Florida State University • University of Florida • Los Alamos National Laboratory

NHMFL REPORTS

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National High Magnetic Field Laboratory

NHMFL Education Programs Showcased in Washington, D.C.

The National High Magnetic Field Laboratory continues to be spotlighted through the activities of its Center for Integrating Research and Learning. In September, the Center was selected as a showcase exhibit for the Science Coalition's Signature Event in Washington, D.C. In Florida, the Center continues to reach more students and teachers through statewide teacher in-service programs, distribution of the *Science, Tobacco & You* curriculum, and mentorship initiatives.

The Science Coalition represents over 400 member organizations seeking to expand and strengthen

Robert Visser, Robert Visser Photography

NSF Director Rita Colwell with NHMFL Education Director Sam Spiegel (left) and FSU Vice President for Research Ray Bye at NHMFL exhibit in Washington, D.C.

NHMFL EDUCATION continued on page 5

NSF Renews National FT-ICR Mass Spectrometry Facility at $5.76 Million

The National Science Foundation renewed its support for the NHMFL's National High-Field Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS) Facility for a second five-year period, 2000-2004. Florida State University's Alan G. Marshall continues as Director of the ICR Facility, with Co-P.I.s, John R. Eyler (University of Florida), Christopher L. Hendrickson (NHMFL), and Mark R. Emmett (NHMFL), and NHMFL staff members John Quinn and Daniel McIntosh. Reviews of the project were sufficiently strong that NSF chose to fund the proposal at its full requested budget ($5.76 million for 2000-2004) without a site visit. The ICR Program has been one of the NHMFL's shining successes, both in instrument and technique development and in applications for a worldwide user base.

History. In 1990, shortly after NSF's decision to fund the NHMFL, Marshall (then at Ohio State

FT-ICR continued on page 13

ATTENTION USERS

Greg Boebinger Director, NHMFL Pulsed Magnetic Field Laboratory

NHMFL Pulsed Magnetic Field Laboratory:

New Experimental Hall Reflects "Full-Multiplex" Operating Philosophy

Over the past several months, the entire experimental hall of the Pulsed Magnetic Field Laboratory has been "boxed up" and moved to a new building…a prodigious accomplishment made possible by long hours and hard work put in by all the NHMFL folks in Los Alamos and two who traveled from

Mike Pacheco (kneeling) supervises the moving of the 60 T Long-Pulse magnet into a new pit located in the Long-Pulse Magnet Building. For safety, this building will be evacuated during 60 T Long-Pulse operations. In the background (at left) is the passage through the two-meter thick safety wall into the New Experimental Hall.

NEW EXPERIMENTAL HALL continued on page 4

Operated by Florida State University, University of Florida, Los Alamos National Laboratory

From the Director's Desk

Jack Crow

The NHMFL is charged by the National Science Foundation with driving a high quality science program in research areas that use the highest magnetic fields, and developing the vision for exploring new field-induced phenomena across broad fields of study (chemistry, physics, biosciences, geosciences, and engineering). These goals can be achieved by advancing facilities, technologies, and instrumentation in close parallel with the science and engineering programs.

Three articles in this issue of *NHMFL Reports* illustrate how the laboratory is already working toward these objectives in a variety of ways: moves to new building space and/or infrastructure improvements; acquisition of new research facilities; development of novel instrumentation; and enhancements of services and support for users.

The NHMFL Pulsed Magnetic Field Laboratory at Los Alamos recently completed a major move into new facilities. The New Experimental Hall and building configurations (described by Greg Boebinger on page 1) were designed in close consultation with users and will better support user demand and prepare for the anticipated growth of the pulsed magnet program.

Likewise, the consolidation of NHMFL magnetic resonance imaging assets at the University of Florida Brain Institute—at the Advanced Magnetic Resonance Imaging and Spectroscopy Facility—continues. Existing instruments like the 600 MHz narrow bore are being moved in; other instruments like the 4.7 T/33 cm instruments are being installed and tested; and new state-of-the-art facilities like the 11.7 T/40 cm system and the 750 MHz wide bore are in transit or are being prepared for shipping. On page 10, Steve Blackband describes these activities and discusses the design and development of a novel rf coil for high frequency application on large samples. Improved performance over a "birdcage coil" is anticipated, and a prototype is being developed for the 11.7 T system.

The NHMFL Ion Cyclotron Resonance Program (page 1) headed by Alan Marshall continues to push the limits of science and technology by continuously upgrading systems (both hardware and software) and by promoting a strong in-house research program that ensures that new techniques are integrated quickly and made widely available to users. The research, publication, education, and industrial collaborative activities of this program have been first-rate—fully justifying NSF's strong $5.76 million renewal.

These glimpses inside several strong programs of the laboratory demonstrate the NHMFL's commitment to employing its outstanding human and facilities resources wisely, efficiently, and in support of world-class science and engineering user activities.

An underpinning of all NHMFL programs is education, and the outstanding efforts of the laboratory's Center for Integrating Research and Learning continue to be dramatically visible and successful. See the education feature on page 1 for a few recent highlights. Education outreach extended to the general public in October when we held our annual open house (see page 8). I would like to publicly thank the over thirty different NHMFL participating research groups and development teams for their extraordinary efforts and inventiveness. This year's presentations were excellent, and our faculty and staff did a truly outstanding job of translating frequently intimidating science concepts into easily understood language—a noteworthy accomplishment!

Before closing, I would also like to thank *you* for responding to recent pleas to write your congressional delegates in support of U.S. investments in science and research. Positive funding decisions in support of the National Science Foundation this fall should help sustain and advance science, education, research and development activities as we enter the 21st Century.

Jack Crow

From the Chief Scientist's Desk


Robert Schrieffer

In this issue, Vladimir Dobrosavljevic and Andrei Pastor discuss the fascinating topic of phase transitions in which random electronic pinning sites and strong Coulomb interactions between electrons lead to a metal insulator transition. As the system approaches the metal insulator transition the energy landscape goes from a smooth function of the configuration coordinates to one with many energy minima in which the system may be trapped. This glassy state exhibits long relaxation times and hysterisis behavior. These minima are due to the joint action of the random pinning potentials and the Coulomb repulsion between electrons. Recently, the antiferromagnet $Fe_{0.31}Zn_{0.69}R_2$ has been studied in a strong magnetic field. These materials are examples of the random field Ising model in which a strong field produces a well-defined transition temperature below which very slow relaxation is observed. These transitions are closely related to the electron metal insulator transition with the theories of these systems being closely related. The understanding of these phenomena is of universal importance in areas such as protein folding. Excellent progress is being made on these problems in the context of the metal insulator transition.

Robert Schrieffer

Vitrification of Electrons and Magnets

V. Dobrosavljevic and A. A. Pastor
Department of Physics and National High Magnetic Field Laboratory
Florida State University

The word *vitrification* may not be familiar to the average solid state physicist, in contrast to a typical chemist or a biologist. And for good reason: According to Webster, it means "*to convert into a glassy substance*," derived from Latin *vitrum* for glass. Indeed, traditional solid state physics capitalizes on the almost perfect periodicity of crystals, while glasses consist of an amorphous, random conglomeration of atoms or molecules.

