# **Francis Bitter Magnet Laboratory**

The Francis Bitter Magnet Laboratory (FBML) has continued to make notable advances in several areas of science and engineering involving high magnetic fields. The Laboratory's research program in magnetic resonance, which includes nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR), and magnetic resonance imaging (MRI), has continued to grow and remains the largest effort at the FBML. The program is funded primarily by the National Institutes of Health (NIH) and the Department of Energy (DOE), and presently involves approximately 30 NMR and EPR magnets and spectrometers.

## **Highlights for the Year**

Professor David G. Cory of the Department of Nuclear Science and Engineering (NSE) and his colleagues continue to make advances in the theory, practice, and implementation of quantum information processing (QIP). They have nearly completed the construction of a simple quantum information processor based on NMR and will start exploring this approach experimentally this fall. In collaboration with the National Institute of Standards and Technology (NIST), Professor Cory and his colleagues have implemented a reciprocal space approach to coherent imaging via a three-blade neutron interferometer, which promises improved contrast and resolution.

Professor Robert G. Griffin of the Department of Chemistry and Professor Gerhard Wagner of Harvard University continue to operate the MIT/Harvard Center for Magnetic Resonance (CMR), a collaborative research effort between MIT and Harvard Medical School. CMR is supported by an NIH Research Resource grant and has been funded continuously since 1976. In September 2005 FBML took delivery of a 900 MHz spectrometer for experiments in liquids and solids that is one of about a dozen such instruments in North America. Professor Wagner is using this instrument in his research program devoted to structural biology and signaling, and Professor Griffin is employing it to develop new methods for solid-state structural investigations, which he is applying to structural studies of membrane and amyloid proteins.

Under the leadership of Dr. Yukikazu Iwasa, the FBML Magnet Technology Division (MTD) is currently involved in four NIH-funded programs on NMR and MRI magnets and two Air Force Office of Scientific Research (AFOSR)-funded projects on stability and protection issues for yttrium barium copper oxide (YBCO)-coated conductors. These projects are briefly summarized below.

Professor Alan Jasanoff of NSE and the Department of Brain and Cognitive Sciences (BCS) and his colleagues are pursuing functional imaging methods aimed at studies of systems-level neural plasticity involved in low-level learning and perceptual behavior. Their experiments are being performed in small animals using prototype imaging agents for "molecular functional MRI."

Senior Staff Scientist Dr. Jagadeesh Moodera continued research efforts in nanoscience condensed matter physics through collaboration with various universities and industries and funding from the Office of Naval Research, the National Science Foundation (NSF),

and the Korean Government (via the Korea Institute of Science and Technology [KIST]). In addition, he has continued his mentoring of graduate students, undergraduates, and high school students by providing research opportunities within his lab. His latest graduating student, Tiffany Santos, won the best PhD thesis award from the Department of Materials Science and Engineering in 2007. Dr. Moodera has also successfully carried out a long-term collaborative project on nanospintronics, called the KIST-MIT Research Laboratory and funded by the Korean Government, which has a provision for the exchange of students and scientists. His group's recent breakthrough published work has attracted extensive media attention in publications such as MIT's *Tech Talk*, *Technology Review*, *Electronic Design*, *IEEE Spectrum*, *Hindustan Times*, and *The Times of India*.

Dr. Moodera was nominated for the International Magnetism Award (given triennially by the International Union of Pure and Applied Physics) for outstanding research breakthroughs. He is currently being nominated to the Oliver E. Buckley Prize of the American Physical Society for outstanding research in condensed matter physics.

Dr. Richard Temkin of Physics and the Plasma Science and Fusion Center and his colleagues are completing the construction of a 460 GHz gyrotron, and they have initiated the development of a 140 GHz gyroamplifier. Another project involves the design and construction of a 330 GHz tunable gyrotron oscillator for use in dynamic nuclear polarization (DNP)/NMR experiments. We anticipate that these developments will ultimately produce a gyroamplifier operating at approximately 600 GHz for use with 900 MHz NMR magnets.

