimental to true single molecule magnetism, exchange interactions can be turned to one’s advantage, as has recently been demonstrated for a dimer system of Mn_4 SMMs;⁵ each half of the dimer acts as a field bias on its neighbor, resulting in a complete suppression of the zero-applied-field QTM. The absence of tunneling at zero field is important if SMMs are to be used for information storage. Similar schemes involving “exchange biasing” are employed in the read heads of some of the latest magnetic recording devices.

The EPR work conducted at UF has been the first to show spectroscopic signatures for exchange interactions among systems of SMMs. In one extreme, large EPR splittings are seen where strong exchange has deliberately been introduced, e.g., the Mn_4 dimers and Ni_4 systems.⁷ In the other extreme, we have demonstrated convincingly that intermolecular exchange interactions are present in prototypical SMMs,⁸ where such effects had previously been neglected. For the weakly interacting cases, evidence

is based on detailed EPR linewidth and shape analyses, as shown in Fig. 2.⁹ These studies were also the first to demonstrate significant distributions in the crystal fields (D and in \hat{H}') in several widely studied SMMs, including the first SMM—Mn₁₂-acetate. These distributions are most likely caused by disorder in the ligand molecules that surround the SMMs. This is particularly interesting in the case of Mn₁₂-acetate, because this disorder may be responsible for the symmetry breaking which gives rise to QTM. This explanation has gained considerable favor with researchers working in this field.¹⁰

None of these investigations would have been possible without the unique instrumentation that has been developed at UF.³ Cavity-based measurements enable studies of extremely small single crystals (< 1×0.3×0.3mm³), with a sensitivity that is on the order of 10⁹ spins.g⁻¹.s⁻¹. The combination of cavities and a phase sensitive detection scheme ensures faithful reproduction of true EPR line shapes (both the dissipative and reactive response). A split-pair superconducting magnet system allows field rotation without compromising the coupling between the cavity and spectrometer, and this capability has

proven essential for all of these investigations. Most importantly, however, the ability to tune the frequency continuously in the range from 20 GHz up to 200+ GHz, as well as the possibility to vary temperature and magnetic field over wide ranges (currently 1.2 K to room temperature and up to 33 T respectively), has enabled us to discriminate between all of the many environmental factors that affect the EPR spectra, e.g., crystal field distributions, intermolecular dipolar and exchange interactions, and spin-lattice effects.⁷⁻⁹ This information is extremely valuable, since fluctuations in these interactions cause quantum decoherence. In the absence of decoherence, QTM generates coherent superpositions of the “spin-up” and “spin-down” states of the molecule, i.e., states that could form the basis for a Qbit. Learning how to reduce decoherence is critical to the future of quantum information processing, and our plans involve probing this coherence via time resolved microwave techniques.

Acknowledgments: We thank George Christou, Naresh Dalal, David Hendrickson, Andrew Kent, Mark Novotny, Kyungwha Park, Per Arne Rikvold, Philip Stamp and Wolfgang Wernsdorfer. Funding is provided by NSF (DMR 0103290 and DMR0196430) and by Research Corporation.

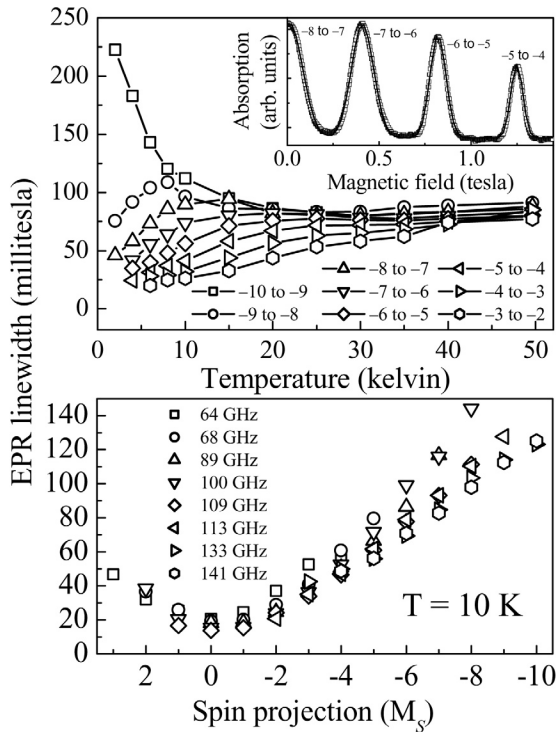
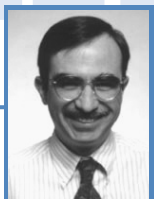


Figure 2. Top panel: Temperature dependence of the easy axis Gaussian EPR linewidths obtained at 116.9 GHz for different spin transitions (indicated in the figure) for the $S = 10$ Fe₈Br SMM from reference 9; the inset shows raw experimental data for several such transitions. Lower panel: A compilation of the M_S (level from which the transition was excited) dependence of the Gaussian EPR linewidths for Fe₈Br, obtained at many different frequencies.

- 1 G. Christou, D. Gatteschi, D.N. Hendrickson and R. Sessoli, *MRS Bulletin*, **25**, 11, 66-71 (2000).
- 2 S. Hill, J.A.A.J. Perenboom, N.S. Dalal, T. Hathaway, T. Stalcup and J.S. Brooks, *Phys. Rev. Lett.*, **80**, 2453 (1998).
- 3 M. Mola, S. Hill, M. Gross and P. Goy, *Rev. Sci. Instrum.* **71**, 186 (2000).
- 4 J.R. Friedman, M.P. Sarachik, J. Tejada, and R. Ziolo, *Phys. Rev. Lett.*, **76**, 3830 (1996); L. Thomas, F. Lioni, R. Ballou, D. Gatteschi, R. Sessoli, and B. Barbara, *Nature*, **383**, 145 (1996).
- 5 W. Wernsdorfer, N. Aliaga-Alcalde, D.N. Hendrickson and G. Christou, *Nature*, **416**, 406-409 (2002).
- 6 M.N. Leuenberger and D. Loss, *Nature*, **410**, 789-793 (2001).
- 7 R.S. Edwards, S. Maccagnano, E-C. Yang, S. Hill, W. Wernsdorfer, D. Hendrickson and G. Christou, *J. Appl. Phys.*, (submitted).
- 8 K. Park, M.A. Novotny, N.S. Dalal, S. Hill and P.A. Rikvold, *Phys. Rev. B*, **66**, 144409 (2002).
- 9 S. Maccagnano, R. Achey, E. Negusse, A. Lussier, M.M. Mola, S. Hill and N.S. Dalal, *Polyhedron*, **20**, 1441 (2001); K. Park, M.A. Novotny, N.S. Dalal, S. Hill and P.A. Rikvold, *Phys. Rev. B*, **65**, 14426 (2002); S. Hill, S. Maccagnano, K. Park, R.M. Achey, J.M. North and N.S. Dalal, *Phys. Rev. B*, **65**, 224410 (2002).
- 10 E. del Barco, A.D. Kent, E. Rumberger, D. Hendrickson and G. Christou, to appear in *Europhys. Lett.*; also cond-mat/0209167.



Attention Users

Tim Cross
NMR Program Director

A unique resource is being installed at the NHMFL in Tallahassee for our NMR Spectroscopy and Imaging users. One of the original goals laid down by the NSF was to achieve magnetic fields in excess of 25 T for NMR spectroscopy. In its first phase towards that goal, the NHMFL is now placing into its final cryostat a magnet designed for 900 MHz (21.1 T) having a room temperature bore of 105 mm. In a recent *NHMFL Reports* (Spring 2002), a thorough report through the early stages of bucket testing was presented. Now, following several months of these tests, the Magnet Science and Technology Group is ready to weld the magnet into its final dewar where the LHe will be at 1.8 K. Full field, high homogeneity, and high stability for NMR experiments ranging from solution and solid state NMR to imaging, diffusion, and *in vivo* spectroscopy are anticipated. Here, I would like to sketch, in general terms, a draft of the scientific vision and its justification for the use of this unique magnet.

The NMR Spectroscopy and Imaging Program at the NHMFL is a national and international user program with access to instruments free of charge. Its mission is to develop technology, methodology, and strategies for very high field applications and to develop the frontiers of the application science through its users and technological developments. Nearly 100 research groups participated in this mission in the past year at these facilities in Tallahassee and in Gainesville at UF. Strong radio frequency efforts are in place at both sites to facilitate the research of both local and external users to accomplish unique spectroscopic and imaging results.

High fields have many advantages:

- Well known enhancements in sensitivity are proportional to $B_0^{7/4}$, resulting in a decrease in signal averaging time proportional to $B_0^{7/2}$.
- Also well known are improvements in resolution at high fields. At constant line width (in Hz), resolution improves linearly with field strength (B_0) for each chemical shift dimension of an NMR experiment.
- Relative magnitudes of field-dependent and field-independent spin interactions change with magnetic field strengths resulting in a reduction of the second-order broadening of quadrupolar nuclei that is linearly dependent on field.
- Magnetic susceptibility effects increase as B_0^2 having important implications for functional MRI, including improvements in spatial resolution and sensitivity.
- Magnetic susceptibility is also responsible for the partial magnetic alignment (as B_0^2) of macromolecules in solution leading to a lowered dependence on liquid crystalline additives for obtaining residual dipolar interactions. Magnetic susceptibility also contributes to the uniform alignment of samples for biological solid state NMR.
- The field dependence of relaxation parameters can lead to improved linewidths (in Hz) and potentially to the use of multiple contact cross polarization at very high fields, thus increasing sensitivity by two, three, or four-fold.
- Increased field strengths provide a greater range of resonance frequencies sensitive to the molecular frequencies of macromolecules, thereby enhancing NMR's ability to provide detailed characterizations of molecular dynamics.
- The relative influence of field-dependent and field-independent relaxation mechanisms can lead to greatly enhanced resolution through the TROSY experiment at high fields for ^{15}N resonances. This experiment at high field will make available NMR as a structural and dynamic characterization tool for many high molecular weight systems and complexes.

- At high frequencies there is a reduction in probe ringing that avoids long delays for detection of signals with short T_2 relaxation.

While these are many of the predicted benefits of high fields, it has been the unpredicted benefits of high fields that are today transforming the NMR community's strategy for macromolecular structure determination and magnetic resonance imaging.

- Spectroscopists over the years have warned that multiple relaxation mechanisms would complicate high-field NMR leading to severe disadvantages. Today, we recognize how to make use of constructive interference between different relaxation mechanisms at high magnetic fields in order to turn this disadvantage into a means for investigating much larger molecules through an NMR experiment called TROSY.
- Until recently, most spectroscopists ignored the slight alignment induced in individual molecules by high fields. Today, this alignment has become a source of new structural constraints that, not only leads to better refined structures, but also enables structural characterization of larger molecules and multi-domain molecules.
- For many years, the NMR community argued against high fields for solid state NMR, in part, due to increased requirements for magic angle spinning speeds, and, in part, due to inefficiencies in cross polarization at high field. Sample spinning rates achievable today are an order of magnitude faster than those 15 to 20 years ago, eliminating the former concern. New strategies for cross polarization have met the latter challenge resulting in better spectroscopy over a broad range of field strengths.
- Concerns about decreased resolution in high field microimaging due to bulk magnetic susceptibility effects were frequently expressed. Today, functional magnetic resonance imaging is the direct result of this problem leading to one of the most exciting new techniques in medical imaging.

This is not to say that there are no disadvantages. Indeed, there will be experiments that are better done at low fields, but there are many advantages of very high fields that will lead to multiplicative effects for sensitivity and resolution in many spectroscopy and imaging experiments. Such significant field effects will open new arenas for scientific pursuit.