In recent years however, the cross-fertilization of ideas and concepts from different fields seems to have given a remarkable boost to modern technology and science. In fact, many of the recently discovered conductors and even superconductors are obtained by introducing a few carriers in an otherwise insulating host—a regime very far from well-understood metals such as copper or gold. By any account, these systems are close to the metal-insulator transition (MIT), a phenomenon that has defied full theoretical understanding for many years. Here, the average kinetic energy of the electrons is not all that large, and even modest perturbations can have a huge effect. The behavior of electrons is then typically dominated by both the strong electron-electron interactions and the disorder due to impurities. Even on the metallic side, these effects can be sufficient to cause drastic deviation from what one expects for standard conductors. Such "non-Fermi liquid" (NFL) behavior is characterized by anomalous temperature dependence of various thermodynamic and transport properties that have been studied by several groups, including the recent effort [preprint, cond-mat/9909215] of J. D. Thompson and collaborators (LANL), on samples grown by Z. Fisk (NHMFL). On the theory side, a possible mechanism that could lead to the disorder-driven NFL behavior has been proposed by Dobrosavljevic (NHMFL) and his collaborators [Phys. Rev. Lett. 78, 290 (1997)].

Further insight in this fascinating regime is obtained by reducing the density of carriers, when the system approaches the MIT. Spectacular and totally unexpected phenomena have recently been reported on several such low carrier density systems. In one example, Fisk and collaborators have revealed the emergence of weak ferromagnetism possibly related to the incipient Wigner crystallization of electrons [Nature 397, 412-414 (1999) and NHMFL Reports, 6-3, 3&6 (Summer 1999)]. Another example that has attracted worldwide attention is the recent observation of a metal-insulator transition in disordered two dimensional (2D) electron systems such as MOSFETs (metal-oxide-semiconductor field effect transistors). This phenomenon, first reported by Kravchenko in 1995, has recently been studied by several groups, including that of D. Popovic at NHMFL, whose typical data [from Phys. Rev. Lett. 79, 1543 (1997)] are shown in Figure 1 (see page 6). Paradoxically, such a transition has been believed to be *impossible* for almost twenty years, since this can be rigorously shown to be true for *non-interacting* electrons. However, recent theoretical work by Dobrosavljevic *et al.* [Phys. Rev. Lett. 79, 455 (1997)] has suggested that the same may *not* be correct for interacting electrons, and that a genuine transition is possible. In addition, simple estimates show that near the critical electron density, the Coulomb energy is more than ten times larger than the Fermi energy—emphasizing the key role of electron-electron interactions in localizing the electrons.

Even though there remains little doubt as to the main driving force for such a MIT in a low carrier density system, providing a satisfactory theoretical description has proven fundamentally difficult. This is most obvious by focusing on the insulating side of the transition. Here, the electrons freeze in a random, amorphous pattern, sometimes denoted the *electron glass*. The resulting low temperature configuration is a compromise between the Coulomb repulsion (which tends to keep the electrons away from each other) and impurities (which favor inhomogeneous distributions). In direct analogy with more familiar "window" glasses (super-cooled liquids), this low temperature state is far from unique. Worse, it is believed

ELECTRONS AND MAGNETS continued on page 6

ATTENTION USERS

Continued from page 1

Greg Boebinger

Tallahassee to lend a much-appreciated hand. Let me take this opportunity to thank my colleagues from Los Alamos and Guy Cochran and John Robinson from Tallahassee for their dedication to the NHMFL's Pulsed Magnetic Field Laboratory.

This laboratory relocation has been accompanied by an extensive re-design of the user support infrastructure to reflect our "full-multiplex" operating philosophy:

> *Since the magnets are inherently pulsed, strive to time-multiplex laboratory operations as well.*

The motivation for this philosophy is straightforward. The Pulsed Magnetic Field Laboratory of the NHMFL currently operates $30 million worth of pulsed power infrastructure. Doubling the scientific breadth, impact, and output of the pulsed magnet program will not come from doubling this investment. Rather it will result from designing operations to exploit more fully the freedom to time-multiplex pulsed magnet experiments.

An aerial view of the new layout. The New Experimental Hall building was originally constructed to house the target for a Los Alamos experiment on inertial confinement nuclear fusion and, thus, is a veritable fortification featuring two-meter-thick reinforced concrete walls. In addition to providing the NHMFL with a clearly defendable perimeter, these walls provide a safety barrier between experimentalists in the New Experimental Hall and the NHMFL's long-pulse magnets (both present and future) that are now located in the adjoining Long-Pulse Magnet Building. Figure 1 shows an aerial view, looking south, of the three buildings comprising the NHMFL's Pulsed Magnetic Field Laboratory. At right, the generator building houses the 1.4 GVA generator and new offices for the generator operations staff. This generator provides power to seven 84 MVA power supplies and the 60 T Long-Pulse Magnet, all of which are now housed in the Long-Pulse Magnet Building at center. The New Experimental Hall, the hub of NHMFL user operations, is in the foreground.

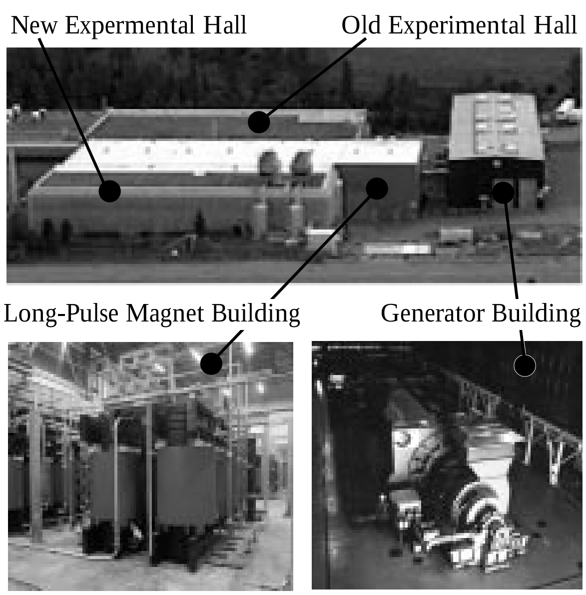


Figure 1. The three buildings comprising the 40,000 square foot NHMFL Pulsed Magnetic Field Laboratory, located at the Los Alamos National Laboratory in New Mexico.

An interior view of the new layout. The floor plan of the New Experimental Hall (Figure 2) was designed in consultation with the NHMFL Users' Committee and reflects the operating philosophy throughout:

- The Short-Pulse and Long-Pulse Magnet Programs have been "de-tangled" and now operate independently in separate buildings.
- The short-pulse magnets and capacitor bank are located in the New Experimental Hall, where magnet cells are designed for independent short-pulse magnet experiments.
- The 60 T Long-Pulse Magnet is located in the Long-Pulse Magnet Building, where additional space has been set aside for the 100 T Non-Destructive Magnet currently under design.