#### **Research Activities**

#### **Professor David G. Cory**

## **Quantum Information Processing**

Professor Cory and his students continue to explore magnetic resonance approaches to QIP through collaborations with Dr. Chandrasekhar Ramanathan (NSE), Dr. Sergio Valenzuela (NSE), Professor Seth Lloyd (Mechanical Engineering), Dr. Raymond Laflamme (University of Waterloo), and Dr. Joseph Emerson (University of Waterloo).

Over the past year they have experimentally demonstrated what were considered two "grand challenges" in quantum information processing: they demonstrated an error correction code that led to an experimentally realizable increase in the process fidelity, and they demonstrated efficient error detection for a physical system. These findings move the theory and practice of fault-tolerant QIP closer together. They continue to use their NMR-based test bed for QIP to develop methods of coherent control and they presently have a system that can robustly operate over a 6-spin Hilbert space. In addition, they have preliminary results from a new setup that will expand the computational space to 15 spins.

They have completed the first series of experiments on coherent spintronics where the electron spin plays an essential role in control of the nuclear spin-based qubits. In particular they have demonstrated that control of the electron spin is sufficient to have universal control over the nuclear spins where the hyperfine interaction is anisotropic. They have also found a logical encoding to protect the nuclear spin's coherence from the finite electron-spin lifetime.

They have installed new electron spin resonance spectrometers to enable further studies of spintronics and are rebuilding the pulses X-band ESR to permit He-4 temperature experiments on systems involving many nuclear spins.

Dr. Ramanathan has led a series of experiments to explore and find applications for multispin dynamics in solid-state systems. This includes the investigation of the transition from classical to quantum dynamics in 1-D spin chains. Applications include using spin chains as channels for quantum information and creating highly polarized spin systems as potential transducers. For example, we report spin pumping by DNP in Si where polarizations as high as five percent are achieved for the first time.

Dr. Valenzuela has carried out a series of experiments aimed at demonstrating spin transport in device structures. In particular, he is interested in showing spin injection in semiconductors.

Professor Cory's group is starting a new program combining spin physics and persistent-current flux qubits (PCFQ). The project is in collaboration with Electrical Engineering and Computer Science (EECS) professor Terry Orlando and Dr. Will Oliver (Lincoln Laboratory). To enable these measurements we are installing a set of refrigerators for low-temperature physics in the lab (two dilution refrigerators and one He-3 system). The aims of the new program are to develop new methods of coherent control for PCFQ and to employ high Q, non-linear resonators as local detectors of magnetization.

### **Coherent Imaging via Neutron Interferometry**

In collaboration with Dr. D. Pushin (NSE) and Dr. M. Arif (NIST), we have demonstrated new models of measurements via a three-blade neutron interferometer. The new approaches enable us to reduce the sensitivity of interferometry to vibrations and to design new scattering experiments that extend the measurement range to lower Q values. We are collaborating with NIST to build a new beam line at their facility and to outfit it with a next-generation neutron interferometry.

#### Robert G. Griffin

### **Structural Studies of Amyloid Peptides and Proteins**

Amyloidosis is a group of disorders created by peptide or protein misfolding and characterized by the accumulation of insoluble fibrillar protein material in extracellular spaces. Twenty different proteins are known to form amyloid-like aggregates involved in several diseases—for example  $\beta$ -amyloid ( $A\beta$ ) in Alzheimer's disease; the prion protein PrPc, which converts to PrPsc, leading to the transmissible spongiform encephalopathy; and the synuclein protein, which is responsible for Parkinson's disease.

