REPORTS
The National High Magnetic Field Laboratory
Operated by: FLORIDA STATE UNIVERSITY • UNIVERSITY OF FLORIDA • LOS ALAMOS NATIONAL LABORATORY
FALL 2000
Volume 7 • No.4

Center for Advanced Power Systems Moves Ahead

The new Center for Advanced Power Systems (CAPS) at Florida State University held a successful two-day workshop on July 25 and 26, 2000. The workshop was held at the NHMFL and attended by over 70 individuals, representing 29 corporations, government agencies, and educational institutions. The keynote speaker for the workshop was Admiral Jay Cohen, Chief of Naval Research, who compared the switch to the all-electric ship to the historic transition from sails to steam powered ships. "This transition to all-electric ships is of that magnitude," said Admiral Cohen.

The conference was presented in three sessions; each session included a series of presentations followed by a panel discussion:

- Future Technologies and Economic Drivers, chaired by Justin Schwartz
- Near Term Systems Issues, chaired by Tom Baldwin
- New Equipment Applications, chaired by Cesar Luongo.

The workshop presented the CAPS staff with a wide variety of industry perspectives and provided guidance in setting organizational and technical priorities. Copies of the presentation materials and the final report were distributed to the attendees via CD-ROM.

Three questions were posed to the workshop participants. The plans developed on the basis of the workshop guidance are summarized.

How should CAPS structure itself to better fulfill its mission?

CAPS should develop two staffing thrusts—one directed to educational and academic research and the other focused on more immediate issues developed in response to near-term problems generated by our industrial and Navy partnerships. The key infrastructure needs are office and lab space and computational and simulation capabilities. A new building is in the works at Innovation Park (between the Magnet Lab and the College of Engineering) that will provide CAPS with 24,000 square feet of lab and office space.

A program is in process to evaluate software and computational platforms through simulation of an actual ship, the United States Coast Guard Ice Breaker Healy. CAPS is working to strengthen relationships with Navy

CAPS continued on page 4

CIRL Educational Program *Science, Tobacco & You* Implemented in Connecticut and Illinois

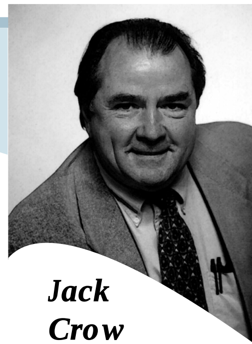
The Center for Integrating Research and Learning (CIRL) continues to develop and disseminate innovative programs for students and teachers and to expand the mission of educational programs at the NHMFL. The *Science, Tobacco & You* program has now been adopted in three states: Florida, Connecticut, and Illinois.

As many as a 1,000 Connecticut fourth and fifth grade teachers are returning to their classrooms this fall with digital cameras, CD-ROMS, stethoscopes, lung bags with mouthpieces, stopwatches, and other tools and knowledge to teach students how the body works and the effects of tobacco on the body. Like

CIRL/ST&U continued on page 5

ALSO IN THIS ISSUE

From the Director's Desk



Jack Crow

National Science Board Approves Increase for NHMFL

It is official. The National Science Board has approved $117.5 million in funding for the NHMFL through 2005. This award represents a 35 percent increase over the last five-year grant of $87.5 million (1995-2000).

Dr. Rita Colwell, NSF director, praised the laboratory in her funding recommendation to the NSB, and I am pleased to share a few of her comments:

> The NHMFL has made outstanding progress in many aspects of this program over the past ten years. The laboratory has successfully developed and put in place a wide and versatile range of high-field magnets and magnetic resonance spectrometers, many with unique capabilities, for users in many disciplines including condensed matter science, chemistry, biology, earth sciences, materials science and engineering, and other areas of engineering. The NHMFL now offers the highest continuous and pulsed fields available worldwide…
>
> The NHMFL requires this level of investment to maintain and consolidate its position of innovation and world leadership for research in high magnetic fields and magnet technology.

Dr. Colwell and the NSF staff also recognized the extraordinary achievements of the laboratory's education program: "The Laboratory has developed and implemented an exciting, multifaceted and highly effective set of educational and public outreach programs…The education programs are absolutely outstanding." This is certainly well deserved praise, and readers of this newsletter need only refer to page 1 of this issue for a glimpse of the laboratory's far-reaching educational outreach activities under the leadership of Drs. Sam Spiegel and Pat Dixon.

The laboratory thanks the NSF for recognizing the important leadership role that the NHMFL has played in advancing science and engineering in the highest magnetic fields possible. We have spent the past decade developing the preeminent center for magnet-related research in the world, and we look forward to a new decade of exploring exciting new science frontiers and technology opportunities.

One example of grasping an outstanding opportunity is the recent establishment of the Center for Advanced Power Systems (see page 1). This center, with its initial funding from the U.S. Navy, is focused on R&D of advanced power systems for transportation and utility systems. The center builds on the expertise of the NHMFL in high field electromagnetics, materials, and superconductivity, FSU, and the FAMU-FSU College of Engineering. All three have unique resources for the development of new equipment and systems for electrical power applications and for training the next generation of electrical power system engineers.

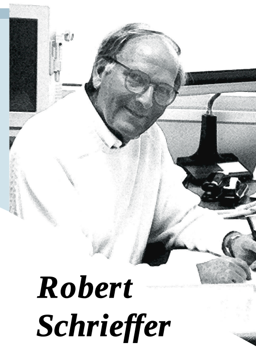
The renewal funding comes with a challenge to, in a timely manner, complete the major 900 MHz NMR magnet project and put the 45 T Hybrid magnet and 60 T Long-Pulse back into full operation for users. These unique, high-priority, and high-risk projects have been and will continue to be the central focus of efforts at the laboratory because we strongly believe that these state-of-the-art systems will open new scientific frontiers and new opportunities for magnet-related technologies.

The laboratory would like to thank, once again, the members of the NHMFL External Advisory Committee and the NHMFL Users' Committee for their time, dedication, and guidance during the renewal process over the last two years. We would also like to recognize the continued support of our institutional partners—Florida State University, the University of Florida, and Los Alamos National Laboratory. Without their ongoing commitment, this model federal-state partnership would be unable to continue to serve its broad international science and engineering communities.

The Committee is very supportive of the research and development activities being conducted at the NHMFL. Based at Florida State University with the University of Florida and Los Alamos National Laboratory as its partners, the laboratory has attracted world-class scientists and engineers and has developed state-of-the-art facilities like no other place in the world. The NHMFL submitted its renewal proposal to the Foundation earlier this year and it is being currently reviewed by NSF and the National Science Board for final funding decisions this fall. The Committee supports strongly the laboratory and the work it has accomplished and hopes that the Foundation continues its support for this outstanding facility.

U.S. Senate Appropriations Committee Report,
September 2000

From the Chief Scientist's Desk



Robert Schrieffer

In this issue, recent NMR studies on $NbBa_2Cu_3O_7$ are discussed. A surprising result is that no evidence for pseudo gap is observed, in contrast to $YBa_2Cu_3O_7$(123); also, the spin lattice relaxation rate is strongly reduced from that in the Y^{123} compound. Furthermore, a minimum in T_1 below T_c is observed in contrast to other superconductors. A spin fluctuation mechanism is considered as an explanation of this effect.

First NMR Experiments in the Hybrid: $NdBa_2Cu_3O_7$

A. P. Reyes, M. Abdelrazek, P. L. Kuhns, T. Caldwell, and W. G. Moulton, NHMFL

Facilities for high field NMR research in condensed matter systems at fields to 30 T have been developed over the past five years by the Condensed Matter NMR group at the National High Magnetic Field Laboratory, with collaboration from the W. P. Halperin group (Northwestern University, NWU) and W. G. Clark (UCLA). A great deal of research in a wide variety of condensed matter systems has been carried out, which has resulted in new physics, a broad based user/collaborator community, and numerous publications. The advent of the Hybrid has extended the available fields to 37 T (the current upper limit of the Hybrid for continuous operation) and hopefully to 45 T in the future. Initial experiments in the Hybrid were very recently carried out on the high temperature superconductor, $NdBa_2Cu_3O_7$, the mixed valent Kondo insulator SmB_6, and preliminary experiments with V. Mitrovic from the NWU group to image the vortex fields. The following reports new results on the high temperature superconductor, $NdBa_2Cu_3O_7$.