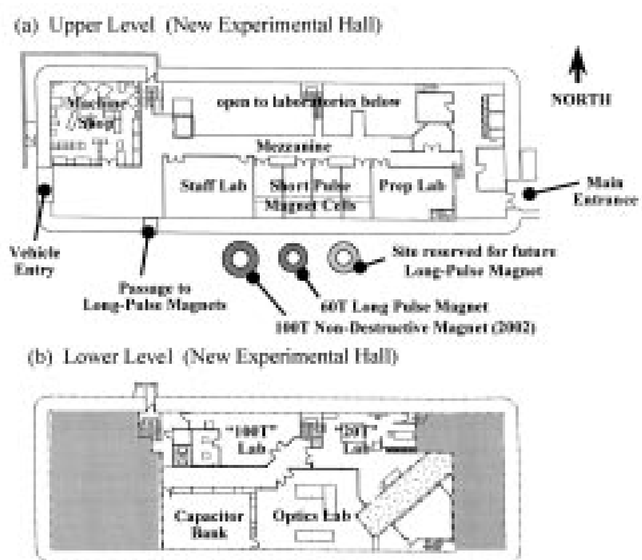


Figure 2. The floor plan of the New Experimental Hall with (a) the upper level featuring the independently-operated magnet cells and user preparation area; (b) the lower level featuring the capacitor bank, optics laboratory and 20 T superconducting magnet laboratory. Magnets are located in the Long-Pulse Magnet Building.

- All newly-purchased infrastructure has been specified to accommodate future growth through increased time-multiplexing of experiments. Examples include a new power supply for sub-minute charging of the users' capacitor bank and automated switching for turn-key capacitor-bank configuration and magnet selection.

Figure 2 details the floor plan of the New Experimental Hall. User activities center around a wide mezzanine on the upper level that connects the four user magnet cells and the user preparation lab. To pulse a magnet, a user need only evacuate his own magnet cell, without interrupting activities in the other magnet cells. The capacitor bank control computer, located at the east end of the mezzanine, automatically configures and controls the capacitor bank. All new infrastructure is being designed and built to be consistent with the possibility that all four user magnet cells could eventually be scheduled for continuous operation. The upper level mezzanine offers easy access to the top of the dewar housing the 20 T superconducting magnet, to facilitate cryogen transfers and setup of 20 T experiments. User offices and instrument storage areas are located at the east end of the upper level, while the machine shop and magnet assembly areas are located in the west end. The staff laboratory provides sheltered bench space for in-house researchers to develop experiments and extend the capabilities of the NHMFL User Program.

The lower level features a sheltered room housing the capacitor bank that powers all short-pulse magnet operations. This room also contains two stations for destructive short-pulse magnet testing; this testing will no longer compete with the Short-Pulse User Program for scheduled time. A greatly-expanded optics laboratory is located beneath the magnet cells for easy access to any of the magnets above. The expanded 20 T laboratory features the DC superconducting magnet, as well as its own user preparation area and magnet control room. The "100 T" Lab houses a fifth short-pulse magnet cell and provides space for development of experimental techniques for use in the NHMFL's 100 T non-destructive magnet, a magnet that is scheduled for initial operations in 2002.

Due to the extreme energies involved, the Long-Pulse Magnet Building must be evacuated whenever a long-pulse magnet is energized. For this reason, a passage has been made for long-pulse magnet users to find shelter in the Experimental Hall during long-pulse magnet pulses. A region in the staff laboratory has been set aside for data-acquisition and analysis for 60 T Long-Pulse experiments.

We anticipate that the positive features of this laboratory re-design will be immediately apparent to users of the NHMFL's Pulsed Magnetic Field Laboratory. The old configuration worked well when pulsed magnets could only pulse once an hour and the pulsed magnetic field user community was small. It began to falter when newer magnet designs doubled and tripled the pulse repetition rate and the NHMFL occasionally scheduled three simultaneous user experiments in response to increased user demand. The new configuration immediately accommodates our current level of multiplexed operations and provides opportunities for significant growth in the future.

NHMFL EDUCATION continued from page 1

the federal government's investment in university-based scientific, medical, engineering, and agricultural research. Its Signature Event was held in the U.S. Senate Hart Building and featured eight selected organizations, one of which was the Center. The NHMFL exhibit focused on its educational efforts that provide resources, experiences, and opportunities to advance science education by capitalizing on the laboratory's unique science resources–distinguished faculty and users, premiere facilities, and advanced technology. Visitors at the exhibit explored our *Science, Tobacco & You* program; investigated how magnetic fields can be used to advance scientific discoveries in biology, chemistry and physics; and in general, gained a heightened understanding of the impact that a national laboratory can have on teachers and learners in both formal and informal education settings from kindergarten through graduate education, as well as the general public.

The Center has received an additional $953,000 from the Florida Department of Health's Tobacco Pilot Program to deliver *Science, Tobacco & You* packages and workshops this year. Last year, over 1,800 4th and 5th grade classes across Florida received a complete package and over 320 teachers were trained to help facilitate the integration of this exciting program into the schools. Twelve additional workshops will be held across Florida this year reaching over 480 teachers and 1,500 classrooms (total distribution to over 3,300 classrooms). The ultimate goal of *Science, Tobacco & You* is to encourage students to become "scientifically literate" citizens by developing their skills to ask questions and determine the answers derived through inquiry. Through scientific analysis and captivating multi-sensory experiences, students can explore and understand the harmful effects of tobacco on their bodies. To learn more about this project, readers may explore the web-based portion of the program at http://scienceu.fsu.edu.

This year we are hosting 26 middle school students for research mentorships as part of the Leon County School's Academic Resource Center. These students come to the laboratory one day a week for a full semester. The students work along-side researchers at the NHMFL conducting experiments, engaging in research, and experiencing the excitement and practice of science. Past projects have included: electrical conduction of materials at different temperatures; analyzing the effects of El Ninõ on stream flow in the southeastern United States; creating a program to calculate and analyze stress and strains in a superconducting magnet; assisting in the creation of a web-based virtual microscope; synthesizing and measuring novel superconductors; exploring photo-illuminescence of a ruby; conducting magnetoresistance measurements for detecting magnetic field strength; and assisting in the development of a web-based application to determine isotope distribution of chemicals. More information on this program is available at http://k12.magnet.fsu.edu/student/k12/arc.html.

For more information on these or other NHMFL educational projects, contact Dr. Sam Spiegel, Director, Center for Integrating Research and Learning, spiegel@magnet.fsu.edu, 850-644-5818.

that there is an exponentially large number of such low energy, random configurations, all very close in energy. As a result, again similarly to other glassy systems, such disordered insulators display extremely slow relaxation processes at low temperature, sometimes described as *non-ergodic* behavior. Such slow dynamics must play a crucial role near the metal-insulator transition, a phenomenon which by its definition describes the slowing down and ultimately the cessation of electronic motion. In addition, this phenomenon is crucial in controlling the extend of electronic *screening processes*, which fundamentally determine the effective magnitude of electron-electron interactions.