To illustrate this multiplicative effect, Prof. Grandinetti of Ohio State University compared the magic angle spinning spectra of ($6\text{-}^{17}\text{O}$) Methyl α -D-Glucopyranoside at 9.4 T (using a 4 mm rotor spinning at 12 kHz) and at 19.6 T (using a 2.75 mm rotor at 20 kHz). The spectrum obtained at 19.6 T in an hour shows far better resolution and sensitivity than the spectrum obtained at 9.4 T with a week of signal averaging time. The comparison shows a sensitivity enhancement factor of about 20 (or B_0^4) by using high magnetic fields. The B_0^4 factor is a combination of gains through the Boltzman factor, resonance frequency, reduced second-order broadening and resolved spinning side bands by the high magnetic field. Such high field spectra are leading to the development of ^{17}O NMR spectroscopy that has great potential for elucidating chemical and biochemical processes in materials and biological macromolecules.

Advantages of Wide Bore Magnets

Wide bores provide opportunities for increased sample size, gradient coils, and probe components. Adult mice, commonly used for biological studies including gene expression and neurological function, cannot be accommodated in narrow bore magnets with compensated gradient coils and large rf coils are required. Perfused rabbit hearts, commonly used to study relationships between metabolism, structure, function, and mechanics, require a bore greater than 52 mm for imaging. Strong rf fields with excellent homogeneity are needed to excite signals in a strong B_0 gradient used for high resolution imaging. They are also needed in solid state NMR, especially for optimal linewidths leading to enhanced sensitivity in magic angle spinning, solid state NMR, and even in solution NMR at high fields where isotropic chemical shift ranges are very large. The ability to achieve such strong rf fields is coupled to the size of the samples and hence the size of the rf coil. Not always is it possible to miniaturize the sample. While *in vivo* specimens are obvious examples, studies of catalytic surfaces, membrane proteins requiring an extensive hydrated lipid bilayer environment, natural abundant samples, dilute environmental samples, or protein preparations that cannot be concentrated may require large sample volumes, and hence high power rf circuitry. Such circuitry requires large size capacitors and insulation to avoid arcing between circuit components. Very low or very high temperature experiments also

(6-¹⁷O) Methyl α-D-Glucopyranoside

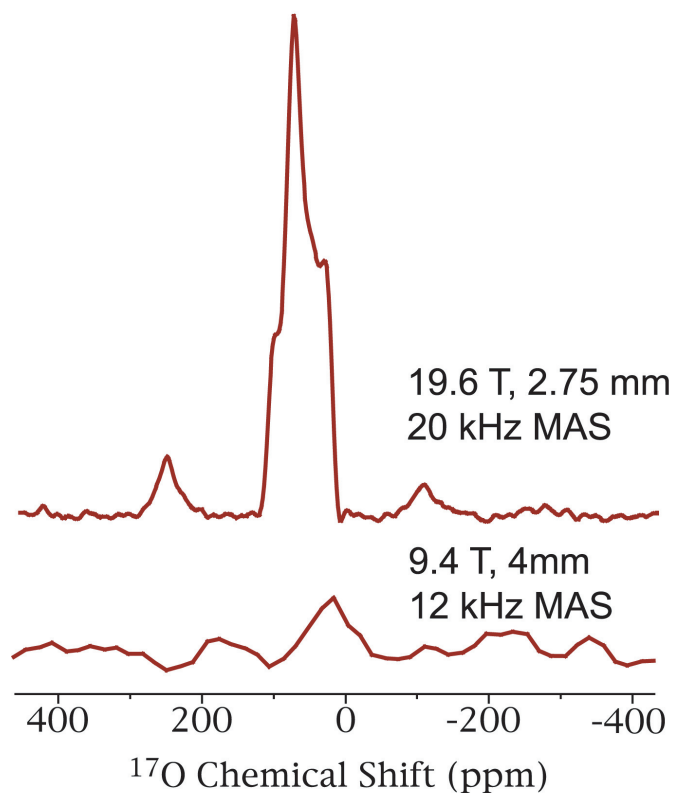


Figure 1. A comparison of magic-angle spinning spectra of ¹⁷O labeled sugar using a 400 MHz (9.4 T) instrument at Ohio State Univ. and the 830 MHz (19.6 T) narrow bore spectrometer at the NHMFL. The data collecting time was 1 hour (19.6 T) and 1 week (9.4 T). (P. Grandinetti/Ohio State and Z. Gan/NHMFL).

require considerable space. For magic angle spinning experiments at temperature extremes, not only is space required for the temperature hardware, but also for increased length of the magic angle spinners so that drive and temperature control air can be separated. As a result, there are many NMR spectroscopy and imaging experiments that can take advantage of the 105 mm bore of the NHMFL's unique 900 MHz magnet.

High Field NMR Spectroscopy and Imaging Science Drivers

Structural and Unstructural Biology

- Structural and dynamic characterizations of high molecular weight macromolecules and macromolecular complexes at high fields
- Characterization of nascent structure in weakly structured macromolecular systems

Membrane Proteins

- High resolution structural characterization of membrane proteins
- Enhanced orientation at high fields of samples for solution and solid-state NMR spectroscopy
- ¹H solid state spectroscopy and multiple contact spectroscopy of membrane proteins uniquely requiring high fields

Materials Chemistry

- Reduction of second order broadening in quadrupolar nuclei through high fields, multiple quantum magic angle spinning (MQMAS), satellite transition magic angle spinning (STMAS), and double rotation (DOR)
- Low gamma nuclei at high fields, characterizations of metal sites in materials including both high and low temperature extremes
- High resolution solid state NMR through high speed ¹H and ¹⁹F MAS at high fields

Cellular Ultrastructure and Kinetics

- Improved temporal resolution at high fields for monitoring metabolic and diffusional rates
- Use of intermolecular zero quantum coherences (iZQC) for enhanced contrast in imaging
- Microimaging for ultrastructural characterization and for monitoring diffusional anisotropy

Based on the above advantages of high fields and wide bores, the following science drivers have been assembled as a guide to the user activities on the 105 mm bore 900 at the NHMFL. We encourage users who are particularly interested in pushing the frontiers of the application science or users interested in the development of technology, methodology, or strategies for high field spectroscopy and imaging. The NHMFL has research faculty who are willing to work with you in any of these areas associated with our mission. For more information, please go to our Web site: <http://nmr.magnet.fsu.edu/>.



Attention Users

Alex H. Lacerda

Director, NHMFL-Pulsed Field User Program

LANL is one of the few places in the world with the infrastructure and the capabilities to investigate plutonium. It is, therefore, crucial for the NHMFL Pulsed Field Facility at Los Alamos to take the opportunity to study Pu under extreme conditions—ultra-high magnetic fields and low temperatures. The following article by C.H. Mielke, A. Migliori and J. Singleton covers work supported by DoE-LANL to develop ultrasonic, thermodynamic, and single-turn coil capabilities for thermal, acoustic, magnetotransport, and spectroscopy studies of Pu in magnetic fields up to 300 T. This work has supported the construction of specific heat and ultrasound capabilities for Pu from 290 mK to 350 K and 0 to 15 T. Previous work on the generation of ultra-high magnetic fields by F. Herlach (Leuven-Belgium) and N. Miura (Tokyo-Japan) were of paramount importance in the development phase of the single-turn project. From the NHMFL user community's view point, this project could evolve, in a couple of years, to be the first in the United States open to qualified users. I encourage the NHMFL user community to read the following article and let us know your ideas about how to further develop this capability in the future to better serve the community.

Actinide Research at Extremes of High Magnetic Field

C.H. Mielke, NHMFL/LANL

A. Migliori, NHMFL/LANL

J. Singleton, NHMFL/LANL

Although many elemental metals are well understood, a few remain mysterious. Perhaps the most interesting and mysterious is plutonium, where a tension between electronic structure and thermodynamics provides a fascinating system for study at extremes of magnetic field and temperature (H - T) space accessible at the NHMFL. Plutonium displays six allotropic phases at ambient pressure (see Fig. 1) which are thought to be driven by the delicate electronic structure near the Fermi energy where temperature, magnetic field energies, and electron energies can be made comparable. This delicate structure, largely unknown, may easily be driven by our magnets, into a field induced phase transition. Because of this, some experts on plutonium assert that “plutonium is one of the most interesting elements in the periodic table, second only to helium.”

As much as scientists welcome theoretical challenge and anticipate undiscovered phenomena, many of the actinides are too difficult to procure, too unsafe to handle, and pose too great a security risk to study effectively. The NHMFL at Los Alamos, however, has

recently implemented the safety, security, and crystal growth infrastructure to enable key studies of these challenging condensed matter systems. Recently, a team at NHMFL/LANL led by John Singleton and Chuck Mielke² has received U.S. DoE-LANL funding to develop the capability to study actinide samples in pulsed magnetic fields up to 300 T. This endeavor is further strengthened by the ongoing work of Albert Migliori and his team who are studying the thermodynamic properties of plutonium in static magnetic fields and have successfully demonstrated that state-of-the-art NHMFL measurement techniques can be applied to plutonium in a safe and secure fashion. These procedures also benefit users of the NHMFL by expanding the user facilities into the new realm of materials previously too difficult to handle.

Recently, John Sarrao and co-workers discovered a new superconducting compound in the 1,1,5 series, which contains plutonium.³ Initial H - T superconducting phase boundary determinations indicate that pulsed magnetic fields of 60 T or greater will be required

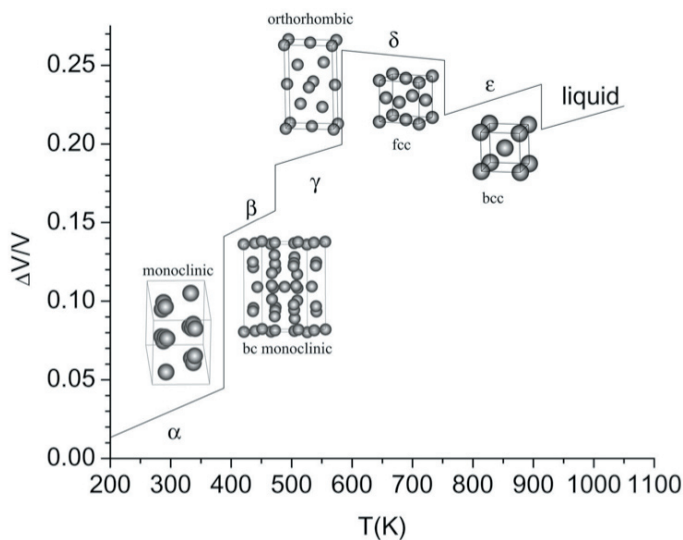


Figure 1. The change in volume of plutonium as a function of temperature, at ambient pressure.¹ Plutonium has six structural phases with intriguing behavior. The fcc phase shrinks on heating and then undergoes a volume collapse as it passes into the bcc phase.

to fully study the superconducting to normal state temperature dependence. This new material can be studied in conventional pulsed fields (to 60 T) at the actinide magnet station that will be part of the new infrastructure at the NHMFL and could eventually be brought to an even more extreme part of phase space with the upcoming 300 T system.

Generation of magnetic fields of up to 300 T will be accomplished by use of single-turn magnets, a concept pioneered initially by Professor Fritz Herlach (Leuven, Belgium), and subsequently developed by Professor Noboru Miura at ISSP, Tokyo, and Professor Michael von Ortenberg of Humboldt University, Germany. Professor Miura has generously offered advice and technical details to the NHMFL/LANL team, so that a reasonably rapid start should be possible; a prototype system is envisaged by mid-2003.

In the single-turn-coil system now being constructed, a low inductance capacitor bank is discharged through

a single sheet of copper bent into a loop that forms the single-turn coil. Very high currents (~3 MA) give rise to very high fields (~300 T), with rise times around 2 microseconds. The coil rapidly turns into plasma and is destroyed; however, all of the forces are directed outwards so that the sample and cryostat usually survive the single-turn shots. This technique is contrasted to the pioneering work of Max Fowler of LANL that used chemical explosives to implode the coil and force the magnetic flux into a smaller volume, hence generating magnetic fields sometimes exceeding 1000 T, subsequently destroying the sample. The single turn technique makes systematic high magnetic field studies to 300 T on the same sample feasible, albeit in smaller volumes.