During the last few years, Professor Griffin and his group have developed methods to prepare large amounts of fibrillar peptide and to maintain this material in a state suitable for magic angle spinning (MAS) NMR experiments. Most recently, they have

used these techniques in a collaborative study of the structure of 11 residue fibrillar peptides of the L111M mutant derived from transthyretin. Using these peptides they have determined the structure with solid-state NMR distance and torsion angle measurements. Their success with the target tracking system has encouraged them to initiate experiments with other systems such as the GNNQQNY peptide from the Sup35 protein. During the past year they have developed methods to determine the interstrand and intersheet alignment of the peptides and have found them to be parallel and antiparallel respectively. They anticipate that they will complete these structures and the structure of a fibril itself during the coming year. Finally, during the past year they have made significant progress toward assigning the spectrum of the SH-3 domain of the protein phophatidylinostol-3-kinase (PI3-SH3) and have initiated experiments on  $\beta$ -2-microglobulin, the protein associated with dialysis-related amyloidosis

### **Dynamic Nuclear Polarization**

The 140 and 250 GHz DNP spectrometers continue to operate reliably and routinely, allowing the group to pursue new methods and applications of DNP. Significant advances have been made in combining MAS with DNP and in the development of new polarizing agents. Specifically, they have improved many aspects of the 250 GHz system so that it is now capable of recording spectra at low temperatures for extended periods (approximately three weeks). The results of these efforts are just being prepared for publication. Specifically, they have obtained excellent spectra of the membrane protein bacteriorhodopsin (bR) and its photo-intermediates that are produced via in situ laser irradiation. The increased signal to noise ratio (S/N) available from DNP is essential for the experiments. In addition they have developed a laser melting experiment, called temperature jump DNP (TJDNP), that yields approximately 150-400 percent increased sensitivity for solution NMR experiments and has recorded the initial 2D 13C-<sup>13</sup>C spectrum with an enhancement of approximately 150. We also have a collaborative program with Professor Tim Swager of the Department of Chemistry to develop new biradical polarizing agents—two TEMPO molecules tethered by a three carbon chain, or BDPA and TEMPO tethered together.

#### **Dipolar Recoupling**

Since Professor Griffin's group initiated <sup>13</sup>C-<sup>13</sup>C dipolar recoupling experiments in the late 1980s, the field has grown enormously and there have been many advances in techniques from multiple laboratories. Over the last decade the Griffin group has been heavily involved in these developments, particularly with regard to techniques for measuring distances and torsion angles in solids. Their goal is to be able to determine the structure of membrane proteins, amyloid fibrils, etc. with solid-state NMR. During the past year they have concentrated on approaches that are applicable to experiments performed at high spinning frequency and at high magnetic fields. In particular, they have developed:

- Methods that permit dipolar <sup>13</sup>C-<sup>13</sup>C recoupling at high MAS frequencies and magnetic fields without application of proton decoupling
- Methods for simultaneously measuring multiple <sup>13</sup>C-<sup>13</sup>C distances in uniformly labeled peptides and proteins, and

• An improved method for cross polarization that was necessitated by experiments at high spinning frequencies and fields.

They anticipate that with increased sensitivity available from DNP experiments, these methods will be applicable to a large number of systems not accessible to solution NMR and X-ray crystallographic investigations. It is also possible that they will be able to measure distances and torsion angles with higher accuracy and precision than is possible with diffraction experiments.

### High Frequency Electron Paramagnetic Resonance

Using the 140 GHz spectrometer and 9 GHz spectra, Professor Griffin's group is studying the inhibition mechanism of ribonucleotide reductase. For the latest version of these experiments they have constructed a rapid freeze-quench apparatus that will trap intermediates on a microsecond to millisecond timescale. They are also performing extensive EPR studies of biradicals that will serve as polarizing agents for DNP experiments. We have also used the 140 GHz spectrometer in experiments to determine the structure of biradicals.