Theoretically, describing this *vitrification*, or glassy behavior of electrons is far from straightforward. Very recently, we have formulated an approach [A. A. Pastor and V. Dobrosavljevic, Phys. Rev. Lett., Nov. 29, 1999] to this problem by combining methods developed for other disorder-driven MITs [V. Dobrosavljevic *et al.*, Phys. Rev. Lett. 78, 3943 (1997)], and earlier ideas used to describe more conventional glassy systems. Several predictions of our theory have immediately found verification in very recent experiments. In particular, we predict the existence of a well defined glass transition temperature T_G below which slow relaxation should be observed; convincing evidence of such behavior has been observed in disordered metallic films by A. Goldman *et al*. [Phys. Rev. B 57, R670 (1998)]. Furthermore, we expect the vanishing of *zero-field cooled compressibility*, as apparently observed in the capacitance experiments on 2D electron gasses by H. W. Jiang and his group [preprint, cond-mat/9909314]. While the first steps to describe this fascinating phenomenon have been achieved, much more has to be done before the metal-insulator transition is fully understood.

To the magnet user, it may be amusing to hear about ways to test our theoretical ideas using strong magnetic fields. A very nice example was discovered in work done by one of the recent NHMFL users F. C. Montenegro and his group (UFPE-Brazil), who studied the behavior of disordered (diluted) antiferromagnets such as $Fe_{0.31}Zn_{0.69}F_2$ in strong magnetic fields. Such materials have long been regarded as experimental realizations of the "random field Ising model" (RFIM), one of the simplest theoretical examples of interacting disordered systems. In these materials, application of even modest magnetic fields is suffcient to suppress any uniform (antiferromagnetic) ordering. At stronger fields, however, a well defined transition temperature is still discovered, where extremely slow, non-ergodic behavior sets in, reflecting the emergence of glassy freezing. Interestingly, the RFIM used to describe these materials is very closely related to models of electron glasses, making it possible for a direct test of our theoretical ideas using strong magnetic fields. To do this, we have computed the magnetic field dependence of the glass transition temperature, and compared it to the existing experimental data [From F. C. Montenegro *et el.*, Phys. Rev. B 44, 2155 (1991)]. Our predictions are in remarkable agreement with the experiments, as shown in Figure 2. In particular, the experiments demonstrate that the glass transition temperature decreases only weakly with the field, viz. $T_G \sim 1/H$, as illustrated in the inset of this figure.

From a more general perspective, the emergence of glassy ordering in electronic and magnetic systems reflects the fundamental differences of phase transitions in disordered and amorphous compounds from those taking place in crytalline materials. Remarkably, very similar phenomena are found in many different fields ranging from physics to chemistry to biology, underscoring the deep connections between these disciplines. Thus from both the practical and the fundamental point of view, the study of effects of randomness and disorder represents a fascinating and *useful* direction for the years to come.

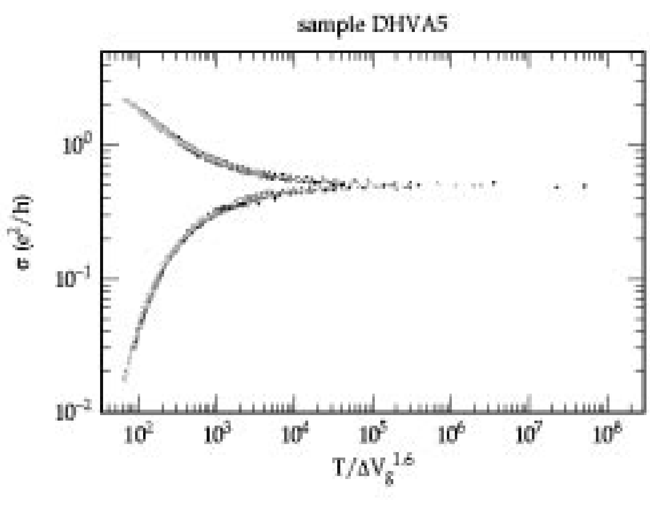


Figure 1. Conductivity of two dimensional electrons in a MOSFET (see text), as a function of temperature for several electron densities, obtained by D. Popovic *et al.* (NHMFL). Here, the temperature is rescaled by a density dependent factor, in order to demonstrate the dynamical scaling behavior expected at a T=0 metal-insulator transition.

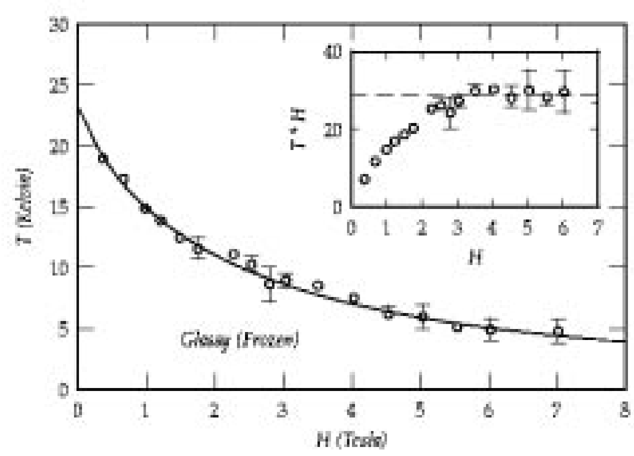


Figure 2. Glassy freezing in the "random-field" magnet $Fe_{0.31}Zn_{0.69}F_2$. The data points are taken from the experiment of F. C. Montenegro (see text), and the full line is the theoretical fit predicted by A. A. Pastor and V. Dobrosavljevic.

Conference and Workshop Activity

16th International Conference on Magnet Technology (MT-16)
September 26-October 2, 1999
Sawgrass Marriott Resort, Ponte Vedra Beach, Florida

MT-16 was—by all accounts—an overwhelming success: 25 percent more abstracts and participants than earlier MT conferences; two-thirds of the attendees came from countries other than the United States; and an industrial exhibition that attracted 21 companies. The growth of this major international conference demonstrates the increasing importance of magnet technology and the progress that is being made in this field crucial for modern industrial applications. A full report on the conference is being developed and will be featured in the next issue of *NHMFL Reports*.

30th Southeastern Magnetic Resonance Conference (SEMRC)
November 4-6, 1999
DoubleTree Hotel, Tallahassee

Over 125 participants attended SEMRC this year. The conference featured invited and contributed papers and posters in NMR, MRI, EPR, and ICR, with topics focusing on Improving Sensitivity, High Field Spectroscopy, New NMR Methods, and Isotope Labeling Strategies.

The closing session of the conference was particularly noteworthy as it honored the life and work of Gitte Vold. Scott Prosser, Kent State University, and Stanley Opella, University of Pennsylvania, were the featured speakers.

International Workshop on Latest Developments in Low-Density and Low-Dimensional Electronic Systems
March 4-7, 2000
University of Florida, Gainesville, FL

The program of this workshop is being organized with ascending dimensionalities in mind: 0D and 1D (dots, wires, nanotubes, etc.) followed by 2D (Hall, stripes, metal-insulator transitions, etc.), followed by quasi 3D and 3D (hexaborides, bismuth, graphite, etc.). An underlying theme in all of these topics will be the relationship between low carrier density, low dimensionality, and the magnetic, metallic and/or insulating properties of novel materials. Some attention will also be focused on the use of high magnetic fields at the NHMFL to induce transitions to new states of matter.