Already working and available for users are an actinide qualified high-precision Physical Properties Measurement System, specific heat system useful from 2 K to 320 K and 0 to 14 T, a moderate-precision specific heat and transport system covering 0 to 14 T and 260 mK to 350 K. Soon, a resonant ultrasound actinide-qualified system covering 0 to 14 T and 300 mK to 350 K and a micro-calorimeter capable of 750 K will be available.

After the systematic investigation of actinides has matured, we intend to examine the feasibility of integrating the single-turn coil facility into the NHMFL User Program, so that the scientific community can have access to measurements in fields of up to 300 T and a controlled environment that allows for samples that would otherwise not be practical in a conventional laboratory.

- ¹ Figure reprinted from, A. Migliori, J.P. Baido and T.W. Darling, *Los Alamos Science*, **26**, 208, (2000).
- ² C.H. Mielke, J. Singleton, N. Harrison, D. Rickel, F. Friebert, J. Lashley, J. Sims, J. Wills, K-H. Kim and R. McDonald, *LDRD-DR proposal*, 2002.
- ³ J.L. Sarrao, *et al.*, to appear in *Nature* (2002).

NHMFL Annual Reporting

Attention Users and Affiliated Faculty!

The National Science Foundation requires that the NHMFL collect and report the scientific activities of the laboratory, which includes brief abstracts of research activities and reporting of publications, presentations, and related activities. The collection of research reports and publications lists is published as the *NHMFL Annual Research Review*.

The online annual reporting system—<http://www.reporting.magnet.fsu.edu>—opened on November 1; the deadline for all submissions is December 13.

Please go to the Web site for complete information and online instructions. If you have questions, contact the appropriate facility director or Kathy Hedick, hedick@magnet.fsu.edu, 850-644-6392.



Power Systems Center on the Move

Peter McLaren, CAPS Director

The Center for Advanced Power Systems (CAPS) is on the brink of its move into the new building across the street from the NHMFL shortly after saying goodbye to its founding director, Jim Ferner. Fortunately, it turns out that the “Goodbye” was only part time and Jim will continue to play a significant role in CAPS’ future activities. He will continue to represent CAPS on the Advisory Board of the Electrical Ship Research and Development Consortium (ESRDC, \$52 million), which comprises Florida State University, Mississippi State University, the University of South Carolina, and the University of Texas at Austin. He will also be available to help CAPS as a consultant on many issues where his expertise and knowledge will be a considerable asset.

Ferner, along with NHMFL Director Jack Crow, participated in the various meetings and workshops that led the U.S. Navy to set up CAPS in 2000, very much to Ferner’s design, here at FSU. The link to the NHMFL was a critical feature of the CAPS initiative. Apart from the obvious technological links, the association with the NHMFL gave CAPS credibility in the national and international engineering theatre. Ferner used this credibility to attract the highly qualified staff needed to launch CAPS on an ambitious program in power engineering (See related article on page 14).

The original funding for CAPS was a 3-year, \$10 million grant from Office of Naval Research (ONR). After two years, this funding was folded into the ESRDC funding but preserved the original commitments under the \$10 million program. Ferner did all the “spadework” to bring the four universities together in the consortium and was instrumental in ensuring that FSU was the lead institution in the administration of the consortium. Getting academics in the same institution to work together is already hard enough, but Ferner had to get

academics in four universities to agree to share the workload in a sensible fashion in order to convince ONR that the consortium could work.

The major feature of CAPS in its new building will be its high bay test area, which will give it the capability to test power apparatus up to the 5 MW level. When the apparatus under testing is coupled to the Real Time Digital Simulator (RTDS), CAPS will have a unique “hardware in the loop” dynamic test capability not presently available elsewhere at this power level. Not to be outdone, CAPS will also have a large magnet on site when the 100 MJ Superconducting Magnetic Energy Storage (SMES) arrives from BWXT (mid 2003). NHMFL personnel will help with the cryostat design for this magnet. So, bit by bit the grand design that Jim mapped out for CAPS will take shape in his “Quasi” absence. We rely on the attraction of seeing it all come together being more than he can resist and look forward to seeing him often in the new facility (particularly between November and March!)



For more information, contact Peter McLaren at 850-644-8075 or mclaren@magnet.fsu.edu.

JAMES FERNER — *A Man for All Seasons*

In August, Jim Ferner retired to the U.S. Great Northwest in the beautiful countryside outside Portland, Oregon. We all wish Ferner and his wife Betty a long and healthy life as new “retirees” and hope that they return to visit us often.

Probably, no other individual in the laboratory has worn more hats than Jim Ferner has over the last decade. He was one of the earliest members of the NHMFL team. In early 1991, Ferner was working with a large construction and engineering firm in Boston. During a business trip to Orlando to check on one of the company’s projects, a colleague suggested that he stop by Tallahassee and meet this Jack Crow, who had out-competed M.I.T. for the new National High Magnetic Field Laboratory. It did not take Dr. Crow long to figure out that he really needed a person with Ferner’s construction and engineering skills to assist in the planning of the laboratory and oversee the construction.

At the time, a magnet laboratory had never been built from the ground up and much of 1991 was spent in the 7th floor conference room of FSU’s Keen Building laying out plans for the new construction and renovation of the existing building space. Ferner kept these long meetings focused and spent the rest of the time working closely with the local architects and

Marshall Construction. Thanks to Ferner’s careful planning and close supervision, all of the new construction was completed on time (in 18 months) and under budget. This was an extraordinary accomplishment for government work and was even highlighted by Vice President Gore during the NHMFL Dedication.

“If you build it, they will come.” Next, Ferner had to recruit and establish the technical support group to keep the facility running. He was closely involved with the design requirements of the 40 MW power supply, which sets the NHMFL apart from other laboratories. As the construction phase was nearing completion, somebody needed to watch the bottom line and budgets, and Dr. Crow, once again, turned to Ferner to be the Chief Financial Officer of the lab.

The role of interim director of the Center for Advanced Power Systems fit Ferner’s managerial and electrical engineering talents perfectly. Thanks to Ferner’s vision and leadership, CAPS has emerged as a key component to the Navy’s efforts to move to an all-electric ship and represents a crowning achievement to a very productive and distinguished career.



NHMFL Director Jack Crow had this to say about Ferner:

Jim Ferner has been a driving force from the start of the laboratory. He has served the laboratory in a variety of areas from administration to guidance of numerous projects. Certainly, during the very early years, Jim was the person given the lead responsibilities in making sure that the design and construction of the laboratory remained on schedule and within budget. His efforts combined with the good support we had from Marshall Constructors, the general contractor for the laboratory, ensured that the laboratory building was completed on schedule and well within cost. In fact, the cost saving realized in the construction phase allowed the laboratory to do much more than originally planned.

After the construction, I asked Jim to stay on and help with the administration of this new laboratory. He led the procurement team for the large power supplies needed at our Pulsed Field Facility in Los Alamos; he provided oversight to the installation and commissioning of the NHMFL DC power supply; and more recently took over the project management for the 900 MHz NMR magnet system. Certainly, some of the successes of the 900 MHz program during the last few years can be directly attributed to Jim’s leadership.

Jim Ferner has stepped up to the challenge at every critical juncture of the laboratory. As the opportunity became clear that the NHMFL had the opportunity to spin out a new program in power engineering, I asked Jim to head it up. He was appointed by Florida State University as Center for Advanced Power Systems interim director and has led the very successful build-up of that program.

I do not know of too many people in this laboratory who deserve recognition more than Jim Ferner. His dedication and commitment to the laboratory over the years should be recognized at every opportunity before he begins retirement in the greater Portland, Oregon area. He has earned our sincerest thanks, and we are genuinely going to miss him as our esteemed colleague and friend.

The NHMFL/NSCL Sweeper Magnet

Mark Bird, NHMFL
Kirby Kemper, Florida State
University, Department of
Physics

Florida State University (FSU) and Michigan State University (MSU) are engaged in a collaboration to build a sweeper magnet for radioactive beam experiments. The magnet is being built at the NHMFL at FSU and will be operated at MSU's National Superconducting Cyclotron Laboratory (NSCL). The NSF is the primary funding source for both laboratories, as well as this project.

Nuclear Physics Opportunities

The NSCL has recently coupled their two cyclotrons such that the older K500 supplies beam to the newer K1200. This new, coupled configuration offers a unique opportunity to create nuclei along the neutron dripline up to the Sulfur isotopes, a capability presently not available elsewhere in the world. Neutron coincidence experiments will be a major part of the future experimental program at the NSCL and a large gap deflection magnet is necessary to sweep away the beam and the charged fragments from the neutrons.

The NSCL has an S800 mass spectrograph, which is a unique device for charged particle detection. The sweeper magnet will add the capability to perform neutron coincidence experiments. The combination of the sweeper magnet with the S800 will allow simultaneous high resolution momentum distribution measurements of the fragments and neutrons in the decay of halo nuclei and full kinematic reconstruction of neutron unbound states (excited states of nuclei close to the driplines and ground states of nuclei beyond the driplines). In both types of experiments, the magnet sweeps the beam away from zero degrees where the neutrons will be detected with the neutron walls. At the same time, the charged fragments are deflected by the sweeper magnet into the S800 (located at 40°).

The magnet will also play an important role in decay studies along the proton dripline. The study of proton decay of ground and excited states along the proton

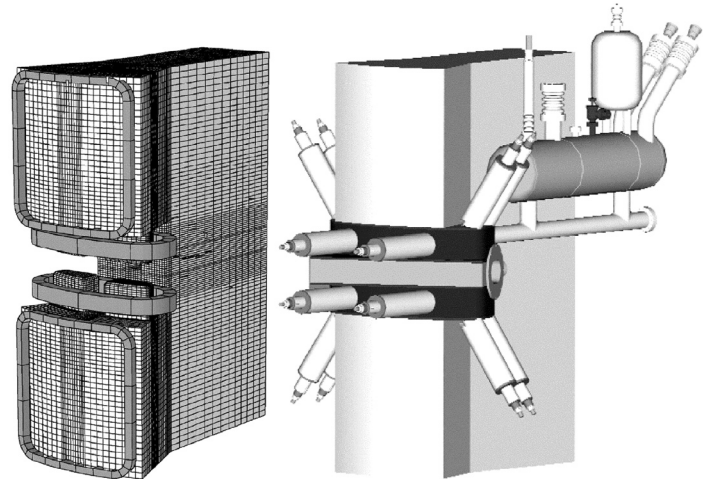


Figure 1. Electromagnetic model of the sweeper magnet (left) with design model (right).

dripline similar to the neutron decay experiments will be possible with its use as will the search for di-proton emitters. For very low decay energy, both the fragments and the proton(s) are emitted near zero degrees in the laboratory rest frame. Thus, a bending magnet is necessary to separate the fragments from the protons before they are detected and identified. Again, the S800 is the ideal detector for the heavy fragment, whereas a high resolution $\Delta E/E$ detector array can be used with the sweeper magnet for proton detection.

In order to use the most rigid beams from the coupled cyclotron facility a focal plane detector similar to the S800 is being built and the sweeper magnet will be used in a "stand alone" mode. The magnet will then be set up in the new N4 vault, which is being extended as part of the coupled cyclotron upgrade. The resulting longer flight path will increase the energy resolution of the neutron walls for the neutron coincidence experiments. Coupled with a quadrupole magnet, the sweeper magnet will also be used as a broad range spectrometer that will allow the gamma rays of higher-lying intermediate energy Coulomb inelastic excitations to be distinguished from the gamma rays produced from excited single nucleon transfer products for masses up to $A = 50$.