### **Center for Magnetic Resonance**

The Center for Magnetic Resonance has completed its 32nd year of operation as a facility providing scientists with access to high-field NMR equipment. In September 2005, CMR took delivery of a 900 MHz spectrometer for performing experiments on liquids and solids. The system became fully operational in August of 2006 with the delivery of the cryoprobe. The 900 operates as part of CMR and will be available to investigators at MIT, Harvard, and other universities and companies. In addition, CMR anticipates purchasing an 800 MHz widebore NMR system in the next year or two and developing a 600 MHz system for TJDNP experiments on liquids and a high-frequency pulsed EPR based on a gyroamplifier.

#### Dr. Yukikazu Iwasa

Under the direction of Dr. Yukikazu Isawa, the MTD is involved in the following NIH-supported programs.

#### High-Temperature Superconducting Insert Coil for 1 GHz NMR Magnet

In Phase 2 of this project, MTD's goal was to complete a 700 MHz NMR magnet comprised of a 600 MHz all low-temperature superconducting (LTS) NMR magnet and a 100 MHz high-temperature superconducting (HTS) insert coil. They achieved a field of 700 MHz in the spring of 2006, but there still remains an important task of shimming the field to improve the field homogeneity. This shimming is continuing at the moment.

## Digital Flux Injector (Flux Pump) for NMR Superconducting Magnets

The ultimate goal of this five-year continuation program on the development of the digital flux injector (DFI) is completion of a DFI to be coupled to the HTS insert of our 1 GHz LTS/HTS NMR magnet. It has been demonstrated that a DFI coupled to a persistent-mode LTS NMR magnet can also be used to shift the frequency of an NMR magnet by pumping in or pumping out a quantified amount of flux from the magnet.

### Development of Low-Cost MgB2/Solid N2 MRI Magnets

The specific aim of this program is to demonstrate the feasibility and practicality of a low-cost, commercially viable superconducting MRI magnet incorporating an MgB2 composite conductor and an innovative cryogenic design/operation concept specifically targeted for use in small hospitals, rural communities, and underdeveloped nations. MTD is achieving this specific aim by building and operating a 0.5 T/80 cm bore demonstration magnet that, except for its lack of an MRI-grade spatial homogeneity, satisfies key operational requirements of 0.5 T/80 cm MRI magnet systems. This prototype system introduces two important firsts to MRI-superconducting magnet technology, both benefiting operation of our type of MRI systems— a trend-setting MgB2 magnet for the next generation of MRI magnets, and an entirely new design/ operation concept for the system cryogenics. The presence of solid nitrogen in the housing that enhances the magnet's heat capacity enormously enables the magnet to maintain its operating field over a limited time period even with its cryocooler shut off, as it would be in the case of a power outage, an event not rare in rural communities and underdeveloped nations. Only during this shutoff period, the magnet will warm up from a nominal operating temperature of 10 K to a design limit of 15 K over a period of 29 hours. The project is moving forward.

## A Cryocooler/Solid Ne-Cooled 500 MHz/20 cm MRI Magnet

The specific aims of this project are to apply a new design/operation concept for MRI superconducting magnets that enable these magnets to achieve operational features that in some respect resemble those of low-field permanent-magnet based counterparts, and to demonstrate the applicability of this concept to high-field MRI (500 MHz and above) magnets by completing a 500 MHz/20 cm superconducting MRI magnet. The completed system will be installed in the FBML for a group of MRI and brain science researchers. FBML strongly believes that the commercial magnet manufacturers for the next-generation MRI magnets will in time adopt this new design/operational concept. These features include a liquid-free system; a quiet, noise/vibration-free system operation over a specific time period (12 hours in this system), if required by the user; and the ability to maintain a constant operating field over this time period, even in the event of a power outage or while the cryocooler is under scheduled maintenance. The proposed MRI magnet will be almost as easy to operate as a low-field permanent-magnet-based system. The program is moving forward.

#### **AFOSR-Supported Programs**

In collaboration with Hyper Tech Research, Troy, OH, and American Superconductor Corporation, Westborough, MA, Dr. Iwasa's group has two air force-sponsored programs to develop reliable protection techniques for high-energy density YBCO-wound superconducting magnet devices.