The three-day workshop will feature over twenty invited speakers (equally divided between experiment and theory) and will provide an opportunity for posters and contributed presentations. The preliminary list of invited speakers includes:

B. Altshuler (Princeton)
R. Ashoori (MIT)
L. Balents (UC, Santa Barbara)
D. Ceperley (U. Illinois, Urbana-Champaign)
S. Chakravarty (UCLA)
C.-L. Chien (Johns Hopkins U.)
S. Das Sarma (U. Maryland)
Z. Fisk (NHMFL, FSU)
M. Fisher (UC, Santa Barbara)
M. Lilly (Cal Tech)
C. Marcus (Stanford U.)
J. Orenstein (UC, Berkeley)
W. Pan (Princeton U.)
V. Pudalov (Moscow)
M. Sarachik (CUNY)
C. Varma (Lucent)
A. Yacoby (Weizmann Institute)

This workshop is sponsored by the University of Florida (Center for Ultra-Low Temperature Physics, College of Liberal Arts and Sciences, Department of Physics, and Institute for Fundamental Theory) and the NHMFL. For further information, see the workshop web site: *http://www.phys.ufl.edu/workshops/ld3.html*.

Physical Phenomena at High Magnetic Fields (PPHMF-IV)
October 19-24, 2001
Santa Fe, New Mexico
Hotel Headquarters: Hilton Santa Fe

Planning continues for this major international conference initiated by the NHMFL in 1991 and held every three years. For information, contact Conference Chair Alex Lacerda, Director of the NHMFL–Los Alamos Users Program (505-665-6504, *lacerda@lanl.gov*, fax 505-665-4311).

Applied Superconductivity Conference (ASC04)
October 4-8, 2004
Site: To be determined

Planning continues for this important international conference that typically attracts over 1,500 participants. For information, contact Conference Chair Justin Schwartz, Associate Professor of Mechanical Engineering and NHMFL Magnet Science & Technology Group Leader (850-644-0874, *schwartz@magnet.fsu.edu*, fax 850-644-0867).

OPEN HOUSE 1999

On a picture perfect autumn day in Tallahassee, the 6th Annual Open House of the NHMFL attracted 2,567 visitors. This included six school buses of students, several large vans of adults, and the State of Florida Commissioner of Education Tom Gallagher. An unscientific poll of visitors indicated that a significant majority of our guests were visiting the laboratory for the first time.

Our guests made a choice to spend the most gorgeous day of the year thus far at the Magnet Lab. And my oh my, did we give them a show. Their exit comments were uniformly in praise of our quality presentations, enthusiasm, ability to communicate, and genuine friendliness. If we were looking for “converts” who support research facilities like the Magnet Lab, we won them hands down.

An important by-product of all the hard work is that we now have many new permanent and semi-permanent displays and demonstrations that will aid the hundreds of *guided* tours that go through the lab each year and attract over 4,000 K-12 students and 1,000 adults.

Amid the Thousands, There Was A Little Boy...

Amid all the wonderful moments on October 23rd, one anecdote focuses on the real significance of efforts like the open house. A little towheaded boy, perhaps 4 years old, ran to the maglev launch demo for one last look. It was 3:00, and the demo had been discontinued for the day. The little boy was stunned. His mother explained that even before coming to the lab, he wanted to be a rocket engineer. The launch demo had been his favorite activity—and they had been here for hours and had toured and enjoyed the whole place. This little free spirit had his heart set on seeing that rocket go off just one more time. Needless to say, we accommodated his special request and were rewarded by his bright eyes and huge smile as "his" rocket soared.

In the aftermath of the open house, we believe we may have identified this little boy, and two NHMFL engineers with space program experience have offered to become involved.

So often, efforts are measured by bottom-line numbers, and dollars and cents. Sometimes, we ought to add a few more variables to the formula.

Kathy Hedick, NHMFL Open House Coordinator

Advanced Magnetic Resonance Imaging and Spectroscopy (AMRIS) Facility

Progress and Research Report #2, Fall, 1999

Steve Blackband, Associate Professor UF Neuroscience Department

AMRIS Progress, October, 1999

The AMRIS facility at the University of Florida (UF) continues to develop close to schedule, and the 4.7 T/33 cm instrument is almost completely functional. In August a Bruker representative (Bob Rycyna) ran an extremely informative programming course for Bruker software (also attended by collaborators from University of Alabama, Birmingham). Most obvious was the extreme complexity of the software. This is due primarily to the overhead that is required when consoles are expected to perform like clinical instruments, and is the unavoidable tradeoff between capability and programming ease. It is clear that a full-time programmer, or at the least a strong tie to the Bruker programmers, will be required.

The 600 MHz narrow bore has been moved into AMRIS facility but is experiencing a problem. Over short time periods the magnet homogeneity is drifting. Extensive experiments are being performed to determine the cause of this (pressure, temperature, building effects), but presently the best bet is a fault in the magnet itself, possibly resulting from the move. It is likely we will be calling in Oxford to take a look. A 500 MHz shielded narrow bore Bruker system with a Magnex magnet was delivered in September and is presently being installed and cryoshimmed.

We await with great expectation (and trepidation!) the delivery of the 11.7 T/40 cm and the 750 MHz wide bore systems. The 11.7 T/40 cm is in transit and delivery is expected in early November. The 750 MHz wide bore is ready and a schedule for delivery is under negotiation subject to final facility preparation. At present we expect delivery in early December. Hopefully both instruments will be fully functional in the spring.

The 3 T/80 cm instrument is presently in pieces and in the process of being upgraded with a state-of-the-art GE console. The upgrade work is ahead of schedule (previously reported as early next year) and should be back in action in early November. The improved system will have stronger and faster switching gradient coils greatly enhancing its imaging capability, especially for fast imaging sequences such as EPI. This will be particularly important for functional magnetic resonance imaging (fMRI). To help in the development of the fMRI program at UF, the Department of Psychiatry has hired a new junior faculty member, Dr Liu. Dr Liu started in October and comes from the prestigious imaging group in Texas run by Dr Peter Fox.

A new development by Barbara Beck in the rf laboratory has been the design and construction of a novel rf coil for high frequency application on large samples. The coil is a rentrant cavity, more similar to a resonant cavity used for microwave applications than a conventional rf wire array, and has performed as well as a birdcage coil at 4.7 T. It is hoped that the cavity will have improved performance over the birdcage at higher frequencies and a prototype is being developed for the 11.7 T/40 cm. The design has been submitted to the International Society for Magnetic Resonance in Medicine meeting; in addition, a publication in is preparation and will form the research section of one of these reports in the near future.

That's it for now. Hopefully the next report will tell of the arrival of our new BIG magnets! The following is the second research report for AMRIS and summarizes some recent spectroscopy work from Dr. Art Edison and his group.

AMRIS Research Report #2

Phosphorylation-Dependent Conformational Changes Induce a Switch in the Actin-Binding Function of MARCKS (in press, *J. Biological Chemistry*, 1999)

Michael R. Bubb, Robert H. Lenox, Arthur S. Edison, University of Florida

Myristoylated alanine-rich protein kinase C substrate (MARCKS) is a prominent protein substrate for protein kinase C that binds calmodulin in a calcium-dependent manner, binds and crosslinks filamentous actin, and is implicated in cellular processes associated with cytoskeletal restructuring, e.g., transmembrane signaling and neurotransmitter release. A highly conserved phosphorylation site domain (PSD) is the binding site for both actin and calmodulin, and may also bind directly to plasma membrane through acidic phospholipids. Considerable work has demonstrated a role for MARCKS in long term events in cell function that are associated with alteration in actin-membrane plasticity in the brain. In particular the regulation of MARCKS expression is involved with brain development, neuronal regeneration, and represents a molecular target in the brain for the action of mood-stabilizers such as lithium in the treatment of manic-depressive illness.