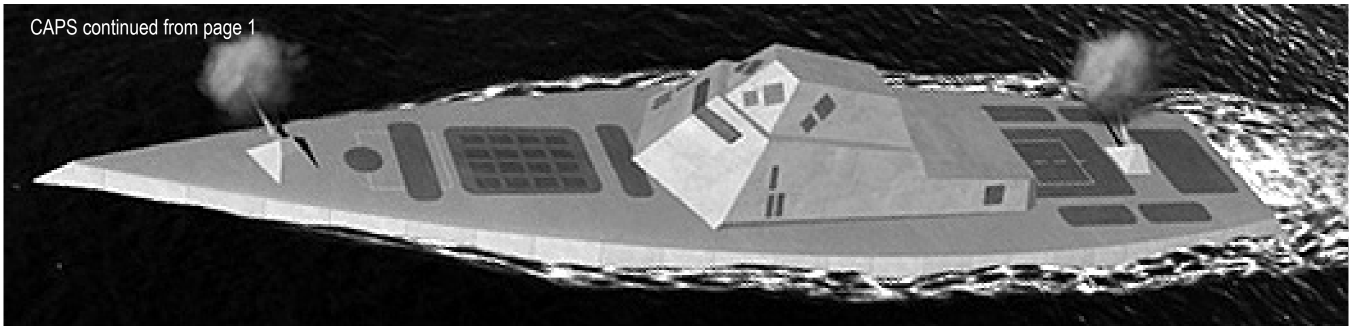
One aspect of high temperature superconducting materials of considerable current issue is the appearance of a pseudo gap and spin fluctuations just above T_c. NMR, primarily through T_1 measurements, has played an important role in the discovery and study of these phenomena. Studies have been carried out as a function of field in optimally doped, underdoped, and overdoped systems[1,2,3,4,5,6] with somewhat different results. This work led to some controversy, recently partially resolved, but the nature and role of the spin fluctuations in superconductivity, if any, are not fully understood. In light of this, an ^{17}O NMR study of $NdBa_2Cu_3O_7$ was undertaken with unexpected results. The Nd is magnetic and like most of the other cuprate superconductors with localized moments, the T_c remains at 92 K. Unlike most RE, however, the Nd ion is known to be too large to fit in the lattice and tends to occupy the Ba-site; the only other case being $PrBa_2Cu_3O_7$. The polycrystalline sample was aligned along the c axis with a magnetic field. The ^{17}O NMR spectra and T_1 were measured for two different O sites as a function of temperature at three different magnetic fields, including 37 T in the Hybrid.

Preliminary data is presented in **Figure 1** which shows T_1 vs. 1/T at various fields for the planar O(2,3) sites. The magnetization recovery at low temperatures is not single exponential due to line overlap, and the values may change slightly with further analysis. There are several features in the ^{17}O T_1 that are very different from the prototypical $YBa_2Cu_3O_7$ superconductor:

a) the spin-lattice relaxation time T_1 at both oxygen sites is nearly 2 orders of magnitude shorter than that of $YBa_2Cu_3O_7$
b) there is no evidence of the "pseudogap" above T_c (92 K), nor a signature of superconducting transition at T_c
c) there is an anomalous field-dependent minimum in T_1 that lies well below T_c.

The Cu NMR in this system is not observable owing to extremely short T_1. The fast relaxation mechanism observed in this system is almost certainly due to Nd spin fluctuations which, in addition to Cu, contributes significantly and possibly dominates and masks the pseudo-gap because of its large moment.

1st NMR EXPERIMENTS in the HYBRID continued on page 6



organizations, particularly NAVSEA, and to develop partnerships with the DOE superconductivity partnership initiative that is developing joint programs. Finally, CAPS is developing formalized industrial relationships around a formal Industrial Advisory Board model with the addition of several focused working groups that will concentrate on specific technological areas.

What are the major systems issues that should be addressed by CAPS?

- System Architecture: The fundamental questions of circuit topology and physical arrangement, voltage levels, and choice of AC versus DC are the key architectural issues. Specifically, ways are needed to evaluate issues of volume, weight, operation and maintainability, and acquisition and life cycle cost in light of mission effectiveness.
- Power Quality Management: The nature of all-electric ship systems calls for re-examination of the issues and methods of power quality management. New ideas and new technologies in filtering and power conditioning are needed.
- Control Technologies: The all-electric ship operating constraints demand a high degree of automation in the electric system which creates a number of control system challenges. In addition, "health monitoring," system state sensing, and automatic system reconfiguration will be a key aspect of control.
- Signatures: It is important that the ship not be readily detected as a result of EMI, RF, or acoustic signatures. These phenomena need to be understood as part of the system R&D.
- Technology Insertion: Finally, a critical aspect of systems studies is looking ahead to the potential adoption of new technologies such as superconductivity. The impact of incorporating new technologies on the system needs to be considered in parallel and even ahead of component development.

What are the technologies that CAPS needs to focus on?

Several technologies may have a profound impact on system development. CAPS needs to maintain a level of involvement in the fields of superconductivity, compact power technologies, power electronics, and advanced machine concepts. It needs to play a role in the evaluation of these technologies, develop simulation models of novel equipment, and study the system impacts of introducing these new technologies into the systems.

In conclusion, the workshop has provided CAPS with major challenges for the future. CAPS is moving forward with the assistance of FSU and the NHMFL in developing the educational program and the research infrastructure needed to support a world-class center for power system research.

For further information on CAPS, contact Jim Ferner, CAPS interim director (850-644-9630, fax 850-644-9462, ferner@magnet.fsu.edu).

CENTER FOR ADVANCED POWER SYSTEMS
FLORIDA STATE UNIVERSITY
Positions Available

Semester Sabbaticals: We have a limited number of positions for semester sabbaticals for faculty who are interested in power systems research, curriculum development, and limited teaching in our new power systems program.

Postdoctoral Positions: A number of postdoctoral opportunities in power systems are available.

Faculty Positions: Several tenure-track faculty positions are available in the EE and ME departments for individuals with interests in power systems and related technologies.

For more information on these opportunities, please contact James Ferner, Interim Director, Center for Advanced Power Systems, Florida State University, Tallahassee, FL 33206-2740, 850-644-9630, ferner@caps.fsu.edu.

CIRL/ST&U continued from page 1

Florida, the Connecticut program is being paid from tobacco settlement funds. *Science, Tobacco & You* is a multimedia, multidisciplinary science curriculum resource that ultimately aims to encourage students to become "scientifically literate" citizens.

The NHMFL, so far this year, has toured and provided outreach for over 4,100 students, teachers, and general public. In addition, CIRL holds several regular events such as the biannual Ambassador Meeting. The fall meeting attracted over 50 area educators, who learned about MagLev train technology, magnetic launching systems, optical microscopy for classrooms, classroom sensory research, and the NHMFL Spanish Moss Project.

This fall, CIRL Director Sam Spiegel, Assistant Director Pat Dixon, and Project Manager Karl Hook are conducting "Train-the-Trainer" sessions in Connecticut and Illinois, as well as training and booster sessions in Florida. "Train-the-Trainer" sessions are for teachers new to the curriculum resource and/or are willing to serve as a facilitator in their school. Booster sessions were recently developed to train teachers who did not receive direct dissemination of the unique curriculum.

Other Center activities and events continue to bridge the gap between real-world science research and classroom science. Recently, an outreach on science in the elementary classroom was conducted with 135 pre-service teachers at Florida State University. The Center actively participated in "Beyond the Blackboard," an event that attracted area teachers to a 2-day mini-conference. Center sessions were well received and well attended. The NHMFL will again host 26 middle school students from the Academic Resource Center for Spring semester mentorships. Students will work in teams with a researcher on a project that gives students a taste of the process of real-world science.

The Spanish Moss Project was developed in collaboration with Dr. Roy Odom and the Geochemistry Department, as part of this summer's Research Experiences for Teachers program. Current research points to the use of Spanish moss as an atmospheric indicator of heavy metal pollutants. To explore this topic, area students and "RET" teachers collected samples of Spanish moss for analysis and started statewide collection efforts. At this writing, over 300 classrooms around the State of Florida have participated. Plans are to expand the project to include all southeastern states where Spanish moss proliferates. Samples will be analyzed and a Web-based database of information set up for teachers and students to access in their classrooms.