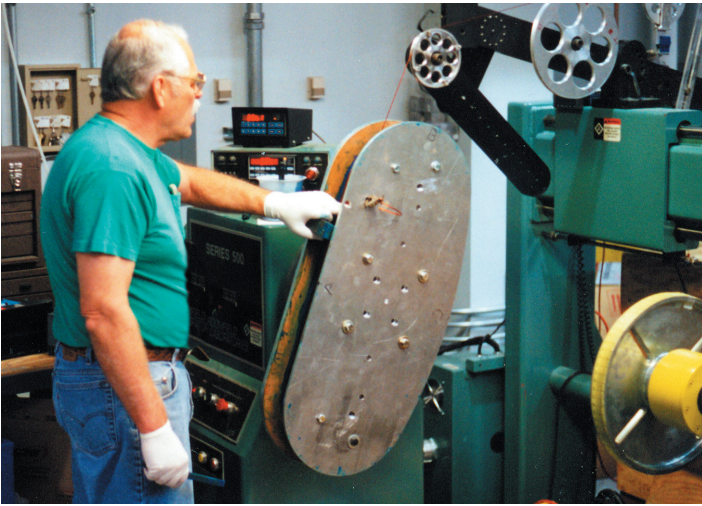


Figure 2. Winding of superconducting coil for sweeper magnet at the NHMFL.

Magnet Design

Electromagnetically, the sweeper magnet consists of two “D” shaped NbTi superconducting coils, a twenty ton “C” shaped iron yoke, and two square resistive trim coils as shown in Fig. 1.

From an assembly perspective, the magnet consists of five major sub-assemblies: the magnet cryostat, the satellite cryostat, the resistive coils, the magnet iron, and the power supplies as shown in Fig. 1. The magnet cryostat, in turn, consists of the two NbTi coils (Fig. 2); a stainless steel bobbin (Fig. 3) that serves as the main structural support and as the helium vessel; structural links from 300 K to 4 K; a nitrogen shield; and a vacuum vessel. The satellite cryostat consists of the helium reservoir, the nitrogen reservoir, nitrogen shields, warm-to-cold links, vapor-cooled leads, bus work and a joint, and a vacuum vessel.

While the magnet provides only modest field (4.0 T on the beam-line and 6.3 T on the conductor) it remains a substantial challenge due primarily to the large gap, non-circular coils, and space constraints. For example, the forces separating the legs of the coils are about 145 metric tons. Such forces require substantial structural support be provided by the bobbin. Not only does the bobbin have to be strong enough to withstand the forces, but it must also be sufficiently stiff to limit coil strain to an acceptable limit.

In addition, the interface between the coil and the bobbin is a very critical design feature. The strain

energy density of the magnet is as high as $39 \mu\text{J}/\text{mm}^3$. The energy margin of the coils is about $7 \mu\text{J}/\text{mm}^3$. If we divide the total electromagnetic stored energy of the coils by their volume, we get $13,240 \mu\text{J}/\text{mm}^3$. Sliding or cracking at the coil/bobbin interface can easily convert sufficient stored energy into heat raising the coil above its current sharing temperature and initiating a quench. Indeed, the smaller “Superbend” magnets that were recently built for the Advanced Light Source at Lawrence Berkeley National Laboratory have similar shape and operate at similar field and current density, and they suffered from numerous training quenches.¹

To fully understand the electromagnetic and structural issues associated with the coil/bobbin interface, several man-months of effort were spent performing detailed three-dimensional finite element calculations of field, body force, and stress distribution with various assumed values of the coefficient of friction. Numerous iterations of coil and bobbin shape were performed to reduce peak stresses and to increase serviceability of the magnet.

Another feature of the design of this coil/bobbin system is the fact that the bobbin has to be welded shut around the coil. The bobbin is made of a stainless steel plate 1/2” to 3/4” thick. Due to the large electromagnetic forces on the coils, the bobbin experiences high stresses, particularly in the weld areas. Nearly full-penetration, crack-free welds are required with very low delta ferrite content to provide sufficient strength, stiffness, and fracture toughness at liquid helium temperatures. In addition, one must avoid overheating the coil during the welding process. Extensive practice welding was performed using various cooling methods to minimize coil heating. The finished practice welds were then tested at low temperature to measure strength, toughness, and ferrite content prior to final selection of welding materials, processes, and operators.

The final coil/bobbin interface system includes a slip surface between the coil and bobbin, an insulating layer between the coil and the slip surface, a helium ventilation scheme, a stiff and strong support, and a low-cost construction, all within a 5 mm space outside the coil.

Finally, the coils and bobbin have to be kept at 4.5 K. While reaching this temperature is typically not a major challenge, in this case the space constraints

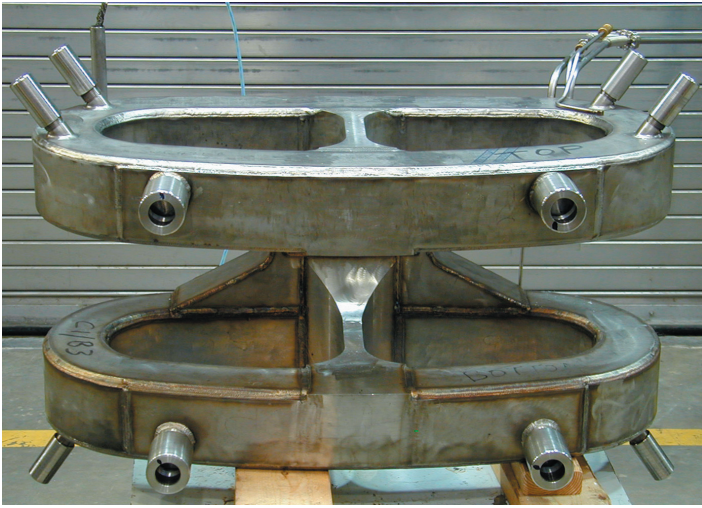


Figure 3. The stainless steel bobbin serves as a helium vessel and the main structural element.

require very small clearance between the 4.5 K bobbin, the 77 K nitrogen shield, and the 300 K vacuum jacket. Over much of the cryostat volume, the space between 4.5 K and 300 K is only 25 mm. The need to combine this tight clearance with a complicated shape lead us to develop a novel laminated nitrogen shield design that provides excellent cooling in very tight spaces. Even with this innovation, however, the cryostat remains a serious challenge.

The wire and coil parameters for the superconducting coils are presented in Table 1. The coils are designed to operate at fairly high overall current density and high stress. The fraction of critical current was intentionally kept low to provide a substantial energy margin to reduce the probability of quenching as well as to facilitate meaningful bucket testing of the coils. The wire is 1 mm x 2 mm with a copper to superconductor ratio of 1.8:1. It is wet wound with stycast and interlayer glass cloth. Stycast was chosen for winding as its thermal contraction on being cooled to helium temperatures is very similar to that of the steel bobbin. Using a dry-wind and impregnation scheme would result in gaps opening during cool-down that may contribute to training and/or degradation.

Three coils were wound between December 2001 and February 2002. Roll bending and welding of the three half-bobbins started in October 2001.

Fabrication Status

The coils were welded into their half-bobbins and tested to high current, field, and strain. The first was

MAGNETIC PARAMETERS AND WIRE SPECIFICATIONS

Peak field on conductor (T)	6.27
Max. field on beam-line (T)	3.96
Coil pack average current density (A/mm ²)	143
Current (A)	365
I/lc	0.28
Stored energy (kJ)	930
Heat load (l/hr of helium)	<10
Turns/layer	46
# of layers	56
Critical current @ 5.27 T (A)	1312
Bare wire height (mm)	1.9
Bare wire width (mm)	0.9
Insulation material	FORMVAR
Insulation thickness (mm)	0.05
Cu:SC ratio	1.8:1
Corner radius (mm)	0.3
Filament size (mm)	46
Twist pitch (mm)	32
RRR	64

completed in May, the second in July, and the third in August of this year (Fig. 4). The test data indicate some variation between the three-coil/bobbin assemblies and the two best (numbers 1 and 3) have been chosen for installation in the final user magnet. The test data suggest that the final user magnet should reach design current with minimal training. The two half-bobbins have been welded together to form the final full bobbin. A joint has been made between the two coils, the lead supports have been installed, and the joint box has been welded shut and leak checked (Fig. 3). As of this writing (late November), construction of the nitrogen shield is underway, to include leak checking.

Then the vacuum jacket will be welded together around the shield, also requiring leak checking. That will complete the assembly of the magnet cryostat.

Satellite cryostat fabrication will follow a similar pattern to that of the magnet cryostat: helium circuit, nitrogen circuit, vacuum jacket, each with an extensive leak check procedure.

Once the magnet and satellite cryostats are complete, they will be brought together and a joint in the



Figure 4. A coil /bobbin assembly is installed in a dewer at the NHMFL for high field testing.

superconducting circuit will be made inside the “services duct” that connects them. The services duct will be closed: again; helium, nitrogen and vacuum, each with extensive leak testing.

When the services duct has been closed, the complete cryostat will be installed in the 20 tons of iron presently located in resistive magnet cell 2, connected to a power supply, energized, and the field will be measured. Once testing is complete, the magnet can be disassembled into pieces less than 2.5 tons and shipped to the NSCL where it will be re-assembled, re-tested, and combined with the beamline, neutron detectors, mass spectrometers, etc., to perform novel nuclear physics experiments as described above.

Acknowledgments

This project has been made possible through the combined efforts and cooperation of numerous persons here at FSU, as well as at the NSCL, and various commercial suppliers. The persons listed below have made major contributions to this project and their efforts are sincerely appreciated. Any omissions are purely accidental. In addition, Denis Markiewicz and John Miller have provided greatly appreciated advice on superconducting magnet design and fabrication.

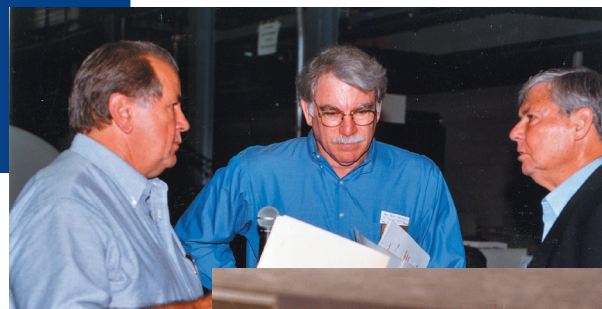
Analysis	Mechanical Design	Testing	Purchasing
Yehia Eyssa	Scott Bole	Iain Dixon	Keith Boockholdt
Andy Gavrilin	Danny Crook	Ke Han	Jim Payne
Soren Prestmon	Scott Gundlach	Mike Haslow	Lee Windham
Gabor Tanacs	Steve Kenney	Vince Toplosky	
Jack Toth		Bob Walsh	
Welding	Assembly	Machining	NSCL Interface
Raymond Lewis	Jerry Kenney	Mark Collins	John DeKamp
Willie Nixon	Ed Miller	John Farrell	Len Morris
Robert Stanton	Ken Pickard	Andy Harper	Mike Thoennessen
		Danny McIntosh	Al Zeller
		Vaughn Williams	
		FSU Physics Shop	

¹ C.E. Taylor, *et al.*, *IEEE Trans. on Appl. Supercond.*, **9**, 2, 479-482. (1999).

For more information, contact Mark Bird at 850-644-7789 or bird@magnet.fsu.edu.

Florida Senator Graham Turns to NHMFL to Help Fight Terrorism

Florida senior Senator Bob Graham visited the NHMFL on August 15 to get a briefing on homeland security related research being explored at the laboratory. Senator Graham is the chairman of the Senate Select Committee on Intelligence and is particularly interested in research and technologies that can help fight terrorism threats. He is especially concerned about the State of Florida's vulnerabilities with its 14 ports and 1,350 miles of coastline.