Using NMR spectroscopy, sedimentation, and molecular dynamics simulations, we have documented for the first time conformational changes in the PSD following phosphorylation. These phosphorylation-dependent conformational changes are correlated with changes in actin crosslinking. In particular, phosphorylated MARCKS-PSD crosslinks actin at significantly higher concentrations than non-phosphorylated MARCKS-PSD. These findings lead to a hypothesis that the actin-MARCKS complex is regulated by specific alterations in conformation of the PSD which changes the availability of actin-binding sites required for crosslinking.

Figure 1 shows NMR spectra of the phosphorylated and non-phosphorylated MARCKS-PSD peptides. The samples leading to these spectra only differ by three phosphate groups; the amino acid sequence is identical. The phosphorylated spectrum (left) shows several signs of structure including a large number of NOE peaks, reasonably large chemical shift dispersion, and limited water accessibility to backbone amide protons. In contrast, the non-phosphorylated spectrum shows no significant long- or medium-range NOE peaks, has reduced chemical shift dispersion, and large interactions with water along the peptide backbone. The data are consistent with structure in the phosphorylated sample but none in the non-phosphorylated sample. Figure 2 shows a family of structures obtained from 100 ps molecular dynamics simulations using NMR restraints. The structures were generated by energy minimizing the dynamics trajectory every 5 ps of the simulation. These structures show multiple contacts between positively charged amino acids and the negatively charged phosphates for the phosphorylated sample and completely extended conformations in the non-phosphorylated sample.

Thus, with a combination of NMR and other techniques, we were able to demonstrate that MARCKS-PSD has significant phosphorylation-dependent changes of conformation. In future work we will be testing the hypothesis that these conformational changes control the functional changes observed for this molecule. For more complete information, please watch out for the paper in a December or January issue of *J. Biological Chemistry*.

Acknowledgements: Work funded by a UF College of Medicine pilot study grant, with data collected on the 720 MHz instrument at the NHMFL.

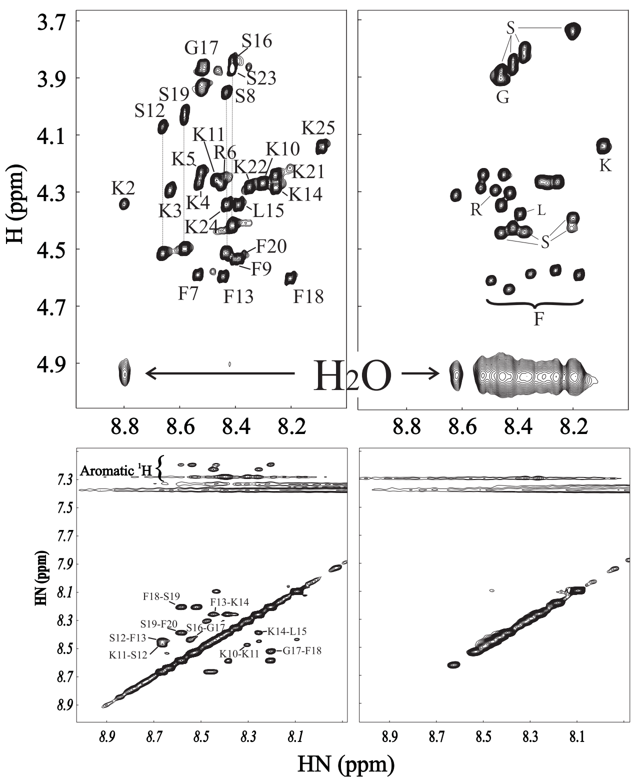


Figure 1. Two dimensional NMR data of MARCKS peptides. 720 MHz TOCSY fingerprint regions (top panels) and NOESY amide to amide regions (lower panels) for the phosphorylated (left panels) and the non-phosphorylated (right panels) MARCKS peptides reveal substantial differences. The sequential assignments for the phosphorylated peptide are shown in the TOCSY spectrum (upper left). The non-phosphorylated peptide residue-specific (not sequential) assignments are shown in the TOCSY spectrum (upper right). The water frequency (just over 4.9 ppm) is labeled. The NOESY spectra were collected with a 200 ms mixing time. The temperature for these experiments was 15 °C.

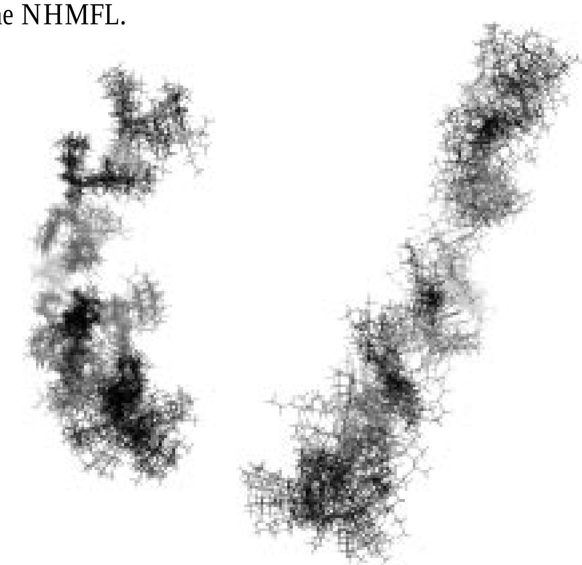


Figure 2. Families of structures from molecular dynamics simulations. Twenty energy minimized structures were produced at 5 ps intervals from a 100 ps molecular dynamics trajectory. The structures were superimposed by overlapping all heavy atoms. All simulations were done with explicit water, which was removed from the figure for clarity. The color scheme for the peptides is blue for lysine or arginine, green for phenylalanine, light green for leucine, yellow for glycine, light blue for serine, and red for phosphates. The phosphorylated MARCKS peptide is on the left and the non-phosphorylated MARCKS peptide on the right, and both are drawn to the same dimensions. The N-termini for the two peptides are facing down. The phosphorylated MARCKS peptide is very clearly bent in the middle, resulting from ionic interactions involving the phosphates and positively charged side-chains. The non-phosphorylated peptide, by contrast, is fully extended.

Tim Cross, director of the laboratory's NMR Program, was recently selected for the Council of the Biophysical Society. Members of the Council are elected by the entire membership of the Society (about 5,000 constituents).

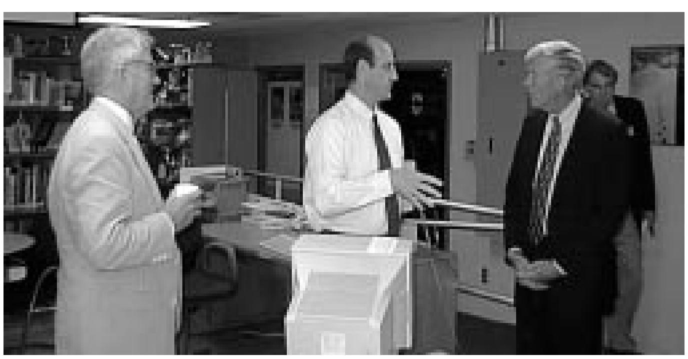
Florida Senator Connie Mack toured the NHMFL in August for the first time since the laboratory's dedication in 1994. His tour focused on NHMFL initiatives in structural biology and biomedical research and applications. Senator Mack met with Drs. Alan Marshall (ICR), Stephen Gibbs (Chemical Engineering), Sam Spiegel (NHMFL Center for Integrating Research and Learning), and others in the laboratory.

