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 20 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). 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. The NIH P41 grant that supports the operation of the 900 and many of the other spectrometers at the FBML was reviewed this past March and renewed until 2014.

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. In addition, Dr. Iwasa recently received Phase 3 NIH funding to begin the design and construction of a 1.3 GHz NMR magnet. This is a long-term project that is very exciting for the magnet design group and the magnetic resonance community.

Professor Alan Jasanoff of NSE and the Department of Brain and Cognitive Sciences 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 (ONR), 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. 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.

Dr. Richard Temkin of the Department 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

David G. Cory

Quantum Information Processing

Quantum mechanics provides a fundamentally new approach that enables us to build devices that exceed the performance of any possible classical device. Quantum mechanics pushes the fundamental physical limits of information processing: by building quantum sensors, actuators, secure communication channels, and computers, we effectively reach the limits in power and accuracy allowed by the laws of physics. The challenge to utilizing quantum mechanics is to control a large enough system so that the efficiency gains offered by quantum mechanics outweigh the technical challenges. Professor Cory and his colleagues have demonstrated control over quantum devices that are so large that they cannot be simulated classically. They are working to turn these quantum systems into practical quantum devices. The program has two stages: the first is directed at laboratory scale devices for characterizing and controlling magnetization, transport and chemistry. These will be enabling for advancing nano- and quantum technology. The second stage aims to construct devices that can operate outside of the laboratory and yet still demonstrate the efficiencies achieved uniquely through quantum mechanics. Professor Cory and his students approach quantum information processing through collaborations with Dr. Chandrasekhar Ramanathan (NSE), Dr. Sergio Valenzuela (NSE), Professor Seth Lloyd of the Department of Mechanical Engineering, Dr. Will Oliver of Lincoln Laboratory, Dr. Mohamed Arif of NIST, Professors Mikhail Lukin and Dr. Paola Cappellaro of Harvard University, Professor Lorenza Viola of Dartmouth College, and professors Raymond Laflamme, X-W Tang, Jonanthan Baugh, and Dr. J. Emerson, all at the University of Waterloo. A few of the highlights from last year are briefly described below.

Ms. Cecilia Lopez has completed an experimental study of efficient error finding. A challenge in quantum computing is that achieving fault tolerance requires some knowledge of the error model. Since the number of terms in a generic error model grows exponentially with the number of qubits, directly measuring all possible errors is not an option. The efficient error-finding schemes that have been developed through collaborations between MIT and the University of Waterloo parameterize reasonable physically relevant models from a polynomial number of measurements.

Mr. Troy Bornamann has demonstrated that the optimal control methods that are used for high-fidelity control in QIP (and which were developed using the NMR test-bed) can be applied to improve performance of traditional applications of magnetic resonance. In particular he has demonstrated the improvement possible for well logging. NMR-based well logging is performed with highly inhomogeneous magnetic fields; here optimal control theory enables uniform control of the spin dynamics even when the control fields are spatially varying.

Dr. Sergio Valenzuela recently succeeded in demonstrating spin injection into Si through a metallic tunnel junction. This has been a long-standing goal of the field, and it opens up the possibility of using spin injection as a polarization source for quantum devices. The key to success in this program was using electron magnetic resonance readout as a monitor of the injected polarization.

Dr. Ramanathan has reported on a series of experiments that use NMR to simulate 1-D multi-body dynamics. This is a system where classical simulations fail to reveal the full complexity of the system dynamics and where it is challenging to set up a clean measurement. One aspect of the study is to investigate 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.

Mr. Chonlagarn Iamsumang has mapped out the changes to the resonance of superconducting striplines as a function of the backing field. He has found that with the stripline in the plane of the magnet the resonance does not vary with the field. When place perpendicularly the Q first increases and then decreases as expected. This observation opens up the potential for using these very high Q systems as efficient spin detectors.

Dr. Dimitri Pushin has reported on a new neutron interferometer geometry that employs quantum error correction to suppress noise from vibrations (which is the greatest experimental challenge to employing neutron interferometry). A new single crystal interferometer has been machined and is being installed at NIST to test these predictions.

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 β -amyloid (A β) 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 wild type and L111M mutant derived from transthyretin. Using these peptides they have determined the structure of the monomer with solid-state NMR distance and torsion angle measurements. Their success with this system encouraged them to initiate experiments with other systems such as the GNNQQNY peptide from the Sup35 protein. During the past year they developed methods to determine the interstrand and intersheet alignment of the peptides and have found them to be parallel and antiparallel respectively. They have now completed the structure and the structure of the WT protofibril during the past year. Finally, during the past year they have also completed assigning the spectrum of the SH-3 domain of the protein phophatidylinostol-3-kinase (PI3-SH3) and have initiated experiments on β -2-microglobulin, the protein associated with dialysis-related amyloidosis.

Dynamic Nuclear Polarization

The 140 and 250 GHz dynamic nuclear polarization (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 were published this past year. 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 (TJ-DNP), that yields approximately 150-400% increased sensitivity for solution NMR experiments and has recorded the initial 2D ¹³C-¹³C spectrum with an enhancement of approximately 150. They 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 ¹³C-¹³C 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:

- Proton assisted recoupling (PAR) methods that permit dipolar ¹³C-¹³C recoupling at high MAS frequencies and magnetic fields without application of proton decoupling
- Similar techniques that are applicable to ¹³C-¹⁵N recoupling
- Methods for simultaneously measuring multiple ¹³C-¹³C distances in uniformly labeled peptides and proteins

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. They 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 33rd 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. Importantly, the grant supporting these facilities was renewed for an additional five year period in March 2008.

Yukikazu Iwasa

The Magnet Technology Division is currently involved in four NIH-funded programs on NMR and MRI magnets and two AFOSR-funded projects on stability and protection issues for YBCO-coated conductors.