Every year about 16 million shipping containers enter United States ports and less than 3 percent undergo immediate inspection upon arrival. Physicist James Brooks of FSU and the NHMFL demonstrated proof of concept work he has conducted in collaboration with CSX Corporation, a major shipping company. A shipping container has a marvelous variety of physical characteristics that depend on its history and contents, which is called its fingerprint. With an integrated sensor probe (sensing physical, chemical, and biological signals), this fingerprint can be checked when the container is lifted from the ship to the dock. Prof. Brooks demonstrated that human motion, sound, temperature, magnetic field, acceleration, and the natural electromagnetic and acoustic behavior of a shipping container can be detected by a simple hand-held device and without entry into a sealed container.

Director of the NHMFL Center for Ion Cyclotron Resonance and Kasha Professor at FSU, Alan Marshall, briefed Senator Graham on the center's unique capability of resolving and identifying hundreds to thousands of chemical constituents of complex molecules. Thus, the center can analyze weaponized bacteria. It is reported that anthrax spores normally stick to surfaces. Weaponizing anthrax consists of coating the spores so that they remain airborne and thus inhalable. The center is proposing to analyze this coating, and with a sufficiently detailed chemical fingerprint, they might be able to compare a given sample with one from a putative source lab to see if they match. Prof. Marshall arranged with the Director of Sandia National Labs to have anthrax spores irradiated there so they are no longer infective.

The FSU Sensory Research Institute is housed within the NHMFL and is directed by Dr. Jim Walker. Recently, the institute developed and validated a procedure that for the first time quantifies dog olfactory capabilities while preserving the key elements of the working dog situation, meaning no food or water deprivation. Results indicate that prior and more traditional laboratory approaches have significantly underestimated the capabilities of the dog. Two key steps to make full use of this research and the dog's capabilities to strengthen the ability to fight terrorism are (1) establishing a database of dog-handler teams under many combinations of chemical markers and situations and (2) devising an explicit testing protocol for comparing dog capabilities to those of machines being considered as replacements for the dog. Senator Graham watched a dog identify the correct chemical markers among numerous situations.

Two months after the terrorist attacks on September 11 in the United States, former NHMFL Deputy Director Hans Schneider-Muntau gave a speech to international exchange students at Florida State University (FSU). His remarks, presented below, signify the importance of international student exchange programs in building international cooperation and trust between nations and cultures.

We can state that science is leading the way in international cooperation. Science, is by definition, the search for truth and learning about the eternal verities. Pure science is non-political, non-religious, and non-historical, in the sense that earlier results are not sacred, because they are re-questioned all the time. Science is a vector of peace, because the vector points to truth through its strict discipline in putting objective truth and its honest and true findings above everything.

Science has been a vehicle for international reconciliation. I remember that after World War II, (you are probably too young to know this) Konrad Adenauer and Charles DeGaulle in their vision to bring peace between Germany and France, decided to create a French-German research institute in Grenoble, right in the heart of the French resistance. This was followed by a cooperation between the Max-Planck-Gesellschaft and the Centre National de la Recherche Scientifique in high magnetic fields. I was the first German scientist of this laboratory to move to Grenoble. Looking back, it has been very successful and rewarding, not only scientifically but also personally. In my own technical field, the cooperation with the French resulted in new ideas, which allowed us to build better magnets than the Francis Bitter Laboratory in the U.S. It also prepared the ground for a Nobel Prize. Klaus von Klitzing, the German Nobel Prize winner, said that it was during measurements in our record magnet, at 2:00 in the morning, when he took a snack, a bottle of French wine together with French cheese, that he had the enlightening idea.

I want to go further and say that international cooperation is only the first step. We know that science is international, so why not have the best international scientists working together at the same place? Let me give an example. Before coming here, I was, as mentioned before, an employee of the Max-Planck-Gesellschaft, a famous research organization of Germany. I was impressed by the fact that this organization always hired the best person worldwide they could find for a specific responsibility. I remember the directors of the German Solid State Physics Institute in Stuttgart were of different nationalities, such as Spain, Denmark, U.S., Russia, and Italy. The MPG is very successful in maintaining its international leadership in basic research thanks to this hiring policy. I know that FSU looks to create the same internationality of its scientific staff here in Tallahassee.

A few words about the National High Magnetic Field Laboratory, which I had the chance to help build up, and I recognize some of you who are working there. Since the beginning, we had the vision and ambition to make it the best magnet laboratory in the world. We obviously needed the best people in the world to achieve this end. I think we have achieved this goal. We count more than 300 people out of which there are 73 people with visitor visas and 30 permanent residents. In other words, about one-third of our staff is from outside the United States. It includes countries like Turkey, Uruguay, Korea, Romania, Moldova, Greece, Egypt, China, Palestine, Tanzania, Austria, Tonga, and many others. We highly appreciate this wide variety, and we consider each of you as an ambassador of your nation.

(Dr. Schneider-Muntau is of German descent and earned his Ph.D. in Munich, Bavaria. He worked five years in Italy, twenty years at the National Magnet Laboratory in Grenoble, France, and ten years at the NHMFL as its Deputy Director).

Design and Optimization of High Sensitivity Small Volume Probes for Improved Limits of Detection in Protein NMR Experiments

Yu Li, Univ. of Illinois at Urbana-Champaign, Electrical and Computer Engineering and Beckman Institute for Advanced Science and Technology

Timothy Logan, NHMFL/FSU, Chemistry and Biochemistry

Arthur Edison, NHMFL/UF, Molecular Biology and Biochemistry

Andrew Webb, Univ. of Illinois at Urbana-Champaign, Electrical and Computer Engineering and Beckman Institute for Advanced Science and Technology

The major focus of the High Resolution NMR program at the NHMFL is the NMR spectroscopy of biological macromolecules, including proteins and RNA, in solution. We determine high resolution three dimensional structures to learn about biological function, and we measure the frequencies and amplitudes of internal motions to investigate the energetics of macromolecule-ligand interactions involved in binding and catalysis. Typical protocols for these experiments require macromolecule concentrations approaching 1 mM (10^{-3} moles/liter) of highly purified protein that is isotopically enriched in ^{15}N , ^{13}C , and even ^2H for high molecular weight proteins. Sample volumes are on the order of 150 to 650 μL , requiring approximately 500 nanomoles (10^{-9} moles) of material. Higher magnetic fields increase sensitivity through Boltzmann factors, but this frequently is insufficient to overcome the inherent lack of sensitivity in the NMR experiment.

One approach we have taken is to develop high sensitivity small-volume probes to improve the limits of detection in protein NMR spectroscopy. This work represents a collaboration between the lab of Andrew Webb at the University of Illinois, who is an expert in designing high-sensitivity “microcoils” for use in small-molecule NMR spectroscopy,¹⁻³ and the labs of Logan and Edison at the NHMFL, who have expertise in multidimensional NMR of biomolecules. The goal of the project was to design and implement triple- and quadruple-resonance rf probes using microcoil technology, with pulsed-field gradient coils, for high resolution macromolecular NMR spectroscopy.

The first approach to making small coils is to simply shrink the saddle-coil geometry used in current commercially-available high resolution triple-resonance probes, but this approach is limited, ultimately, by the low filling-factor and poor rf coupling of these designs. Instead, we use solenoidal coils, which have a higher intrinsic sensitivity than saddle-coils due to stronger coupling with the sample. The major

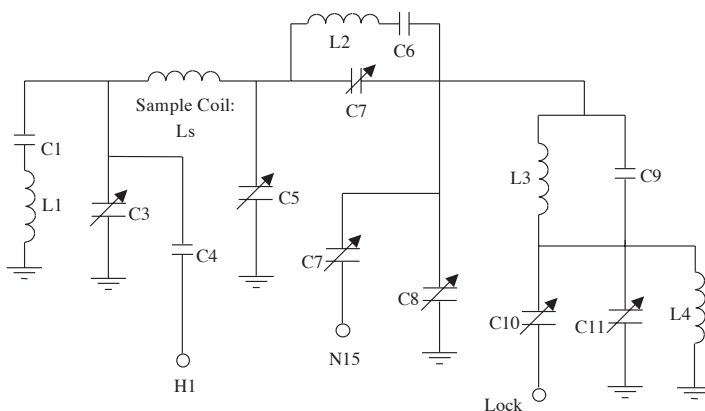


Figure 1. (a) RF circuit for the three-channel, double resonance, or “HX”, probe.

issue in the use of solenoids is the poor rf homogeneity. Webb uses perfluorinated susceptibility-matched fluids to reduce homogeneity problems. Using this approach, he has collected NMR spectra on molecules in as little as 5 nL sample volumes. In our work, we show that efficient multi-frequency coils can be designed using a variable-pitch solenoidal coil. The sample volume in these coils is about 15 μL as a compromise between small sample volumes and the limited solubility of most proteins. These coils produce high quality multidimensional NMR spectra on less than 50 nmoles of protein sample in as little as two hours.

Coil Design

Different impedance matching network designs were modeled to optimize the probe sensitivity. The typical heteronuclear NMR experiment utilizes the high spin polarization of protons to enhance the polarization of lower-gamma nuclei followed by detection on the proton spin, so the designs were performed to optimize the sensitivity, in particular, of proton channel and to minimize rf coupling between ^1H and ^{13}C , ^{15}N , and ^2H . The rf circuit for an optimized H{X} probe, where X is a second frequency, either ^{15}N or ^{13}C , is shown in Fig. 1. Note that probe is referred to as “double” resonance, but it is

in fact triple resonance because it includes a separate circuit tuned to ^2H for field-frequency lock. Since LC (inductance-capacitance) trap circuits are used extensively to separate channels, circuit losses arise mainly from these traps. The L1-C1 trap presents a short circuit at low frequencies and an open circuit at high frequencies. The proton channel matching is balanced, but matching for the other channels is at least partially unbalanced. To optimize ^1H sensitivity, this channel has the shortest electrical path to the sample and the highest quality (Q) factor. A high Q factor L2-C6-C7 tank results in a high impedance at the proton frequency and a short-circuit path at the ^{15}N frequency. Inductive matching was used for the ^2H lock channel because the lock frequency is higher than the ^{15}N frequency and because there is little need for high efficiency of this channel. A parallel LC (L3-C9) trap, resonant at the ^{15}N frequency, is used between the ^{15}N channel and lock channel. The rf coupling between the ^{15}N and ^2H channels is relatively high at the lock frequency, but an external filter having a high impedance at the ^{15}N frequency provides an additional 30 dB of isolation for these two channels.

In the triple-resonance probe, additional trap circuits at both ^{15}N and ^{13}C frequencies are added between the ^{15}N and ^{13}C channels. The lock channel is attached to the ^{13}C channel with a trap circuit at the ^{13}C frequency via capacitive matching. In comparison to the HX probe, the Q value of the proton channel drops slightly, while the Q values of the ^{15}N and lock channels are both higher.

The sample coils in the two probes use the same design. A six-turn solenoid with diameter 2.5 mm and length 4 mm was fabricated using 26 AWG (405 μm diameter) copper wire. The coil was wound on a fused-silica capillary with an inner diameter of 2.2 mm. The active volume of the coil is 15 μL . Initial designs used a constant-pitch solenoid suffered from poor B_1 homogeneity, compromising performance on a range of NMR experiments. Subsequent designs introduced a variable pitch,^{4,5} increasing the $810^\circ/90^\circ$ ratio of the coil by 50% over that of the constant-pitch coils.