For more information on "Science, Tobacco & You," *please visit the Web site at* ***http://scienceu.magnet.fsu.edu****. For the Center for Integrating Research and Learning, go to* ***http://k12.magnet.fsu.edu****.*

1st NMR EXPERIMENTS in the HYBRID continued from page 3

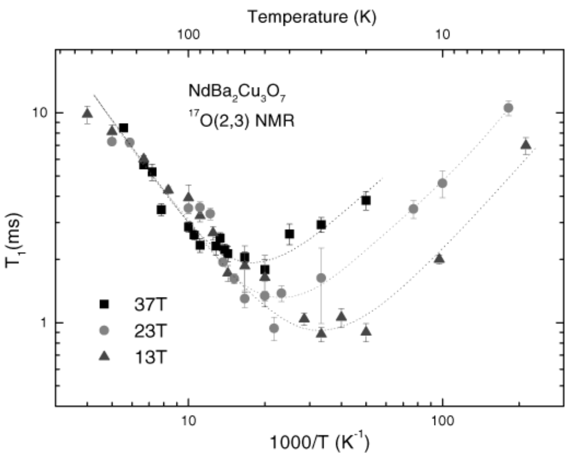


Figure 1. Plot of T_1 vs. 1/T for ^{17}O NMR at the O(2,3) sites in $NdBa_2Cu_3O_7$ for various fields. Lines are guides to the eye.

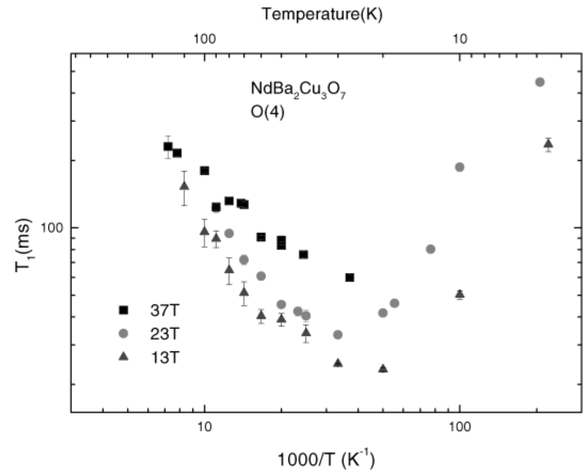


Figure 2. Plot of T_1 vs. 1/T for ^{17}O NMR at the apical O(4) site.

The minimum in T_1 below T_c has not been observed in other cuprate superconductors. The physical origin of this behavior is not clear at present and unexpected considering the fact that the antiferromagnetic ordering of the Nd occurs more than an order of magnitude lower in temperature. Typically, T_1 minimum (or a peak in rate $1/T_1$) is understood as a signature of critical slowing down, and possibly "freezing," of the spin fluctuations. The minimum therefore corresponds to $\omega\tau_c \sim 1$, where τ_c is the correlation time of the Nd spins and is the NMR frequency. In this picture, the field dependence originates from the behavior of spin-fluctuation power spectrum beyond the $1/\tau_c$ cutoff, which goes as $\propto \omega^2$. The magnitudes of T_1 at temperatures below the minimum qualitatively scale with field as expected from this speculation. Data on the apical O(4) site (**Figure 2**), however, also shows a minimum in T_1 at about 20 K, but it is somewhat less field independent, and thus appears inconsistent with the speculations as to the mechanism. On the other hand, the O(4) is much more weakly coupled to the Nd than the O(2,3), as indicated by the almost one order of magnitude longer T_1 and may possibly have considerable contribution from Cu. We currently have no explanation for these interesting new phenomena, and while they are probably unimportant to the superconductivity, they do raise interesting questions as to how, in spite of a very tight coupling of the charge and spin in this system, the critical balance with magnetism is maintained to preserve superconductivity. More experimental and theoretical work is required to understand this behavior.

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1 K. Gorny, O. M. Vyaselev, J. A. Martindale, V. A. Nandor, C. H. Pennington, P. C. Hammel, W. L. Hults, J. L. Smith, P. L. Kuhns, A. P. Reyes, and W. G. Moulton, *Phys. Rev. Lett.* **82**, 177 (1999).

2 Guo-qing Zheng, W. G. Clark, Y. Kitaoka, K. Asayama, Y. Kodama, P. L. Kuhns, and W. G. Moulton, *Phys. Rev B. Rapid Communications* **60**, 9947 (1999).

3 H. N. Bachman, V. F. Mitrovic, A. P. Reyes, W. P. Halperin, M. Eschrig, J. A. Sauls, P. Kuhns, and W. G. Moulton, *Physical Review B* **66,** 7591 (1999).

4 V. F. Mitrovic, H. N. Bachman, W. P. Halperin, M. Eschrig, J. A. Sauls, A. P. Reyes, P. Kuhns, and W. G. Moulton, *Physical Review Letters* **82**, 2784 (1999).

5 Guo-qing Zheng, H. Ozaki, W.G. Clark, Y. Kitaoka, P. Kuhns, A.P. Reyes, W.G. Moulton, T. Kondo, Y. Shimakawa and Y. Kubo, *Phys. Rev Lett* **85**, 405 (2000).

6 G. Q. Zheng, W. G. Clark, Y. Kitaoka, K. Asayama, Y. Kidama, P. L. Kuhns, and W. G. Moulton, *Phys. Rev B. Rapid Communications* **60**, 9947 (1999).

Advanced Magnetic Resonance Imaging and Spectroscopy (AMRIS) Facility Progress and Research Report #5, October 2000

Steve Blackband, Associate Professor, University of Florida Neuroscience Department

AMRIS Progress, October 2000

1. 750MHz:

In the last report, we described that over a few hours the magnet homogeneity falls off significantly. The instrument is fine for short spectral acquisitions (a couple of hours), but sub-standard for longer (overnight or more) runs. The Bruker engineer came in July to look into the problem and determined that there existed a small, but significant, coupling between the wide bore gradient shim set and the cryoshims of the magnet. Consequently, when the narrow bore (high resolution) shim sets are placed in the magnet, the wide bore shims are disconnected and perturb the cryoshims. This coupling takes several days to stabilize. To circumvent this issue, Bruker will supply a second shim set power supply and control boards so that the wide bore shims may be left powered on when the narrow bore shims are used. It is anticipated that this will cure the long term spectral stability issue. The new equipment has arrived and the engineer comes back on October 16th to effect the modifications. Incidentally, this is the first wide bore Bruker has installed requiring imaging and high resolution capabilities, so it was a surprise for Bruker and an important development for their future sales.

The imaging capabilities of the instrument continue to be quite astounding. Using a 15 mm diameter Bruker birdcage coil, images with a 47 micron isotropic resolution with an SNR of 32 (no filtering) can be routinely obtained in 2 hours and 43 minutes of fixed biological samples.

2. 11.7T/40cm:

Last time, we reported that the 11.7 T had made field and that we were awaiting corrected gradient coils for completion. Since that time, however, we have had severe difficulty filling the magnet—an indication of a developing ice blockage in the cryogenics. Magnex returned and, to cut a long story short, a very large ice block was revealed. Upon further investigation, much of the cryogenic supply and pumping lines in fact are very leaky! Magnex has resolved to fix the situation and, so far, an engineer has been working on the job for five straight weeks. To make the magnet safe for this operation, the field was lowered to 9.4 T where the magnet is stable without pumping. When the vacuum and pumping lines are finally satisfactory, we will return to 11.7 T. This has been a learning curve for Magnex (this is their first pumped system) and we remain grateful for their continuing efforts to solve the problems. Many thanks especially to Alwyn Smith, who has taken over as the senior installation engineer following the Magnex shakeup and now virtually lives in Gainesville!

In the meantime, we have an upcoming NIH site visit to develop AMRIS as an NIH Resource. To provide preliminary data, Bruker has been extremely supportive and supplied rf amplifiers enabling the system to operate at 9.4 T. Despite being quite ill, Mark Mattingly came down in early October and made the instrument functional at 9.4 T, providing us with our first phantom data and then *in vivo* images of a rat. The magnet is not optimally cryoshimmed at 9.4 T, but the images were nevertheless quite good. Additionally, Barbara Beck was able to demonstrate, at least at 400 MHz, that her new ReCav rf coil (described in AMRIS report #3) out-performed a conventional birdcage coil with an SNR improvement of 45%. This data is crucial for the site visit on October 16th. Many thanks indeed Bruker. We hope to be returning to 11.7 T later this month.

Ben Inglis has announced that he will be leaving us by the end of the year. Ben has been crucial for the development and installations at AMRIS and will be sorely missed. He is moving on to a new position at Stanford—good luck Ben. Consequently, a search has begun for a replacement, recently advertised in *Magnetic Resonance in Medicine and Science*. Please bring this to the attention of anyone you think may be appropriate.