Ray Bye (FSU Interim Vice President for Research), Senator Mack, Greg Williams (Senator Mack's aide), Janet Patten (NHMFL Director of Government and Public Relations), and Alan Marshall, during the tour of the FT-ICR Facility.

FSU Faculty Promotions

In the Summer Issue of this newsletter, we reported the promotion of several NHMFL physics colleagues at the University of Florida. Here, we are pleased to announce similar recognitions at Florida State University and the NHMFL:

Yusuf Hascicek, to Scholar/Scientist, Magnet Science and Technology
Jurek Krzystek, to Associate Scholar/Scientist, EMR Program
Adriana Moreo, to Full Professor, Physics
Justin Schwartz, to Full Professor, Mechanical Engineering
Sam Spiegel, to Associate in K-12 Education
Robert Walsh, to Associate in Research, Magnet Science and Technology



Sam Spiegel explains the laboratory's extensive educational activities to Senator Mack, as Sandy D'Alemberte (FSU President) and Alan Marshall look on.

Senator Mack talks to the media following his half-day tour.

FT-ICR continued from page 1

University) and Eyler asked NHMFL Director Jack Crow if any of the NHMFL magnets could be made available for FT-ICR MS applications. Although ICR was not included in the original NHMFL budget, Crow offered to stage a two-day workshop in 1991, at which more than a dozen ICR researchers and vendors met to discuss magnet specifications and potential impact for high-field (>7 tesla) experiments. Armed with three or four main "thrust" directions from that meeting, Crow, Marshall, and Eyler made several trips over the next two years to federal funding agencies, seeking a match between proposed ICR projects and existing federal grant programs. In 1993, Marshall accepted the position of Director of the NHMFL ICR Program and Professor of Chemistry at FSU, and Dr. Shenheng Guan joined him as Assistant Scholar Scientist to direct instrumentation and technique development. Alan left for Tallahassee on the same day that he submitted the FT-ICR MS Facility preproposal to NSF's newly created "Chemical Research Instrumentation" Program. A full proposal followed the next spring, and after a two-stage, competitive, peer review, NSF elected to fund the FT-ICR MS Facility at $5 million for 1994-1999, matched by $2 million from the State of Florida to acquire 9.4 T and 15-17 T superconducting magnets. In 1996, Marshall led an effort that resulted in an additional $600,000 grant from the W. M. Keck Foundation to develop a 25 T high-resolution resistive magnet. (The Keck magnet project has since been developed by Dr. Mark Bird (Magnet Development), Dr. Timothy Cross (NMR), and Dr. Louis-Claude Brunel (EMR).)

Organization and Operation. Prior national NMR and mass spectrometry facilities had typically been funded for three to five years, usually with a large complement of commercial instrumentation in the first year. As a result, after a few years, the equipment required updating, and new spectrometers and/or upgrade modules were requested when the project came up for renewal. In contrast, NHMFL's ICR Facility upgrades *continuously*, in both magnets (with obvious benefit from NHMFL's magnet expertise) as well as ICR hardware and software.

A second premise of the ICR Facility is a strong in-house (FSU and UF) FT-ICR MS research program, which ensures that new techniques (whether developed locally or elsewhere) are rapidly reduced to practice and made available to a wide user base. For example, the NHMFL ICR Facility is currently helping two new assistant professors (Neil Kelleher at University of Illinois and Michael Freitas at Ohio State University) to build their own FT-ICR spectrometers with special capabilities not commercially available. Based in part on their NHMFL results, Pat Limbach (Louisiana State University) and Troy Wood (State University of New York at Buffalo) each won Young Investigator Awards in 1998 from the American Society for Mass Spectrometry.

A third principle of the Facility is to operate with a minimum of permanent staff. Apart from Hendrickson and Emmett, the Tallahassee Facility employs one full-time machinist (Daniel McIntosh) and one full-time technician (John Quinn). Much of the external collaborative effort depends on postdoctoral fellows. The expertise developed at the Facility is thereby regularly exported back into the external community as each postdoctoral fellow leaves for a permanent position elsewhere.

One of the most successful features of the ICR Facility has been its visitor program, funded equally by NSF and the State of Florida at $60,000 per year. These funds provide economy air fare for visitors, and lodging at two permanently rented local apartments, so that a visitor can stay as long as it takes to complete a project. The Facility offers stipend support (six months for a graduate student or three months for a postdoc) for research involving an extended stay (a few weeks to a few months) at the Facility to develop new experiments and/or applications. The visitor budget is critically important in helping the Facility to attract users and develop external collaborations.

Service. The Facility provided pilot data for the University of California at Berkeley, contributing to their recent successful NSF proposal to acquire their own departmental FT-ICR mass spectrometer. NHMFL high-field data also triggered funding of FT-ICR instruments at the University of Illinois, Ohio State University, University of Maine, University of Florida, and the University of Konstanz (Germany). National 9.4 T FT-ICR MS Facilities modeled after the NHMFL are now

FT-ICR continued on page 14

FT-ICR continued from page 13

in place in England and Sweden. At the industrial level, the Facility provided data for Wyeth-Ayerst to justify their acquisition of the first 9.4 T industrial FT-ICR MS system; similar NHMFL data led to purchases of two FT-ICR MS systems each for Bayer and Ibis. The Facility is currently setting up the world's first fee-for-service FT-ICR MS, for commercial applications.

External Profile and Recognitions. The most important product of the ICR Facility's first five years of operation has been its 107 refereed publications/manuscripts (48 from external users and another 59 from the Facility "core" group), and more than 337 invited and contributed presentations (i.e., more than one per week at conferences and institutions; 115 from external users and another 222 from the Facility "core group"). Technical achievements from the ICR Facility have been featured more than 20 times in the past six years in (e.g.) *Science*, *Chemical & Engineering News* (including a cover feature), and *Analytical Chemistry*, as well as numerous trade publications from magnet, instrument, and chemical vendors. Since 1994, research carried out at the ICR Facility has contributed to four national awards for the P.I., plus two national awards and several local awards to ICR graduate students, and two national awards to Facility external users.