The 90° pulse widths were 4.0 μs , 3.8 μs , and 1.8 μs for ^1H , ^{15}N , and ^{13}C , respectively. In comparison, these values are 12 μs , 43 μs , and 14 μs , respectively, for a typical 5 mm saddle-coil probe. As expected, the pulse widths are considerably shorter for the solenoidal coils, reflecting the increases in sensitivity from a more efficient intrinsic design and a reduced diameter. In particular, the 90° pulse widths for the ^{15}N and ^{13}C channels decrease dramatically compared to the standard probe due to an enhanced filling factor and optimized impedance matching circuitry.

Fig. 2 shows a $^1\text{H}\{^{15}\text{N}\}$ correlation spectrum (HSQC) of ubiquitin acquired with the HX solenoidal probe outfitted with a pulsed-field gradient coil. Solvent suppression was

performed using a WET pulse sequence element.⁶ In this probe, a protein sample volume of 45 μL was used. Although the active volume of the coil is 15 μL , we found that it was necessary to have some volume of liquid outside of the coil for reasonable shimming, although this requirement can be reduced by introducing perfluorocarbon plugs into the capillary without any degradation in spectral resolution compared to an infinite cylinder of sample.⁷

Fig. 3 compares the sensitivity of the HX solenoidal probe and a commercial 5 mm probe in HSQC spectra collected under identical conditions, using the same sample mass. In the solenoidal probe 45 μL of 1 mM ^{15}N -labeled IA-3 was used, whereas in the 5 mm probe, 600 μL of 0.1 mM IA-3 was used. The signal-to-noise ratio of the spectra acquired using the solenoidal coil is approximately ten times greater than that of the 5 mm probe.

Conclusion

The microcoil probes designed as a result of this study will have an immediate impact in several areas of structural biology. First, the high sensitivity and reduced sample requirements will allow structural biologists to investigate the structures and dynamics of proteins produced in eukaryotic cells. Currently, most proteins for NMR studies are isotopically enriched by expression in bacteria, which lack many of the post-translational modifications found in eukaryotic cells, such as glycosylation. Isotopic enrichment in eukaryotic cells is considerably more difficult than in bacteria, and cost estimates for producing enough protein for use in standard 5 mm NMR probes are greater than \$30,000 per sample! By reducing the required sample mass by at least an order of magnitude, the micocoils developed here make the study of these proteins economically feasible. Second, and more relevant to the NHMFL mission, the small

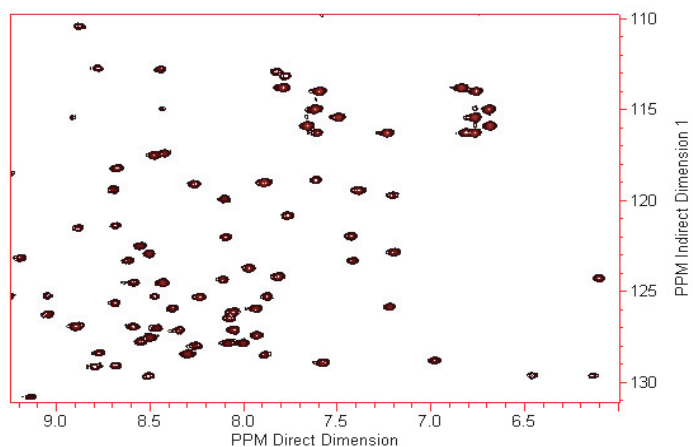


Figure 2. Gradient $^1\text{H}\{^{15}\text{N}\}$ HSQC spectrum of ubiquitin (1.25 mM, 50 μL) using the HX solenoidal probe. Experimental parameters: sweep width (number of complex points): ^1H = 3000 Hz (1712); ^{15}N = 1300 Hz (96), 64 scans per complex t1 time point, relaxation delay 1.5 s, total data acquisition time 2 hours. Solvent suppression used a WET sequence.

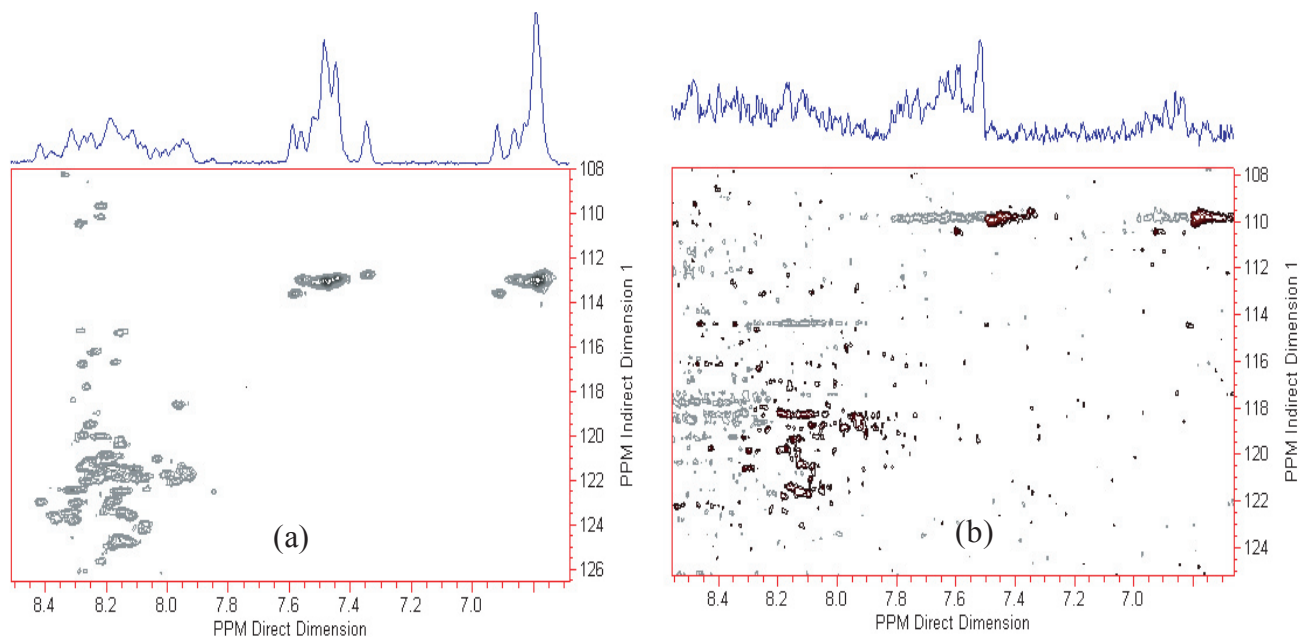


Figure 3. A sensitivity comparison of the HX solenoidal probe and the standard 5 mm probe using equal amounts of ^{15}N -labeled IA-3 and an $^1\text{H}\{-^{15}\text{N}\}$ HSQC sequence. Experimental parameters were the same as in Fig. 2. The solenoidal probe contains 60 μL of 1 mM ^{15}N -labeled IA-3, the 5 mm probe contained 600 μL of 0.1 mM ^{15}N -labeled IA-3. The trace shows the maximum intensity projection of the HSQC plot in either spectrum.

sample volume of microcoils reduces the requirements for the spatial homogeneity in high magnetic fields, potentially allowing us, and external users, to extend results obtained from lower-field NMR studies to much higher fields. In addition, the short 90° pulse widths and high rf homogeneity obtained in the microcoils will provide efficient excitation over the large bandwidths with reduced power demands (for ^{13}C , in particular) encountered in these high fields. Finally, the results of this study represent the first step in producing triple-resonance multi-microcoil probes.^{8,9} These probes support the simultaneous investigation of multiple samples in a single magnet, leading to true, high through-put NMR spectroscopy and very efficient use of the limited magnet time on high-field magnet systems.

Cryo-cooled technology provides an attractive approach for increasing the sensitivity of standard geometry triple resonance NMR probes. In these commercially-available systems, the rf coils are maintained at cryogenic temperatures, thereby reducing Johnson noise in the probe, resulting in approximately 4-fold sensitivity increases. The microcoils provide an interesting alternative for the cryoprobes. Microcoils provide comparable sensitivity increases with considerably simpler technology and reduced cost. Microcoils also provide higher rf coupling with higher rf homogeneity, resulting in significantly shorter pulse widths on all three rf channels.

Acknowledgments: We would like to thank Vedrana Marin and Terry Green for production of the labeled proteins, and William Brey (NHMFL), Peter Gor'kov (NHMFL), and Jim Norcross for helpful discussions on probe design. Feng Lin and Paul Molitor of the VOICE lab at UIUC aided greatly with running the spectra. This project was funded by grants from the NIH (P41 RR16105), the NHMFL (IHRP Grant #5032), and the Alexander von Humboldt Foundation.

- 1 D.L. Olson, T.L. Peck, A.G. Webb, R.L. Magin and J.V. Sweedler, *Science*, **270**, 1967-1970 (1995).
- 2 A.G. Webb, *Progress NMR Spectroscopy*, **31**(1), 1-42 (1997).
- 3 M.E. Lacey, R. Subramanian, D.L. Olson, A.G. Webb and J.V. Sweedler, *Chemical Reviews*, **99**, 3133-3152 (1999).
- 4 K.R. Minard and R.A. Wind, *Concepts Magn Reson.*, **13**, 128-142 (2001).
- 5 K.R. Minard and R.A. Wind, *Concepts Magn Reson.*, **13**(3), 190-210 (2001).
- 6 S.H. Smallcombe, S.L. Patt and P.A. Keifer, *J. Magn. Reson. Ser. A*, **117**, 295-303 (1995).
- 7 B. Behnia and A.G. Webb, *Analytical Chemistry*, **70**, 5326-5331 (1999).
- 8 Y. Li, A. Wolters, P. Malawey, J.V. Sweedler, and A.G. Webb, *Analytical Chemistry*, **71**, 4815-4820, (1999).
- 9 X. Zhang, J.V. Sweedler and A.G. Webb, *J. Magn. Reson.*, **153**, 254-258 (2001).

LANL UPDATE

Recently, Los Alamos National Laboratory featured NHMFL/LANL in its bi-monthly newsletter. The story profiled the lab and its development since inception in 1990. It explained how the lab hosted just one user in 1992, when it set up the first magnet, and now hosts over 100 users annually.

The story focused on how facility changes and magnet capabilities have accompanied the growth of the lab. It also explained the NHMFL's mission and how the three campuses work together not only to create world-class user facilities, but also to produce outstanding in-house research.

The Pulsed Field Facility was also pleased with the recognition it received from NSF's new National Facilities' Director, Hugh Van Horn, regarding his recent visit. In September, Van Horn took the opportunity to visit each of the NHMFL campuses to meet the personnel and observe the facilities. Van Horn came to Los Alamos on September 23.

The visit began with a tour of the facility—from the 1.4 GVA generator to the user cells. Center Leader Greg Boebinger and Alex Lacerda, led the tour. Staff engineers accompanied them for part of the tour, explaining the details of the equipment. Then staff scientists and users met them in the experimental hall to elaborate on some of the unique techniques featured at the lab.

After seeing the extent of the laboratory, Van Horn met with various individuals from the NHMFL and associated groups in Los Alamos, including MST division leaders Ross Lemons and Don Parkin; Bill Press, Deputy Director for Science and Technology; Alan Hurd, Group Leader for the Lujan Neutron Scattering Center, and Alan Hartford, Director of LANL Science and Technology Base Program.

"Hugh's visit was a complete success," said Boebinger. "Not only was his enthusiasm and support for the magnet

A few weeks after the publication of the newsletter story, the article was featured in the U.S. Department of Energy's Research News. The web version can be found at: <http://www.eurekalert.org/features/doe/2002-09/danl-lah090302.php>

"I think this publicity is very important to the NHMFL," said Alex Lacerda, Director of the Pulsed Field User Program. "Since the NHMFL is not specifically a DOE User Facility, it is significant to receive their recognition."



Hugh Van Horn's visit on Sept 23. Van Horn is looking at pieces of the 60 T long pulse magnet with engineer Jim Sims (left of Van Horn) and engineer Joe Schillig.

lab readily apparent, but he also clearly understood the nature of the magnet lab and the challenges that lie ahead of us."