We would like to take this opportunity to pass on our sincerest condolences to the family and friends of the young Magnex engineer fatally injured on a recent magnet installation in New York. This tragic incident serves to remind us of the inherent dangers of the systems with which we work and that we must remain vigilant and careful around them. The AMRIS facility is well set up with oxygen sensors in all rooms; however, the installation of additional ground level sensors is under consideration. May I suggest that we all take a moment to review the SOPs of cryogenic facilities to ensure that such unfortunate circumstances do not occur again.

AMRIS continued on page 8

AMRIS continued from page 7

The following research report briefly describes single cell diffusion data obtained on the 600 MHz instrument at the NHMFL that has just been submitted for publication.

AMRIS Research Report #5

Diffusion Imaging of Isolated Single Neurons

S. Grant, University of Chicago, Illinois
D.L. Buckley, University of Florida Department of Neuroscience and the McKnight Brain Institute
S. Gibbs, NHMFL
A. Webb, University of Illinois
S.J. Blackband, UF Department of Neuroscience, McKnight Brain Institute, NHMFL

Several groups have now demonstrated that the diffusion signals observed in biological tissues, mainly in neurological studies, is multicompartmental in nature (see references in 1 and 2). The origins of these compartments, however, remains unclear. We have demonstrated that the diffusion of water in perfused brain slices is multiexponential.[1, 2] To a first approximation, fitting to a biexponential may grossly approximate the intra and extracellular spaces in the tissue, as supported by data acquired following physiological perturbation on perfused brain slices.[1, 2] In this study we examine diffusion signals in isolated single neurons with a view to aiding the interpretation of diffusion measures on macroscopic cell assemblies.

L7 *Aplysia* neurons were isolated and placed in a susceptibility-matched microcoil 700 microns in diameter[6] and experiments were performed in a 600 MHz Bruker wide bore instrument at the NHMFL. Ten increasingly-diffusion-weighted images were acquired in 3 hours with b values up to 12264 s/mm^2. In these experiments the spatial resolution is relatively low (40 x 40 x 150 µm) to provide adequate SNR for curve fitting.

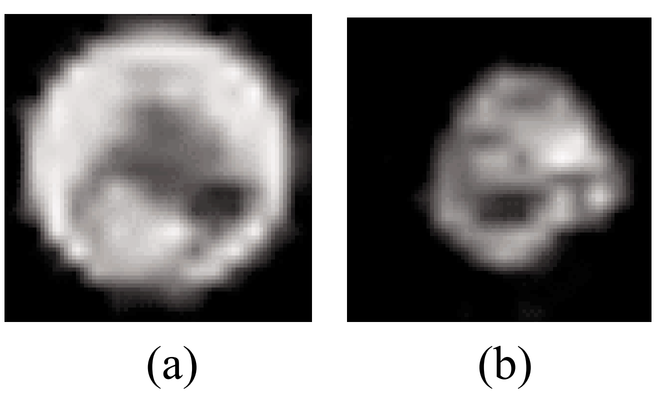


Figure 1. Diffusion weighted images of a single cell. (a) With virtually no diffusion weighting (b = 302s/mm^2) the central bright nucleus is surrounded by the dark cytoplasm, which in turn is surrounded by artificial sea water. (b) With strong diffusion weighting (b = 7856 s/mm^2), the fast diffusing water and nuclear signal is lost, leaving only the slow diffusing cytoplasmic signal.

Figure 1 shows example images from one cell demonstrating the slow diffusion component of the cytoplasm. **Figure 2** shows a diffusion curve obtained from a series of diffusion weighted images that were segmented manually to isolate the nuclear and cytoplasmic compartments. The non-linear log curve demonstrates clearly that diffusion in the cytoplasm is multiexponential, indicating multiple components of water diffusion. Excluding seawater contamination the ADCs from the cytoplasm (n = 6, with relative fraction) were 0.54 ± 0.14 x 10^{-3} mm^{2}s^{-1} (65 ± 10%) for the fast component and 0.043 ± 0.013 x 10^{-3} mm^{2}s^{-1} (35 ± 10%) for the slow. The nuclear curves appear primarily monoexponential, but fitting a biexponential gives 1.1 ± 0.3 x 10^{-3} mm^{2}s^{-1} (89 ± 8%) for the fast component and 0.036 ± 0.031 x 10^{-3} mm^{2}s^{-1} (11 ± 10%) for the slow. Thus it appears that the slow diffusing component from the nucleus arises from a small degree of volume averaging with the cytoplasm at these relatively low spatial resolutions.

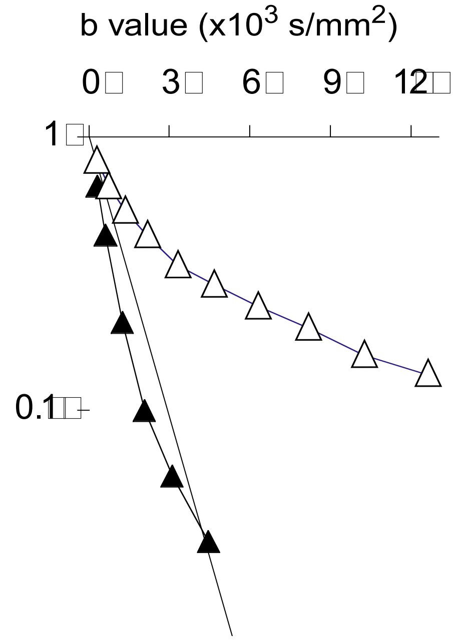


Figure 2. Normalized diffusion curves measured in the cytoplasm (open symbols) and nucleus (filled symbols) of a typical cell. Data were acquired using diffusion times of 10 ms.

These data demonstrate directly, for the first time that the diffusion of water within the cytoplasm of single cells appears multicompartmental. This has implications for the interpretation of diffusion signals from intact tissues. It may explain why the compartmental size of the extracellular component is overestimated when a simple intra/extracellular model is employed.[2] Rather, it may be that the fast diffusing component exists intra and extracellularly, while the slow diffusing component is primarily intracellular. We are presently developing new model systems to further investigate these possibilities.

1 Buckley *et al.*, *Magn Reson Med* **41**, 137 (1999).
2 Bui *et al.*, *Neuroscience* **93**, 487 (1999).

Conference & Workshop Activity

US-Japan Joint Seminar on Innovative Measurement Techniques in Cryogenics
December 3-6, 2000
NHMFL, Tallahassee, Florida

The NHMFL, NSF International Programs Division, and the Japanese government are co-sponsoring a small workshop of approximately 30 attendees. For three days, researchers involved in the development of cryogenic measurements and instrumentation will discuss new devices and techniques, and their use in measurements and applications. Invitation only, the small seminar is expected to provide a very effective forum for focused exchange. Contributions by world leaders in the field will be of a tutorial nature; shorter ones on more narrowly defined topics will be given by junior scientists and graduate students. For further information, contact Steve Van Sciver, director of NHMFL Magnet Science and Technology Program, 850-644-0998, fax 850-644-0867, *vnsciver@magnet.fsu.edu*.

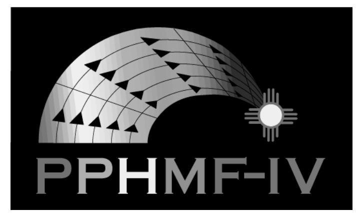
Third North American FT-ICR Conference
March 22-24, 2001
Austin, Texas
Hotel Headquarters: Omni Austin Hotel
Pre-Conference Registration Deadline: February 1, 2001

The NHMFL ICR Program initiated this biennial conference in Tallahassee in 1997. The deadline for poster/talk titles and application for Student Award, group hotel rates, and early registration is February 1, 2001. For updated information, contact Mark R. Emmett, 850-644-0648, emmett@magnet.fsu.edu; Chris Hendrickson, 850-644-0711, hendrick@magnet.fsu.edu; or visit the Web page at http://www.magnet.fsu.edu/news/events/icr.html.

Fifth MRS/ISTEC Joint Workshop on High Tc Superconductivity
June 24-27, 2001
Honolulu, Hawaii

The NHMFL is a partial sponsor for this workshop. The general theme is Processing and Applications of High Tc Conductors, with a special focus on HTS Coated Conductors. Other U.S. sponsors include Oak Ridge National Laboratory, Los Alamos National Laboratory, Argonne National Laboratory, and the University of Wisconsin. ISTEC is a Japanese organization; MRS is the Materials Research Society.