These projects are briefly summarized below.

NIH-Supported Programs

HTS Insert Coil for 1-GHz NMR Magnet

In Phase 2, which ended on May 31, 2008, we successfully completed a 700 MHz NMR magnet comprised of a 600 MHz all-LTS NMR magnet and a 100 MHz HTS insert coil.

Digital Flux Injector (Fluxpump) for NMR Superconducting Magnets

The ultimate goal of this program on the development of a digital flux injector (DFI) is completion of a DFI to be coupled to the HTS insert of our 1-GHz LTS/HTS NMR magnet. Coupled to a persistent-mode LTS NMR magnet, it has been demonstrated that a DFI 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. We achieved 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. The program is scheduled to end on August 31, 2008. Since September 2007 we have been concentrating to develop a technique to superconductively splice MgB2 wires to enable MgB2 magnets to operate in persistent mode. So far we have achieved MgB2-MgB2 splices that are superconducting up to a current of 200 A when evaluated at 4.2 K in zero background field.

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 enables 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 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 had two air force-sponsored programs to develop reliable protection techniques for high-energy density YBCO-wound superconducting magnet devices. Both programs ended in September 2007.

Alan Jasanoff

Professor Jasanoff has been a faculty member at the FBML since the autumn of 2004. As of July 2008 he will become an associate professor in the Department of Biological Engineering.

In the past year, the Jasanoff laboratory continued to make progress in the development of MRI contrast agents for the molecular imaging of brain activity. Work on an MRI dopamine sensor, including in vivo studies which are among the first to demonstrate real-time noninvasive monitoring of dopamine transport in living animals, is now being completed by graduate student Mikhail Shapiro and postdoc Gil Westmeyer. Next steps will use the sensor to examine patterns of dopamine released during rewarding stimulation in animals. A zinc sensor developed last year in collaboration with Steve Lippard's laboratory is being applied to detect labile zinc distributions in mice; ongoing

work being performed by postdoc Xiao-an Zhang may ultimately allow functional imaging of neuronal activity using sensors of this family. Much of the newest work of the lab now concentrates on genetically encoded contrast mechanisms. These methods will allow functional imaging of targeted neuronal elements. A recent step toward this goal has been the creation of ferritin-based protein contrast agents sensitive to neuronal signal transduction pathways (the work of Mikhail Shapiro).

Professor Jasanoff was awarded a 2007 NIH Director's New Innovator's Award, a highly competitive \$3.5 million dollar grant.

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 (MBE) 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 micro-disc 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 has introduced the MRAM chips into the market. In this context, Dr. Moodera's group is 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 the technical advisor to a company that is developing MRAM chips and has research collaboration with another one to develop THz radiation sources and detectors. He and his colleagues have successfully developed a research program in the new superconductor (MgB₂) science and technology for Josephson junctions that has a potential for hybrid superconducting electronics in areas such as computers, logic elements, mixers switches, and sensors. They intend to start a new collaboration with Department of Electrical Engineering and Computer Science (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 the materials aspect for quantum computing. In a parallel approach, they are investigating injecting spins into two-dimensional electron gas semiconductors to create spin-field effect transistors. Another program they have embarked on is a new approach to read the Q-bit 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 future goal of reaching mechanically flexible, cheap, and highly efficient spin-based multifunctional devices for bottom-up electronics. They have begun a new collaboration with another group in EECS after their initial success in this area.

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 at the national level magnetism committee policies and meeting initiatives, and has served as well 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.

Highlights

Dr. Moodera obtained a major instrumentation grant from ONR that allows his group to buy a latest scanning electron microscope with E-Beam writer capability to create nanostructures and chemically analyze and image them as well. His latest graduated student, Tiffany Santos, was awarded a prestigious postdoctoral fellowship and joined Argonne National Laboratory in fall 2007. His postdoctoral fellow, Jenny Shim, has joined LG Electronics as a scientist in the research division. Dr. Moodera has also secured the second three-year phase of his long-term collaborative project on nanospintronics with KIST. His article published in *Physical Review Letters* 74 (1995): 3273–3276 on magnetic tunnel junction and TMR is the fourth most cited paper in PRL since 1995.

Dr. Moodera was nominated for the International Magnetism Award (given triennially by International Union of Pure and Applied Physics) for outstanding research breakthrough. He is currently being nominated to the Oliver Buckley Award of the American Physical Society for outstanding research in condensed matter physics and also for the Nishikawa Award of the Institute of Electrical and Electronics Engineers. He was selected as American Competitiveness and Innovation Fellow by the NSF (2008–10) and was cited "for his achievements and world-leading role in the field of spintronics and his dedication to diversity while educating the next generation of scientific and technological leaders of the world."

Richard J. Temkin

Dr. Temkin's research on millimeter wave and THz gyrotrons for EPR and DNP is continuing with support from the NIH /National Institute of Biomedical Imaging and Bioengineering. The goal is the development of stable sources that produce 10 to 50 watts of continuous (CW) power or up to 1 kW of pulsed power at frequencies of 140 to over 600 GHz. The 140 GHz gyrotron was rebuilt in 2008 to achieve true CW operation and it is now fully operational under computer control. The 250 GHz gyrotron is being used for DNP research and has been operated under computer control for periods of weeks at a time. These gyrotrons have permitted unique experimental DNP/NMR measurements. The 460 GHz gyrotron has been rebuilt to operate at higher efficiency. Preliminary results are very promising, with a power level above 12 watts achieved in first tests. A 140 GHz amplifier has achieved a power level of 820 watts and 34 dB of gain with a bandwidth of 1.5 GHz in microsecond pulsed operation. 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.

Robert G. Griffin Director Professor of Chemistry

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