As for Van Horn's opinion of the visit, he wrote the following in a thank you e-mail: "I had an exceptionally interesting visit, and I learned a LOT! ... I came away even more impressed than I had expected to be."

A child using one of the NHMFL demos of a motor that powers a light bulb. This was taken at the family day event in April. This is an example of one of the hands-on demos we intend to share with the Bradbury Museum and one that we routinely use with tours for students. Rebecca Mcintosh is holding motor to keep it still.



Todd Barrick

Finally, in an effort to reach out to the local community, the Pulsed Field Facility has begun collaboration with the LANL Bradbury Science Museum. Inspired by the NHMFL/Tallahassee Center for Integrated Research and Learning (CIRL), the LANL group decided to look for a way to enhance its education outreach. Until this point, individuals in the group took it upon themselves to give talks at area schools, judge science fairs, or participate in career days. Additionally, over the years, the Bradbury museum, as well as other educational groups, has come to the NHMFL to tour the lab facility. Certainly, staff at the magnet lab will be encouraged to continue individual school visits, however, this new initiative hopes to make outreach a group effort as well.

This collaboration intends to help enhance the Bradbury's two education programs (*Science on Wheels* and *A Day in L.A.*) by sharing ideas and expertise with the educators who run the program,

and also by sharing hands-on activities. The magnet lab hopes to share its hands-on demonstrations with the Bradbury programs and also to gain new ones from the museum in return. The NHMFL/LANL plans to enhance its tour-giving capability with help from the Bradbury staff (such as adding curriculum and hands-on activities) as well as increasing the number of tours given in an effort to reach more students.

“Collaboration of our demos with those from the Bradbury both here (at the lab) and there (at the museum) represents a substantial development in our ongoing relationship with the museum and the community,” said Boebinger.

Naturally, this project is in the very beginning stages, and will ultimately be of much smaller magnitude than that in Tallahassee. For a small facility, however, such as that in Los Alamos, it represents a significant first step.



Donovan Hall, an NHMFL magnetometry specialist, has left the User Services Group of the DC facility in Tallahassee to be an editor of *Physical Review Letters*. He helped many users with magnetic measurements, built a solid, well-documented set of magnetic measurements instruments, and trained others in their use. His research and development projects include a SQUID magnetometer for high magnetic fields and superconductivity. He received his B.S. in Physics in 1991 from the University of Dallas and his Ph.D. in Physics in 1997 from Louisiana State University.



Michael Hoch, professor of physics and former chair at University of Witwatersrand, South Africa, is spending a year sabbatical with the Condensed Matter NMR group, working on the magnetic properties of the cobaltites. He received his Ph.D. from the University of St. Andrews, and has worked closely with Don Holcomb and others in the Cornell group. His research interests include: experimental solid state physics, magnetic resonance, and the metal-insulator transition.



Joanna Long, UF assistant professor and biological solid state NMR spectroscopist, has joined the faculty at the UF Department of Biochemistry & Molecular Biology and McKnight Brain Institute. She has a Ph.D. in Physical Chemistry from M.I.T. where she used solid state NMR to study protein structure and dynamics under the supervision of Bob Griffin. As a postdoc, she joined the laboratory of P.S. Stayton and Gary Drobny at the University of Washington where she studied protein and peptide mediation of tissue engineering using solid state NMR dipolar recoupling techniques. In 2000, she

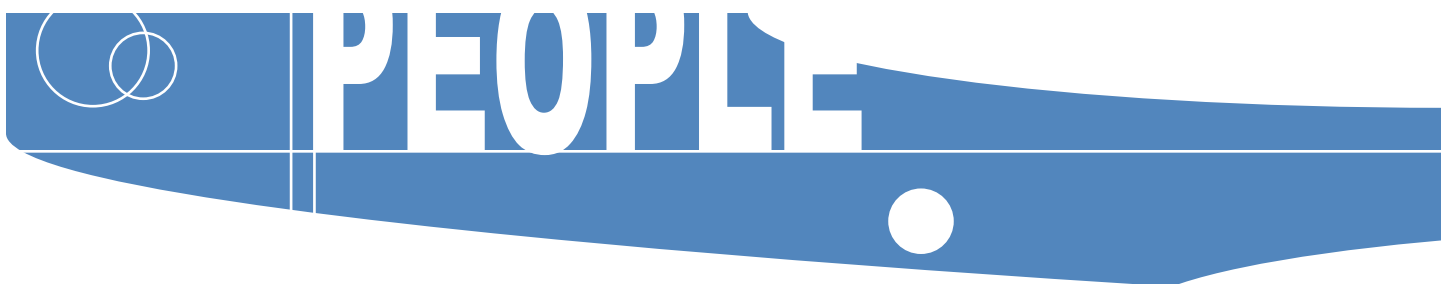
joined the UW Department of Chemistry as the Director of the NMR Facility. Her research interests cover many areas of biology and bioengineering including proteins and peptides on solid supports for biomaterial design and membrane associated proteins and receptors. As part of her recruitment, the AMRIS facility is adding solid state capabilities to its existing Bruker Avance 500 and wide-bore 750 spectrometers.



Cesar Luongo, who has affiliations with the NHMFL MS&T group, the Center for Advanced Power Systems (CAPS), and FAMU-FSU College of Engineering, has been elected to the Board of Directors of the Applied Superconductivity Conference (ASC), the largest and most important meeting in the field of superconductivity. He will serve a 6-year term on the board and will also be Program Chair for the next ASC being organized by the NHMFL (Dr. Justin Schwartz is Conference Chair). ASC-04 will take place in Jacksonville, Florida, October 3-8, 2004.



Vincent Salters, director of the NHMFL Geochemistry Program, has been published in the July 4, 2002, issue of *Nature*, along with J.B. Dicks of the Woods Hole Oceanographic Institution, for their discovery that not one, but two, types of rocks are involved in the production of sea floor basalt, a volcanic rock, during the process of sea floor spreading. This can effect estimates of how much rock material melts, the temperature structure of the Earth's mantle, and how volcanic activity is generated in the first place. Their paper, "Mineralogy of the Mid-Ocean-Ridge Basalt Source from Neodymium Isotopic Composition of Abyssal Peridotites," is a result of their three-year, NSF research project that analyzed samples of rock taken from the floor of the Indian Ocean.



The FSU President and Provost's Named Professorship Program,

established in 2000, has chosen a third round of professors. The professorships, implemented to honor outstanding tenured professors, consist of a title and an annual salary supplement. The recipients exemplify standards of excellence in the teaching, research, and service within their discipline and profession. They hold the appointments until they retire, resign, or leave the university. Three of the new named professors are affiliated with the NHMFL.

Elbio R. Dagotta, professor of physics, was named the Edward A. Desloge Professor of Physics. His research interests include the Theory of Condensed Matter and Materials Science, mainly computationally oriented and Quantum Field Theory and Particle Physics. He received his Ph.D in Physics in 1985 from the Instituto Balseiro in Bariloche, Argentina. In 1998, he was an Elected Fellow of the American Physical Society, and in 1995 received a Developing Scholar Award from FSU.

Naresh S. Dalal, professor of chemistry and chairman of the FSU Chemistry Department, was named the Dirac Professor of Chemistry. He earned in his Ph.D. in Physical Chemistry in 1985 from the University of British Columbia in Vancouver, Canada.

Stephan von Molnar, director of the FSU Center for Materials Research and Technology and long-time colleague of the NHMFL, was named the Robert A. Kromhout Professor of Physics.

FSU Faculty Promotions

Congratulations to the following NHMFL faculty on their recent promotions:

Zhehong Gan to Associate Scholar/Scientist. Gan, a member of the NMR Program, has research interests in solid state NMR, pulse sequence and hardware development, and theory.

Stephen Gibbs to Associate Professor. Gibbs, a member of the NMR Program, has a Ph.D. in Chemical Engineering from the University of Wisconsin. His research interests include magnetic resonance (NMR and MRI), mass transport, and separations.

Ke Han to Associate Scholar/Scientist. Han, a member of the MS&T Program, received his Ph.D. in Materials Science from the University of Oxford. His research interests include high strength conductors and high strength structure materials, plastic deformation, thermodynamic simulation, and nanostructure materials.

Yang Wang to Associate Professor. Wang works in the Isotope Geochemistry Laboratory located at the NHMFL. She is currently researching coastal wetland formation and its significance to carbon sequestration; the source and fate of dissolved organic carbon and phosphorous in Florida Everglades; the factors and processes controlling carbon emission from soils; and the paleodiet and paleoenvironment of fossil mammals in China. She received her Ph.D. in Geology and Geophysics from the University of Utah in 1992.

NHMFL in the News

The laboratory was featured on the History Channel's special "Magnets and Marvels" on August 27. It contained footage and interviews from the laboratory, including physics professor James Brooks and NHMFL Director Jack Crow. They explained unique properties of magnets and detailed how they are used in everyday things like TVs and computers. A 50-minute VHS tape of the special is available from A&E Television Networks.

Their Web address is <http://store.aetv.com/html/>.



EDUCATION PROGRAMS

The new school year brings with it new challenges for the Center for Integrating Research and Learning (CIRL). With standardized testing the focus of education in Florida, teachers are looking to resources such as CIRL to help them with science in their classrooms. For the first time in Florida, science will be tested as part of the battery of tests completed in grades 5, 8, and 10. This fact has driven much of what CIRL has planned for students and teachers.

At its Fall Ambassador Meeting, the NHMFL attracted 70 educators from North Florida and South Georgia. Discussions at the Ambassador Meeting yield valuable information about what teachers want from educational outreach. There was no doubt that our outreach to schools and classrooms provides a valuable alternative to field trips. With budgets tight, teachers are forced to cut back on information science education opportunities unless it is brought to the children. Consequently, CIRL has increased its educational outreach to, on average, two to three classrooms/schools each week.

In addition to classroom and school outreach, CIRL educators are reaching out to larger groups of students, parents, and teachers through events such as Magnet Lab Night at a local school for mathematics and science, Science Night at another local school, teacher events at the local art and science museum, and other community events. CIRL is actively planning, with other community educational outreach groups, a series of workshops for teachers sponsored by the Smithsonian Institution.

After attending and presenting at the “Bringing Research Into Science Classrooms” (BRISC) conference last April, CIRL was asked to serve on two panels at the NSF Research Center Educators Network (NRCEN) workshop at the University of California Santa Cruz. The networking and partnerships that have resulted from this expanded outreach are valuable in creating new educational outreach programs and enriching existing programs. CIRL expects to take a leadership role in creating and maintaining a network of educational outreach programs.

Planning has already begun for Summer 2003 programs including a two-week summer institute for elementary



and middle school teachers that focuses on science content. CIRL has chosen to focus on areas that teachers have reported as weaknesses—physics concepts and integrating other content areas into science. Follow-up is planned with teachers who attended the Summer 2002 institute on magnets and optics.

Another new avenue of focus for CIRL is evaluation. The diverse nature of educational programs at the NHMFL, and the fact that the programs are constantly changing in reaction to issues in education locally, statewide, and nationally, have created a need to evaluate what we do. It is important to identify those features of educational outreach that define CIRL, that are applauded by teachers, and that have become signature programs for the NHMFL. CIRL has increasingly turned to scientists, engineers, and researchers at the laboratory for support with K-12 outreach. Answering questions such as, “What makes for a successful outreach program?” and “How does informal science education affect student attitudes toward science?” helps us as we work with scientists and researchers as they struggle with trying to fit educational outreach into their busy schedules.

The Center for Integrating Research and Learning continues to develop new programs and enhance existing programs as an extension of the NHMFL. The challenges that are provided for us by new local, state, and national educational policy strengthen our resolve to provide quality educational experiences for students, teachers, and the general public. Maintaining successful programs and developing creative new programs will continue to be the focus of CIRL with continued support of laboratory faculty and staff.