Physical Phenomena at High Magnetic Fields (PPHMF-IV)
October 19-25, 2001
Santa Fe, New Mexico
Hotel Headquarters: Hilton of Santa Fe



This major international conference was initiated by the NHMFL in 1991 and is held every three years. After three meetings in Tallahassee, PPHMF-IV is moving to New Mexico! The key dates and deadlines are as follows:

- December 15, 2000, Final Call for Papers
- May 24, 2001, Pre-Registration
- June 1, 2001, Abstract Deadline

For updated information, see the conference Web site at *http://www.lanl.gov/mst/nhmfl/PPHMF4/*.

Applied Superconductivity Conference (ASC04)
October 4-8, 2004
Site: Jacksonville, Florida

This important international conference is held every two years and typically attracts approximately 1,800 participants. In September 2000, ASC00 was held in Virginia Beach, Virginia; in August 2002, ASC02 will be in Houston, Texas, and in October 2004, ASC04 comes to Jacksonville, Florida. For information, contact ASC04 Conference Chair Justin Schwartz, project leader in NHMFL's Magnet Science & Technology program, 850-644-0874, fax 850-644-0867; *schwartz@magnet.fsu.edu*.

Attention Users

Gregory S. Boebinger, Director, NHMFL–Los Alamos

Alex H. Lacerda, Director, NHMFL–Los Alamos User Program

NHMFL Pulsed Field Facility Update

60 T Long-Pulse Failure

At approximately 9:15 a.m. on Friday, July 28, the 60 T Long-Pulse (60 T LP) magnet failed during otherwise normal operations at the Pulsed Field Facility of the National High Magnetic Field Laboratory (NHMFL). Initial indications are that the full 90 MJ of peak magnetic field energy contributed to the destruction of the magnet. Analysis of the debris is underway and will continue for another month. One emerging theory is that the magnet failure nucleated as a stress-induced failure of a reinforcing shell around one of the middle layers of the magnet.

The NHMFL is committed to rebuilding the 60 T Long-Pulse magnet.

The 60 T LP Magnet Recovery Plan

Although a final recovery plan will await the outcome of the 60 T LP debris analysis, a preliminary plan calls for the construction of a replacement magnet, the 60 T LP-II, which follows the same general design as the original 60 T LP. The design margins in the new 60 T LP-II are expected to be dramatically increased by the incorporation of stronger conductor and reinforcing materials that have been recently developed as part of the NHMFL's 100 T magnet project. Under the current plan, the 60 T LP-II magnet is scheduled for commissioning in two years.

The 60 T LP Scientific Recovery Plan

The 60 T LP magnet was commissioned in August 1998. During its lifetime, the magnet was pulsed approximately 900 times, from which data was collected for 22 submitted manuscripts, of which sixteen are already in print. Among these articles are six *Physical Review B* articles, three *Phys. Rev. B Rapid Communications*, a *Physical Review Letter*, and an article in *Nature* magazine (A second manuscript containing data from the 60 T LP magnet was recently submitted to *Nature* magazine). Research on the 60 T LP magnet has led to fifteen invited talks at international conferences.

The staff of the NHMFL Pulsed Field Facility is working to minimize the scientific impact of the loss of the 60 T LP magnet by migrating the 60 T Long-Pulse Magnet Research Program to other unique NHMFL magnets, by developing entirely new experimental techniques, and by dramatically increasing the experimental capacity of the NHMFL Pulsed Field Facility.

(1) A newly-designed 50 T "Mid-Pulse" magnet, energized by the 1.6 MJ capacitor bank, will address many of the needs of the NHMFL Optics Program, which had constituted the bulk of the research performed on the 60 T LP magnet. In addition, the 50 T Mid-Pulse magnet will provide a platform for developing new AC specific heat and thermal conductivity measurements, as well as new low-noise magnetotransport measurements. Specific heat and magnetotransport measurements accounted for the rest of the 60 T LP Research Program.

(2) A "Quick-Cool" magnet design is in the early stages of development. This magnet could have a dramatic impact on the scientific productivity of all existing Short-Pulse Magnet programs, because of the expected doubling of the pulse repetition rate, the anticipated quieter experimental environment, and the possibility of extending the peak magnetic fields available to users.

(3) Adiabatic specific heat measurements, which demanded the pulse-shaping capability of the 60 T LP magnet, will be developed for use in the hybrid magnet at the NHMFL in Tallahassee.

(4) Finally, and most importantly, much hard work over the past six months has led to the early commissioning of all four Short-Pulse User Cells in the new experimental hall. This doubles the capacity over the old building and provides magnet stations for the many magnet design strategies and

experimental techniques currently under development.

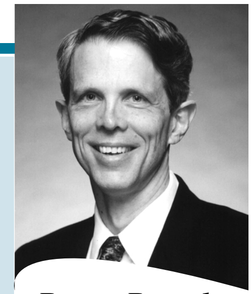
In summary, the NHMFL Pulsed Field Facility has developed plans to recover in roughly two years the unique experimental environment provided by the 60 T Long-Pulse magnet. We have developed plans to dramatically reduce the impact of the 60 T Long-Pulse magnet failure. The future looks bright because of the expanded capacity of our new experimental hall.

Annual Reporting Notice

NHMFL users, scientists, engineers, and affiliated faculty report their research and publication activities to the laboratory each year. Reporting comprises the submission of one-page research reports and evidence of science productivity, such as publications, presentations, software, patents, and various related activities.

The outstanding efforts of our users and faculty are recorded in the NHMFL *Annual Research Review* (*www.magnet.fsu.edu/publications/annualreview/*). This volume has grown significantly—from 131 research reports in 1994 (the year the laboratory was dedicated) to 310 reports in 1999. In an effort to streamline the submissions process and to take advantage of new technologies, all submissions for the *2000 Review* will be made online at http://*reporting.magnet.fsu.edu.* Contributors should check the Web site for complete instructions. The deadline is December 15.

On a related note, the laboratory will be publishing the *2000 Review* principally in CD format.



Bruce Brandt,
Director,
NHMFL DC
Field User
Program

I recently received the following message:

Dear Bruce,

I am writing to let you know that during the week of September 24, 2000, one of the graduate students working with me, Umit Alver, was at the NHMFL taking data on his dissertation project. He had been there for this purpose on two previous weeks this year with me, and we worked together while he learned how to operate the magnets. On this latest trip he went by himself. I was able to monitor his progress during the week from my office in Baton Rouge using the software suggested to me by you, Scott Hannahs, and Donavan Hall —Timbuktu Pro.

It was a great experience in that I could be in my office in Baton Rouge and see on a real-time basis the data Umit was collecting. I was able to communicate with him using the Chat Box feature of this software. Perhaps in the future, if both computers are equipped with microphones, the communication can be by voice. Thus, my input to the experiment was essentially the same as if I were there without the cost of time and money of my actually making the trip. I was able to teach my classes, attend local committee meetings, etc., while the data collection was going on with periodic monitoring by me.

I would like to point out that I did this with a trial version of Timbuktu Pro that I downloaded from the Web. I now have purchased a copy of this software because I plan to use it in the manner I have described many times in the future. This really is a very cost effective way to take data at the NHMFL, enhancing one's ability to do "Science at a Distance" as well as the student learning to become an independent investigator through "Learning at a Distance."

Yours truly,
Roy G. Goodrich
Department of Physics and Astronomy
Louisiana State University

The NHMFL's DC High Field Facility has offered the capability that Professor Goodrich describes for some time. Timbuktu has been used regularly by User Services and Hybrid Operations staff to diagnose problems, assist users, and run systems remotely. We have found it to be easy to use, fast, and robust. We'll be happy to assist other users who want to duplicate Professor Goodrich's experience.

Transient Electron Magnetic Resonance at High Frequencies

H. van Tol, NHMFL, Center for Interdisciplinary Magnetic Resonance
L-C. Brunel, NHMFL, CIMAR, EMR Program Director

Recently, the field of Electron Magnetic Resonance (EMR) has seen a considerable drive to increase the operating frequency of the spectrometers. At the NHMFL we have been on the forefront of the high and very high frequency electron magnetic resonance with frequencies up to 670 GHz, about 70 times higher than the X-band frequencies, which is (still) considered the standard EMR frequency.

There are several principal reasons for increasing the measurement frequency:

- **Resolution of Zeeman splitting.** This is of great importance especially in the study of biological systems with small g-anisotropies.
- **Increased sensitivity.** The sensitivity of an EMR experiment for a standard S=1/2 system is proportional to $\nu^{11/4}$, where ν is the frequency. As the available sample volume decreases with ν^3, the sensitivity enhancement is especially advantageous for samples available in small quantities or as small single crystals.
- **High-spin systems.** Spin systems with S (or J) >1/2 may have a zero-field splitting that is large with respect to the frequency of the spectrometer. An increase in frequency thus extends the range of spin-systems that can be studied by EMR. This is of great importance in the study of the transition ion complexes and rare-earth ions.
- **Faster measurement.** The "characteristic timescale" of the experiment is inversely proportional to the applied frequency.