Technical Innovations. The ICR Facility's first magnet, the world's then highest field 9.4 T, was the first shielded ICR magnet (virtually all commercial FT-ICR magnets are now shielded). The magnet also included a "Gabrielse" stabilization coil, also now available commercially. The Facility's next ICR magnet (11 T) will be the first pumped-dewar ICR magnet (another feature likely to be imitated commercially). The Facility introduced external ion accumulation, a technique that provides for near-100% duty cycle to couple inherently continuous ion sources (e.g., electrospray ionization) to inherently pulsed ICR detection. The Facility has built six of its own data acquisition systems, and has exported another six to external users around the world. These and other technical innovations have enabled the ICR Facility to establish (and continue to hold) several world records for mass resolving power (unit mass resolution for a protein of 112,000 Da; sub-ppm mass accuracy throughout a wide-range mass spectrum of environmental mixtures; resolving power of ~10,000,000 for proteins up to 16,000 Da, allowing for resolution of isotopic "fine structure" from which the number of (e.g.) sulfur atoms in a protein can be counted directly; detection of biological components at concentrations as low as 10 attomoles per microliter; isotopic depletion to extend upper mass limit by an order of magnitude; and ultrahigh-resolution elemental analysis. The Facility has ordered a 15-17 T superconducting magnet that will become the world's highest-field for FT-ICR MS.

Analytical, Chemical, and Biological Applications. Various FT-ICR MS applications have been chronicled in *NHMFL Reports* and the *NHMFL Annual Reports*. One new direction for the next five-year grant period will be environmental and forensic applications. As one example, Figure 1 shows FT-ICR electron-ionization mass spectra of turpatine (the modern petroleum-based equivalent of turpentine formerly obtained from trees) and the extract from a couch onto which turpatine had been poured, burned, and doused. The ultrahigh resolution of FT-ICR makes it possible to identify *all* 190 species in the raw turpentine according to their unique chemical formulas ($C_cH_hO_o$). Moreover, 178 of the 190 species could be identified in the couch extract, positively proving that turpatine was the accelerant. Finally, an *additional* 350 chemically distinct species in the couch extract could be identified as pyrolysis products and constituents of the original fabric and stuffing. (The best match was obtained to turpatine that had been allowed to evaporate to 15% of its original volume, presumably because the heat of the fire volatilized much of the original accelerant.) It was even possible to distinguish between the same accelerants (e.g., mineral spirits) purchased from different suppliers. The Facility is working with the State of Florida Fire Marshal to

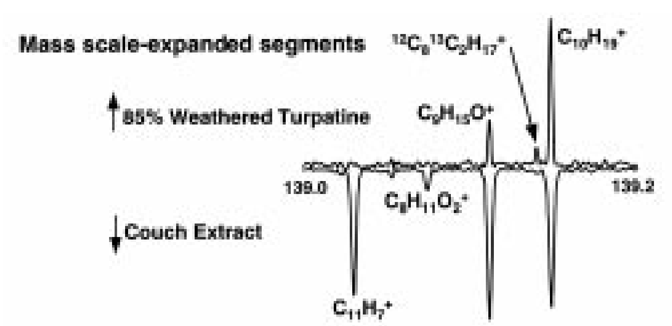


Figure 1.

develop an FT-ICR library of accelerants for use in future arson investigations.

Industrial Collaborations. The Facility has published with Dupont Marshall Lab on the composition of butylmethacrylate:glycidylmethacrylate copolymers used in automotive coatings (requiring ultrahigh mass resolution to distinguish the copolymer subunits at up to 7,000 Da), as well as a paper with Amoco on identification of components of crude oil distillates at 3 T, and a paper with Haldor-Topsoe (a Danish catalyst company) showing how to monitor the removal of dozens of sulfur-containing organics simultaneously at various stages of hydro-desulfurization catalysis (requiring broadband mass accuracy of ~300 ppb at 5.6 T). As another example, the Facility has just completed a project with DuPont Pharmaceuticals on H/D exchange to map the interaction surfaces in binary and tertiary complexes of p19:cyclin d2:cdk6, the enzyme complex that determines whether or not a biological cell will divide.

Education and Outreach. In 1997, the ICR Program hosted the first North American FT-ICR MS Conference at NHMFL in Tallahassee. That meeting drew approximately 90 non-local attendees, and brought virtually all of the leading North American (and some foreign) FT-ICR groups together. The attendees recommended that the meeting be repeated every two years, and the second North American FT-ICR MS Conference was held in March, 1999, in San Diego, with 128 attendees. One measure of interest is that $21,000 in support for that conference was contributed by all three FT-ICR mass spectrometer vendors (ThermoQuest, IonSpec, Bruker), three magnet vendors (IGC, Magnex, Oxford), as well as Isis (drug development) and Cambridge Isotopes.

Publication of the *ICR/Ion Trap Newsletter* moved to NHMFL with the P.I. on September 1, 1993. The newsletter, now in its fourteenth year of publication, is sent quarterly to 250 principal investigators, and probably circulates to several times that number of researchers. The newsletter connects the user community by exchange of technical contributions and problems, conference announcements, positions available announcements, etc.

The ICR Program has logged more than 26 student-semesters of undergraduate research, including several African-American students from Florida A&M University. One of our FAMU students (Ms. Kali-Nicole Hodge) went on to win an NSF Graduate Fellowship and is now a Ph.D. candidate at the University of Florida.

Placement of Former Graduates. The ICR Program has an excellent record of placing its Ph.D. and postdoctoral personnel as university faculty members and as senior researchers at government and industrial laboratories. A partial list over the past five years includes: Shenheng Guan (Symyx), Forest White (University of Virginia), George Jackson (PRIME Lab, Purdue University), Weiqun Li (Rigel), Stone Shi (SmithKline Beecham), Jared Drader (Isis), Ljiljana Pasa-Tolic (Battelle Pacific Northwest National Lab), Yulin Huang (PerSeptive), Michael Senko (Thermo), Touradj Solouki (University of Maine), Michael Freitas (Ohio State University), Guo-Zhong Li (Waters), Christopher Hendrickson (NHMFL), Mark Emmett (NHMFL), and Zhongqi Zhang (Amgen).

For further information on the ICR Program, contact Alan Marshall (850-644-0529, marshall@magnet.fsu.edu, fax 850-644-1366).

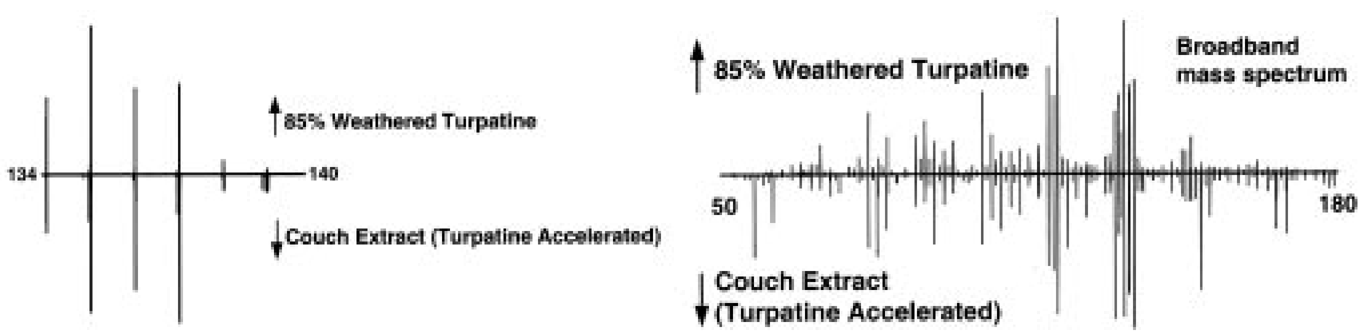


Figure 1. (Continued)

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