2002

High Field EMR Workshop

December 13-14, 2002

NHMFL, Tallahassee, Florida

<http://www.magnet.fsu.edu/news/events/iemrw.html>

This workshop, co-sponsored by the NHMFL, the Italian CNR (Consiglio del Reserche), and the FSU Chemistry Department, will focus on applications and future developments of multifrequency electron magnetic resonance in chemistry, biology, and materials science. A variety of topics will review the role of electron magnetic resonance (EMR) in current and future science, with an emphasis on multi- and high-frequency applications. The sessions planned include: protein structure, photosynthesis, molecular and single-molecule magnets, protein dynamics and simulation, catalysis, low-dimensional magnetic materials, instrument development, and quantum computing.

See the Web site for complete information. Register by e-mail to emr2002@magnet.fsu.edu. The organizing committee includes representatives from the NHMFL (L.C. Brunel, J. Krzystek, and J. van Tol), Istituto per i Processi Chimico-Fisici, CNR Pisa (M. Martinelli and L.A. Pardi), FSU Department of Chemistry and Biochemistry (N. Dalal), and the FSU Department of Biological Sciences (P. Fajer). For more information, contact emr2002@magnet.fsu.edu or call Louis-Claude Brunel at (+1) 850-644-1647.

2003

43rd Sanibel Symposium

February 22 - March 1, 2003

St. Augustine, Florida

Hotel Headquarters: Ponce de Leon Resort

Abstract Deadline: January 3, 2003

<http://www.qtp.ufl.edu/~sanibel/>

This symposium held by the Quantum Theory Project at the University of Florida will focus on forefront theory and computation in quantum chemistry, condensed matter physics, molecular dynamics, quantum biochemistry and biophysics. A new feature is Thursday tutorial lectures on simulation methods. There will be two special plenary sessions for everyone, and a computationally-oriented, hands-on Workshop for Graduate and Advanced Undergraduate students. Invited and poster sessions, as well as informal discussions, will include topics on carbohydrates, coherent control, advanced materials, energy transduction, electronic structure theory, and more. Short course topics include force fields and molecular dynamics. Organizers include NHMFL-affiliated UF faculty, Rodney Bartlett, Hai-Ping Cheng, Henk Monkhorst, John Sabin, and Samuel Trickey.



IBM is the sole corporate sponsor. For more information, e-mail sanibel@qtp.ufl.edu or visit the conference Web site.

4th N. American FT-ICR Conference

April 3-6, 2003

Marconi Conference Center, Coastal Lodge, and Retreat

<http://www.magnet.fsu.edu/news/events/icr4.html>

The 4th North American Fourier Transform Ion Cyclotron Resonance Mass Spectrometry Conference is being organized by the NHMFL ICR Program, and will be held at the Marconi Center, located north of San Francisco (7 miles north of Point Reyes Station) in the quiet hamlet of Marshall, CA. The conference will feature 24 invited plenary lectures (no parallel sessions) plus posters and a feature lecture by Prof. Helmut Schwarz from Berlin. Partial support for a number of graduate student/postdoc posters will again be available. Local arrangements are being organized by Professor Evan R. Williams of the Department of Chemistry, University of California, Berkeley, CA. Complete details about the program, registration, and lodging are available on the Web site. Interested participants may also contact members of the organizing committee: NHMFL/FSU (Alan G. Marshall, Christopher L. Hendrickson, Mark R. Emmett) or NHMFL/UF (John R. Eycler).

VI Latin American Workshop on Magnetism Magnetic Materials and their Applications (LAW3M)

April 7-11, 2003

Chihuahua, Mexico

Advanced Materials Research Center (CIMAV)

Extended Abstract Deadline: November 15, 2002

<http://www.law3m.org.mx/>



The NHMFL is assisting in organizing this biennial meeting initiated in La Habana, Cuba in 1991, and followed by workshops in Guanajuato, Mexico (1993), Merida, Venezuela (1995), Sao Paulo, Brazil (1998), and San Carlos de Bariloche, Argentina (2001). The workshop is designed to support scientific exchanges in the Americas. The LAW3M is a great forum to support scientific exchanges among researchers and institutions interested in recent developments in all branches of fundamental and applied magnetism.

A primary goal during the 2003 LAW3M will be to provide an open forum that promotes exchanges among researchers (including students and postdocs) and discussions of new concepts and developments in materials research and magnetic applications. Workshop proceedings will be published as a special issue of the Elsevier Science B.V. journal, *Journal of Alloys and Compounds*.

SPIE's First International Symposium on Fluctuations and Noise

June 1-4, 2003

Sante Fe, New Mexico

Hotel Headquarters: La Fonda Hotel

<http://spie.org/conferences/calls/03/fn/>

The use of noise techniques to study materials has grown steadily over the past few decades, and the goal of this symposium is to bring together people from around the world working on the most exciting applications of noise to serious material problems. These applications are largely but not exclusively to problems in glassy systems and disordered materials, for which probes that do not average over many dissimilar regions are particularly valuable. Another emerging theme is the use of shot noise to characterize conductance mechanisms in unconventional regimes.

The first meeting on Fluctuations and Noise (FaN) comprises six parallel conferences. The NHMFL is pleased to support the conference on Noise as a Tool for Studying Materials. For complete symposium information, see the Web site, or contact Michael B. Weissman (chair), University of Illinois/Urbana-Champaign, at (217) 333-7897, mbw@uiuc.edu.

XIIth International Quantum Atomic and Molecular Tunneling in Solids Workshop (QAMTS)

June 22-25, 2003

Gainesville, Florida

Hotel Headquarters:

Reitz Union Hotel and

UF Hotel & Conference Center

Abstract Deadline: March 22, 2003

<http://www.clas.ufl.edu/QAMTS/>



The XIIth QAMTS will be held on the campus of the University of Florida in Gainesville. NHMFL Principal Investigator and UF Dean of the College of Liberal Arts and Sciences Neil Sullivan and Juergen Eckert of Los Alamos National Laboratory are the principal organizers. The topics for this important international meeting include Macroscopic Tunneling in Nanomagnets and Related Molecular Systems; Rotational Tunneling of Symmetrical Groups; Proton Tunneling in Hydrogen Bonds; Molecular Dynamics Simulations; Coupled Rotors; Tunneling in Life Sciences; and Tunneling in Glasses and Amorphous Systems.

Sponsors for XIIth QAMTS include the NHMFL, LANL, Spallation Neutron Source, National Institute of Standards and Technology, and UF.

Interested scientists and students should note the following key dates:

March 15, 2003	Deadline for registration and payment
March 22, 2003	Deadline for submission of abstracts
May 20, 2003	Deadline for hotel reservations

For further information, contact Carol Binello at the conference office, cbinello@clas.ufl.edu; (352) 392-0780; fax (352) 392-3584.

2004

16th International Conference on High Magnetic Fields in Semiconductor Physics

August 2-6, 2004, Tallahassee, Florida

Contact: Yong-Jie Wang (Chair)

850-644-1496

wang@magnet.fsu.edu

Applied Superconductivity Conference (ASC04)

October 4-8, 2004, Jacksonville, Florida

Hotel Headquarters: Adam's Mark

Contact: Justin Schwartz

850-644-0874

ASC04ConfChair@magnet.fsu.edu

15th Conference of the International Society of Magnetic Resonance (ISMAR 2004)

October 24-29, 2004, Jacksonville, Florida

Hotel Headquarters: Sawgrass Marriott Resort

Contact: Tim Cross

850-644-0917

cross@magnet.fsu.edu

<http://www.ismar.org/>

2005

Physical Phenomena at High Magnetic Fields - V

August 2005 (tentative)

Tallahassee, Florida

Contact: Mary Layne

850-644-3203

layne@magnet.fsu.edu

24th Low Temperature Physics Conference

August 10-17, 2005

Orlando Hyatt Conference Center

Orlando, Florida

Contact: Gary Ihas

352-392-9244

ihase@phys.ufl.edu

GRANTS

Mark R. Emmett, Ph.D. (FT-ICR program, NHMFL) and Carol L. Nilsson, M.D., Ph.D. (Medical Biochemistry, Göteborg University, Sweden) were recently funded for their application to the Swedish Foundation for International Cooperation in Research and Higher Education (STINT) entitled “An international consortium for structural glyco- and phosphoproteomics as studied by 2D electrophoresis and high resolution mass spectrometry, and applied in neuroscience.” The funding for the academic year 2002/2003 was set at 500,000 SEK (approximately \$50,000 U.S.), with continued funding for up to four years. The grant will cover travel and living expenses during the exchange period. This grant will be pivotal, helping to secure goals that are outlined in other proposals like the R21/R33 recently submitted to the National Cancer Institute by Emmett and his Co-P.I.s Nilsson and Charles A Conrad. These funds will permit the exchange of students/post doctoral fellows/scientists between Göteborg University and NHMFL/FSU to permit training of true multidisciplinary scientists.

In the STINT application, it was specifically stated that the entire consortium should meet once a year, in Göteborg, Sweden and in Florida in alternate years. In order to best coordinate the research consortium’s efforts, the first meeting of this research group was held in Göteborg during August 24-31, 2002. Consortium members from the United States who attended this meeting were Emmett, Michael J. Chalmers, Kristina Håkansson, and TuKiet T. Lam (all members of FT-ICR program, NHMFL) and Charles A. Conrad (M.D. Anderson Cancer Institute-Houston, TX).

Elisabet Gustafsson, a Ph.D. student from the laboratory of Dr. Nilsson at Göteborg University, arrived at the NHMFL on October 25, 2002. Ms. Gustafsson will be learning about FT-ICR MS while analyzing membrane proteins from *Helicobacter pylori*. Ms. Gustafsson will also be learning the technique of Hydrogen/Deuterium exchange for monitoring protein/protein interactions

and sharing her expertise in 2D PAGE separations with the FT-ICR group. Ms. Gustafsson is the first of the visiting scientists from Göteborg University to be funded by the STINT grant.

Zachary Fisk, professor of physics and member of National Academy of Sciences, and **Bob Schrieffer**, NHMFL Chief Scientist and Nobel Laureate, received a research grant from the Department of Energy (DOE) National Nuclear Security Administration (NNSA) Office of Research, Development, and Simulation in the total amount of \$1.8 million over the next 3 years, for their project entitled, “Electron Interactions in Actinides and Related Systems under Extreme Conditions.”

The Center of Advanced Power Systems (CAPS), in collaboration with Georgia Tech, won a contract from NASA to conduct research on superconducting motors and power systems architecture for future aircraft. The NASA work supplements the present CAPS thrust in support of the Navy all-electric ship initiative as aircraft power systems share the need for high reliability and reduced weight and volume. The collaboration with Georgia Tech is part of a NASA initiative to establish a center of excellence in aeropropulsion and power. The CAPS portion of the grant amounts to \$1.5 million over 5 years, with Cesar Luongo (CAPS, MS&T, and Mechanical Engineering) as the Principal Investigator. The funding will be used to initiate research toward the development of very compact superconducting motors. For more information on CAPS activity, see page 13.

Chuck Mielke and **John Singleton**, both NHMFL/LANL scientists, received a \$1.5 million grant for three years (total \$4.3 million) from the Los Alamos Laboratory Directed Research and Development (LDRD) Program. This program provides the flexibility to invest in long-term, high-risk, and potentially high-payoff research activities.



REPORTS

National High Magnetic Field Laboratory
1800 East Paul Dirac Drive
Tallahassee, FL 32310-3706
Tel: 850 644-0311
Fax: 850 644-8350
www.magnet.fsu.edu

Non-Profit
Organization
U.S. Postage
PAID
Tallahassee, FL
Permit No. 55