#### **Professor Alan Jasanoff**

Professor Alan Jasanoff has been a faculty member at FBML since the fall of 2004. Last year, he accepted a joint appointment in the Department of Biological Engineering along with his previous appointments in NSE and BCS. Professor Jasanoff's work and recent

publications continue to focus on the development of MRI contrast agents for next-generation functional brain imaging.

His lab made significant progress on its core focus of developing molecular probes for next-generation functional imaging in animals. They introduced a new family of calcium sensors for MRI, and are in the process of applying them in single cells and intact organisms. They collaborated with chemistry professor Stephen Lippard's group to develop porphyrin-based cell-permeable contrast agents that address the key problem of in vivo delivery and could be important for future neuroimaging work. Newer projects focused on several types of genetically-controlled contrast agents; most advanced is work on a protein dopamine sensor they plan to use for mapping reward-related signaling in rodents. They recently completed a project to study development of neural connectivity and hemodynamic responses in juvenile rats, in collaboration with BCS professor Martha Constantine-Paton's lab. They found that systematic changes in blood oxygen level-dependent time courses take place from P13-adulthood, and may be related to changes in carbonic anhydrase expression occuring at this age; changes also coincided with gross repatterning of neural activity in response to somatosensory stimuli in these animals.

Professor Jasanoff has received the McKnight Foundation Technological Innovations in Neuroscience Award and the Dana Foundation Brain and Immuno-Imaging Grant, and holds the N. C. Rasmussen Career Development chair in NSE.

## Dr. Jagadeesh S. Moodera

In nanoscience condensed matter physics, in particular in magnetism and superconductivity, the Moodera group's research continues to make significant contributions to both fundamental science and industrial applications.

Their basic investigation emphasizes spin transport in thin film nanostructures (spintronics), specifically in semiconductors including organic semiconductors. Using their molecular beam epitaxy system, their research seeks to contribute to the understanding of the spin properties of conventional materials and to unravel the spin properties of certain novel magnetic compounds that have a high potential for technological application. Their research into the structure of these materials is being further developed by various companies such as IBM, Motorola, Seagate, TDK, and Fujitsu for application in digital storage. In fact, these companies have introduced into the market mini- and microdisc drives with unprecedented capacity that have read head sensors based on magnetic tunnel junctions. Another important area of application includes nonvolatile magnetic random access memory (MRAM) elements as well as reprogrammable logic circuits that will potentially have a significant and highly profitable impact on memory technology. Freescale (an offshoot of Motorola) has introduced the MRAM chips into the market. In this context, we are continuing national and international collaborative research efforts with scientists and faculty from industry and from national laboratories and universities, including the Eindhoven University of Technology, the University of Twente, the University of Gottingen, Ewha Women's University, Tohoku University, the KIST, Boise State University, UCLA, and the Institute of Physics (Bhubaneswar, India). Exchange of scientists and graduate students is a part of this program.

Dr. Moodera is technical advisor to a company that is developing MRAM chips and is collaborating on research with another to develop THz radiation sources and detectors.

The Moodera group has successfully developed a research program in the new superconductor (MgB2) science and technology for Josephson junctions that have potential for hybrid superconducting electronics in areas such as computers, logic elements, mixers switches, and sensors. They intend to start a new collaboration with EECS to develop Josephson junction-based ultra-fast circuitry that is useful for the navy. There is an ongoing collaboration with scientists from Lincoln Laboratory as well.

They also have research programs in the fields of nanoscience for single-spin transistors as well as in the materials aspect for quantum computing. In a parallel approach, they are also investigating injecting spins into two-dimensional electron gas semiconductors to create spin-field effect transistors. Another program they have just embarked on is a new approach to reading the qubit information using quantum dot structure and the spin filter method.