Here we will focus on the latter point. Even in continuous-wave EMR spectra the timescale will show up in the study of dynamics of spin systems. At higher frequencies, the averaging of anisotropy due to molecular movements will be less, and the resulting spectra will be more anisotropic or more 'rigid.' But more importantly, in the context of time-resolved EMR, this enables the measurement of systems with shorter lifetimes and/or shorter relaxation rates. This would be of great benefit for pulsed EMR at these frequencies, but currently no practical sources and components are available to create very short, high power pulses at frequencies above 200 GHz.

Nonetheless, we can take full advantage of the increased time-resolution in so-called transient EMR. In this technique the measurement of the EMR signal is combined with optical excitation of the sample with a fast laser-pulse. Transient EMR thus extends the scope and applicability of EMR to the study of excited Magnetic states and (reaction) intermediates. With the generous help of an NSF grant, we have built a unique multi-frequency transient EMR spectrometer operating at 120, 240, and 360 GHz that not only increases the g-resolution but also extends the time-resolution to the sub-ns range.

The design of the spectrometer on the one hand is quite traditional in its layout as a CW super-heterodyne spectrometer (see **Figure 1**). On the other hand, it is quite unique in its implementation with multi-frequency, quasi-optical elements, consisting of mirrors and wire grids. This ensures conservation of the polarization and a virtually loss-less free-space propagation of the (sub) millimeter-wave radiation.

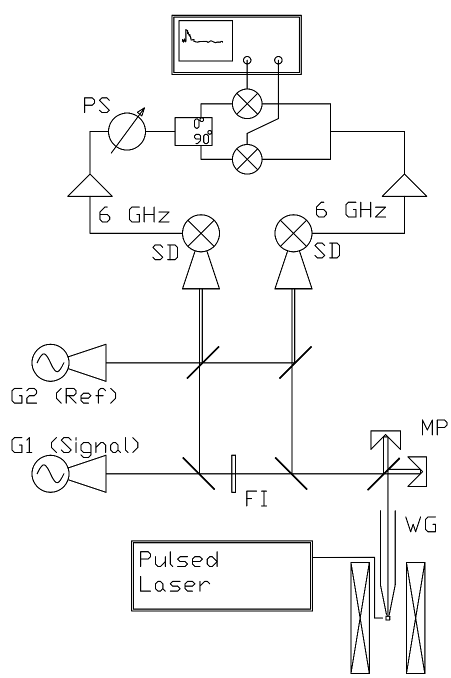


Figure 1. Schematic layout of the transient superheterodyne EMR spectrometer. G1 is the signal Gunn diode phase-locked source operating at 120, 240, or 360 GHz. The reference oscillator G2 is tuned to 6 GHz below that. FI: Ferrite Isolator. MP: Martin-Pupplet serving as polarization converter. WG: Corrugated oversized waveguide. SD: Schottky diode mixer. The 6 GHz IF signals are amplified and mixed down to 0-2GHz, and recorded with a 1.5 GHz digital oscilloscope.

As opposed to the CW system with a homodyne hot-electron bolometric detection with a bandwidth around 1 MHz, here the detection is based on Schottky diodes and has a 1 GHz bandwidth. The CW-sensitivity we obtained is of the order of 10^{11} spins/gauss at room temperature without a cavity (1 Hz bandwidth). With the 50 µl sample volume this corresponds to a concentration sensitivity of 3 nmol/(l*gauss). With a Fabry-Perot type cavity, the room temperature sensitivity is 10^{9} spins/gauss.

The optical excitation of the short-lived Magnetic systems is achieved with laser-pulses from either a 5ns Q-switched Nd:YAG laser (1064, 532, 355, and 266 nm) or a 120 ps mode-locked Nd-YAG with an Optical Parametric Generator (460-670 and 750-2000 nm). The time-resolution of the system was measured by looking at the transmission of a Si-wafer in response to a 120 ps lightpulse, and was found to be 600 ps (see **Figure 2**).

The instrument enables the study of short-lived Magnetic species, or fast changes in stable Magnetic species, at relatively high magnetic fields and is intended to be a research tool for different disciplines like solid-state physics, chemistry, and biophysics. Projects being envisioned include studies of photosynthesis of green plants and bacteria; intermediates in charge-transfer reactions; short-lived excited triplet states; photo-induced orientation changes of spin-probes on protein molecules; paint degradation by UV light; and light-induced changes of cyclotron resonance with sub-nanosecond resolution.

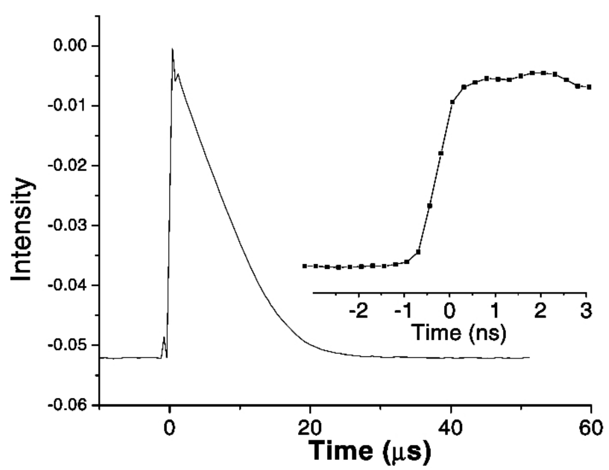


Figure 2. Measured response of Si-wafer transmission at 240 GHz to a 120 ps laser pulse (532 nm) at room temperature. The fast decrease of transmission (95%-5%) was measured to be 600 ps. The decay of the conduction-electrons is in the ms timescale.

As an example of a typical result that can be obtained, **Figure 3** shows the spectrum of the lowest excited spin-triplet state of a tetra-phenyl porphyrin molecule dissolved in a polymer. This porphyrin molecule is a basic unit of many biologically important systems, like hemoglobin, chlorophyll, and other cofactors that play a role in photosynthesis. The high-frequency delivers information about the Zeeman splitting in the lowest excited triplet state, which cannot be resolved at lower frequencies, as is shown in **Figure 3**. The spectrum was measured 1 µs after laser excitation at 532 nm. The population of the triplet sublevels is governed by the singlet-triplet intersystem crossing and results in both emission and absorption in the spectra. A fit of these spectra gives the zero-field splitting, g tensor, and relative population rates. By studying and comparing similar biological systems in cooperation with several external researchers, we hope to supply a meaningful contribution to the understanding of photosynthesis and other electron transfer processes in proteins.

In the near future, we intend to extend the possibilities of this spectrometer to pulsed EMR and pulsed ENDOR (Electron-Nuclear Double Resonance). The fast detection of the spectrometer makes it very suited for this purpose. The optical access will also enable us to use it for high-field, optically detected magnetic resonance (ODMR).

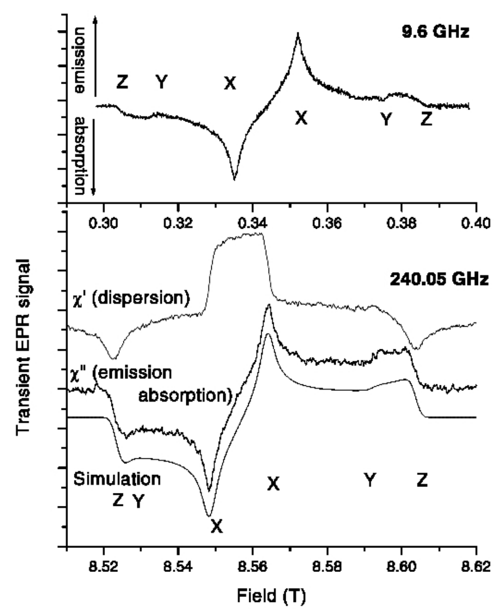


Figure 3. Transient EMR spectra of TPP in polystyrene at X-band (top), and at 240 GHz (bottom), taken at 290 and 170 K respectively. The X, Y, and Z labels indicate the spectral positions corresponding to the magnetic field oriented along the zero-field splitting axes. The asymmetry of the 240 GHz spectra is due to g-anisotropy.