Another recent research area the group is leading is in spin transport studies in organic semiconductors with the goal of creating mechanically flexible, cheap, and highly efficient spin-based multifunctional devices for bottom-up electronics. They began a new collaboration with another group in EECS as a result of our initial success in this area.

Seven postdoctoral scholars, three visiting scientists, three graduate students, three undergraduates, and several high school students have taken part in Dr. Moodera's research. The high school students have won several science competitions, and some of these students have been admitted to MIT as undergraduates. The group's research has resulted in several publications (including four in *Physical Review Letters* this year), reviews, book chapters, and invited talks at various national and international conferences and universities. During this year two of Dr. Moodera's patents have been licensed to a company that is developing MRAM.

Dr. Moodera continues his collaboration with Eindhoven University of Technology as a visiting professor. He is the expert advisor for a spin-related nanotechnology national program in the Netherlands and at KIST. He has taken part in national-level magnetism committee policies and meeting initiatives, and has served on the scientific board of international meetings. For example, he is a review panel member for NSF's Partnership for Research and Education in Materials, a multidisciplinary educational activity of the W. M. Keck Computational Materials Theory Center at California State University Northridge and the Princeton Center for Complex Materials at Princeton University. Dr Moodera was invited to be part of an international review board to set the scientific orientations and objectives on nanosciences at the frontiers of nanoelectronics by the National Center for Scientific Research in France. He was the chairman of the Gordon Research Conference on Magnetic Nanostructures at Oxford in August, 2006.

#### Dr. Richard J. Temkin

Dr. Temkin's research on 140, 250, 330 and 460 GHz gyrotrons for EPR and DNP is continuing with support from the NIH National Institute of Biomedical Imaging and

Bioengineering. The 140 GHz and 250 GHz gyrotrons are operational and are being used for DNP research. The 250 GHz gyrotron has operated continuously for about one year, a major technological accomplishment. This has permitted unique experimental DNP/NMR measurements. The 460 GHz gyrotron has operated for a 24-hour trial run. A new version of this gyrotron aimed at increasing efficiency has been designed and built and is now undergoing tests. A 140 GHz amplifier began operation in early 2007. A power level of over 500 watts at 31 dB of gain with a bandwidth of 1 GHz was obtained in early testing. A novel 330 GHz gyrotron oscillator with up to 2 GHz of frequency tunability has been designed and is now under construction. A program of research on techniques for transmitting and radiating THz frequency microwaves supports the program of source development.

### **Facilities**

Renovations for the 900 MHz instrument in NW15 were completed in January 2005 and the instrument was delivered in September 2005. Installation and initial operation of the equipment was completed in July 2006 when the solution-state cryoprobe was installed and became operational.

#### **Education and Personnel**

The FBML contributes to undergraduate education by participation in the Undergraduate Research Opportunities Program (UROP) a program that encourages and supports research-based intellectual collaborations of MIT undergraduates with Institute faculty and research staff. In addition, the laboratory has 25–30 full-time graduate students and approximately the same number of postdoctoral associates and fellows performing research.

#### **Future Plans**

In the longer term FBML plans to complete renovations of the second floor magnet hall. Instruments currently housed on the fourth and fifth floors and new high field magnets will be relocated to this space in order to create a comprehensive CMR. This will involve the acquisition of an 800/89 magnet and a wide bore 600 MHz magnet currently being used in tests of HTS material by Dr. Iwasa and his colleagues.

FBML is also participating in national efforts to start the development of a 30 T magnet (1.3 GHz for <sup>1</sup>H) and to plan the installation of such a system at MIT. At present these systems are proliferating in Europe.

The health of the Research Programs in QIP, imaging, magnet design, spintronics, and high field magnetic resonance at the FBML is excellent, and we anticipate that the lab will continue to grow in the next few years.

Robert G. Griffin Director Professor of Chemistry

More information about the Francis Bitter Magnet Laboratory can be found at http://web.mit.edu/fbml/.