People in the News

Heidi S. Bond, an NHMFL 1998 summer intern and FSU graduate, has received an NSF Fellowship to study Theoretical Chemistry at the University of California at Berkeley. Heidi is the third child in her immediate family to receive an NSF Fellowship, and she attributes her work at the laboratory with Professors Jack Quine and Tim Cross as her first exposure to work in theoretical chemistry, general chemistry, and models of complicated chemical systems. Heidi says, "I can't even begin to estimate the value of the conversations and support that I got from the people who I worked with on a regular basis. The advice and information from professors, the graduate students, and the postdocs in the Cross/Quine group have been invaluable."

Michelle V. Buchanan, founding member of the ICR Facility Advisory Panel (1994 to 2000) and member of the NHMFL Users' Committee (1999 to 2001), has been appointed Director of the Chemical and Analytical Sciences Division (CASD) at Oak Ridge National Laboratory. She has provided valuable advice and assistance in setting priorities for new ICR techniques and experiments at NHMFL, and in the initiation and staging of the first two North American FT-ICR Mass Spectrometry Conferences. Dr. Buchanan's research interests include development of gas phase processes for elucidation of molecular structure with particular emphasis on mass spectrometry. She has published more than 150 scientific papers and reports and received an R&D 100 Award in 1986 for development of ionization detectors.

Helen Cooper, formerly of the Institute of Mass Spectrometry, University of Warwick, where she managed the National FT-ICR service, has joined the ICR Group. As the primary contact for external users of the ICR Facility, Dr. Cooper logs and coordinates both fee-for-service and research collaborations. She operates the facility's FT-ICR mass spectrometers, conducts independent research, collaborates with internal ICR users, and assists with grant proposals. Her research interests have been in the field of gas-phase ion chemistry of fullerenes and mass spectrometry of calcium-binding proteins.

Jan Jaroszynski has been visiting the NHMFL from the Instituite of Physics of the Polish Academy of Sciences. He has been here scince last October studying noise in silicon field effect transistors in collaboration with Dragana Popovic of the CM/T Group

Rajiv Singh, professor of materials science and engineering at UF College of Engineering, has made pioneering contributions in the fundamentals and technical applications of laser-solid interactions in materials ranging from microelectronics to pharmaceutics.

John Singleton, a Reader in Physics at the University of Oxford and member of the Correlated Electron Systems Research Group, is visiting NHMFL-LANL on a year-long sabbatical. His research interests include crystalline organic molecular metals and magnets, magnetic oxides, oxide superconductors, superluminal light sources, semiconductors, and biophysics. He has written over 260 publications, including a recent review article on organic metals. His undergraduate textbook, *Band Theory and Electronic Properties of Solids* is due for publication in December. While at LANL, Singleton is developing techniques for high-frequency measurements of metals in pulsed magnetic fields.

FSU Faculty Promotions

Four NHMFL colleagues were recently recommended for promotion:

Nicholas E. Bonesteel, to Associate Professor and for tenure
Timothy M. Logan, to Associate Professor and for tenure
Piotr G. Fajer, to Professor
Hamid Garmestani, to Professor

Development of High Field High Resolution Solid State NMR Spectroscopy of Quadrupolar Nuclei

Zhehong Gan, NHMFL, Center for Interdisciplinary Magnetic Resonance

About two thirds of all magnetically active nuclei in the periodic table possess half-integer spins S>1/2 with nuclei like ^{11}B, ^{17}O, ^{23}Na, ^{27}Al, ^{71}Ga and ^{87}Rb that are commonly found in solid materials such as glasses, minerals, catalysts, ceramics and semiconductors. Solid state NMR spectroscopy, with its capabilities of resolving individual chemical sites separated by a few ppm in chemical shift, has become a powerful tool to probe structure at the atomic levels of these solid materials. High magnetic fields and NMR technique development play an important role in improving spectral resolution, especially for half-integer quadrupolar nuclei. Reported here are some activities of high field NMR and recent development of NMR methodology at the NHMFL in solid state NMR of quadrupolar nuclei.

NMR spectroscopy of quadrupolar nuclei is dominated by quadrupolar couplings typically in the orders of several or even tens MHz. High resolution solid state NMR becomes possible for half-integer quadrupolar spins because the central m_z=1/2↔-1/2 NMR transitions are not affected by the first-order quadrupolar interactions. The second-order quadrupolar effects, however, can still widen resonance lines to several kHz and prevent the resolution of chemically inequivalent sites. High magnetic fields reduce the second-order quadrupolar effects while increasing spectral dispersion through the field-dependent chemical shift. The combined effects result in a quadratic gain in resolution in solid state NMR spectra of half-integer quadrupolar nuclei. The advantages of high magnetic fields are demonstrated clearly by spectra in **Figure 1** obtained at the 14 T, 19.6 T superconducting magnets and the 25 T Keck resistive magnet at the NHMFL (courtesy of Dominique Massiot, CNRS of France in Orleans for the $9Al_2O_3$+$2B_2O_3$ sample). The combination of high fields and high speed magic-angle sample spinning narrows resonance lines that become resolved at 25 T among the 4, 5, and 6-coordinated aluminum sites with quadrupolar coupling constants ranging from 6 to 9 MHz.

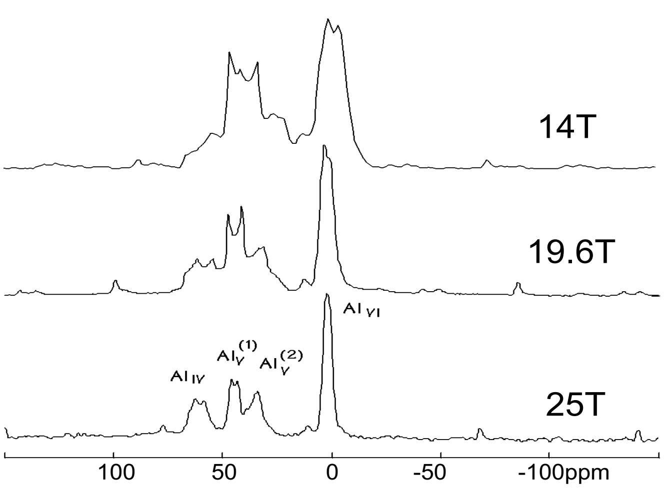


Figure 1. ^{27}Al magic-angle spinning solid state NMR spectra of $9Al_2O_3$+$2B_2O_3$.

In parallel with the increasing magnetic fields, NMR techniques continue to be developed to enhance spectral resolution of half-integer quadrupolar nuclei. First, magic-angle sample spinning was applied to average out dipolar coupling and chemical shift anisotropy interactions. Magic-angle spinning also reduces the second-order quadrupolar effects and narrows resonance lines.[1] The long-time goal of isotropic NMR spectra with all anisotropic terms in the second-order quadrupolar effect averaged was achieved more than ten years ago with the invention of double rotation[2] and dynamic angle spinning.[3] Several years later, the multiple-quantum magic-angle spinning (MQMAS)[4] method was introduced that achieves isotropic NMR spectra with single axial sample spinning in the form of two-dimensional NMR spectra. Very recently, a new method that uses satellite transitions and magic angle spinning (STMAS) has been developed at the NHMFL to generate isotropic NMR spectra with high efficiencies.[5] The STMAS method enhances spectral sensitivity by an order of magnitude over the MQMAS experiment.

The STMAS experiment correlates satellite transitions with the commonly observed central transitions of quadrupolar nuclei. The first-order effects to satellite transitions are averaged out by magic-angle spinning with carefully calibrated magic-angle and pulse sequence. Correlation of satellite and central transitions generates coherence transfer echoes that refocus signal decay by the second-order quadrupolar effects. The creation of coherence transfer echoes achieves the goal of isotropic NMR spectra. The STMAS spectrum of the $^9Al_2O_3$+$^2B_2O_3$ sample is shown in **Figure 2** as an example.

QUADRUPOLAR NUCLEI continued on page 16

QUADRUPOLAR NUCLEI continued from page 15

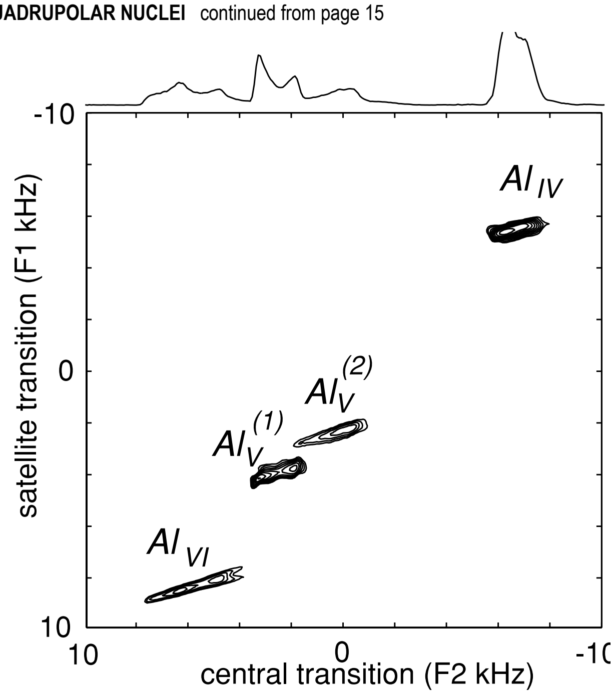


Figure 2. 2D STMAS spectrum of $9Al_2O_3+2B_2O_3$ acquired at 19.6 T and with 20 kHz magic-angle sample spinning.

Both satellite and central transitions are single quantum transitions that can be directly excited and detected. High efficiencies in excitation and conversion of satellite transitions improve spectral sensitivity of the STMAS experiment by an order of magnitude over the MQMAS experiment. The gain in sensitivity makes rapid acquisition of isotropic NMR spectra possible for half-integer quadrupolar nuclei. To average out the first-order quadrupolar interactions typically in the order of several MHz, the STMAS experiment requires sample spinning axis at the magic-angle within 0.002 degree! Probe engineers at Bruker are improving their probe design to meet this requirement to facilitate applications of the STMAS experiment.

Taking advantage of high magnetic fields, NHMFL has been enhancing hardware capabilities for solid state NMR spectroscopy of quadrupolar nuclei. In collaboration with Dr. Ago Samoson of the National Institute of Chemical and Biophysics of Estonian, inventor of double rotation technology,[2] the NHMFL will soon become one of the few places in the world with DOR capability. A MAS probe designed for low-gamma nuclei has been built and an ultra fast (40 kHz) MAS probe is expected at the end of the year, both by Peter Gor'kov. The fast MAS probe is designed to be compatible with all high field magnets: the 833 MHz, the 25 T Keck, and the 45 T hybrid magnet at NHMFL. High magnetic fields, hardware, and methodology developments will continue to attract users around the world to the NHMFL for solid state NMR spectroscopy of quadrupolar nuclei.

1. E. Kundla, A. Samoson, and E. Lippmaa, *Chem. Phys. Lett.* **83**, 229 (1981).
2. A. Samoson, E. Lippmaa, and A. Pines, *Mol. Phys.* **65**, 1013 (1988).
3. A. Llor and J. Virlet, *Chem. Phys Lett.* **152**, 248 (1988).
4. L. Frydman and J. S. Harwood, *J. Am. Chem. Soc.* **117**, 5367 (1995).
5. Z. Gan, *J. Am. Chem. Soc*. **122**, 3242 (2000).

Interested readers and prospective users may contact Dr. Zhehong Gan at 850-644-4662, gan@magnet.fsu.edu.

Universities of Florida, Chicago to Lead Way for Ultra-Powerful Computer Data Grid

Reprinted with permission from UF News, Aaron Hoover and Steve Koppes, September 13, 2000.

The Universities of Florida and Chicago will lead an $11.9 million initiative that will lay the groundwork for a computer data grid of unprecedented speed and power. The initiative, called the Grid Physics Network, or GriPhyN, is funded by the largest grant in the National Science Foundation's new Information Technology Research program, which supports long-term basic research on networking and information technology.

"GriPhyN initially aims to give scientists a tool to interpret the vast amounts of data expected to flow from the world's most ambitious physics and astronomy experiments, but it also could have applications in the business world and elsewhere," said Paul Avery, lead scientist and UF professor of physics.

"We need to plan for these experiments now, because we can't wait till they start," Avery said. "A personal computer today can do about a billion operations per second. The overall computing power we need is about 1 million times more than that."

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GriPhyN involves more than a dozen institutions nationally and will pioneer a new concept called virtual data, in which the entire resources of a scientific collaboration become a single vast computing and storage system. "GriPhyN could be thought of as a Napster for scientists, where the tunes being downloaded are not purloined hits but crucial insights into the nature of the universe," said project co-leader Ian Foster, professor in computer science at the University of Chicago and associate director of the Mathematics and Computer Science Division of Argonne National Laboratory.

"Results will be computed only if and when needed," Foster said. "Much of the time, the result you need will already have been computed by one of your colleagues, and the system will know where to find it."

The initiative initially will benefit four physics experiments that will explore the fundamental forces of nature and the structure of the universe. Two experiments at the European Laboratory for Particle Physics near Geneva will search for the origins of mass using the Large Hadron Collider, which will become the world's highest-energy particle collider when it begins operation in 2005. The Laser Interferometer Gravitational-wave Observatory, based in Louisiana and Washington, will probe the gravitational waves of pulsars, supernovae and other phenomena. The Sloan Digital Sky Survey, conducted from Apache Point Observatory in New Mexico, is carrying out a massive automated survey of the stars.

Each of these experiments will produce huge amounts of data that scientists at different institutions around the world will want to search and manipulate. "Genomics is another major area of science where data volumes are increasing much faster than analysis capabilities," Foster said. So large are the data collections that scientists anticipate they will be measured in petabytes, where one petabyte is roughly the amount of data that can be contained on 1 million personal computer hard drives. A personal computer hard drive contains approximately 1 gigabyte, which equals 1 billion bytes.

The world's most powerful supercomputers today can store and process data measured in terabytes, each of which equals 1,000 gigabytes. By tapping into the computer power of multiple institutions around the world, a computational data grid could significantly boost both storage and calculating capacity. The result will not reside at one location or one supercomputer but rather will be spread throughout the institutions, much like power plants connected to an electrical grid.

"The electrical grid is a useful analogy, because users ranging from individuals to large organizations will consume computing and data resources in greatly differing amounts, and they will not care where those resources are located," Avery said.

Scientists will need to have access to the data, but also the ability to carve out chunks of it and manipulate the chunks to produce results. Because of their size or the available computing power, the movement of these data chunks around the network will have to be scheduled at different times, a task that will require a kind of "intelligent" network.

"A worldwide community of perhaps thousands of physicists want to be able to have their combined computer, storage and network resources used as a single computing engine to solve their problems," Foster said. "This requires new technology that can coordinate potentially thousands of processors, petabytes of storage and a variety of high-speed and low-speed networks and cause them to operate in some sense as a single analysis engine."

GriPhyN will build on a base of proven grid technologies, in particular the Globus toolkit, to provide the basic services and capabilities of a computational grid.

"Although intended initially for science, GriPhyN could also prove useful for large business applications," Avery said. For example, companies with multiple sales outlets don't always store sales data in one central location. But marketers hoping to identify consumer buying habits may wish to comb through all the company's sales data to ferret out buying habits. "There's a huge amount of interest in the technology that would allow companies to actually study these large archives of commerce data," Avery said.

The $11.9 million NSF grant is for research and development only, with no money for hardware. Researchers seek a total of $70 million in NSF grants for further research and equipment to build the system. Research and construction should take place simultaneously, with a target completion data of 2005.

The institutions participating GriPhyN are the University of Florida; University of Chicago; Stanford University; University of Southern California; California Institute of Technology; Harvard University; Indiana University; Johns Hopkins University; Northwestern University; University of California, Berkeley; University of California, San Diego; University of Illinois, Chicago; University of Pennsylvania; University of Wisconsin, Madison; University of Wisconsin, Milwaukee; and the University of Texas, Brownsville.

Professor Paul Avery is a member of the NHMFL extended family at UF. Many other NHMFL-affiliated faculty, representing Physics, the McKnight Brain Institute, Astronomy, Fine Arts, Computer Sciences and Engineering, and Humanities at UF, will also be participating in GriPhyN.

Neil Sullivan, NHMFL co-principal investigator at UF notes, "this effort is very important to the future of NHMFL because it will create a national network by which researchers across the U.S. can share large amounts of data at high speed. This ability is critical to some NHMFL research areas, notably in NMR and MRI where large volumes of data are associated with images and spectra that are central to the research activities. Active participation, in real-time, on projects associated with time-limited operations such as experiments in the Hybrid magnet and high field pulsed magnets can also benefit considerably."

R E P O R T S *The National High Magnetic Field Laboratory*

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FALL 2000 Volume 7 • No. 4

Published by :

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