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NHMFL and Los Alamos National Laboratory Dedicate the World's Most Powerful Pulsed Magnet

The National Science Foundation and the U.S. Department of Energy celebrated a significant engineering achievement and a scientifically important partnership when the 60 T Long Pulse Magnet was commissioned on August 28 at the NHMFL facilities at Los Alamos National Laboratory (LANL). This unique user facility represents a 50 percent increase in peak-field capability over existing magnets of its class and offers unprecedented flexibility to experimentalists in pulse shape variability, duration, and experimental volume at peak field. Recent data obtained from the magnet is reported on page 8.

Over forty scientists and dignitaries attended the event, including Chancellor Adam Herbert of the Florida State University System; Dr. Robert Shelton, representing the University of California; LANL Director John Browne; NSF Science Advisor Karl Erb; Florida State University Vice President for Research Susan Allen; and University of Florida Interim Vice President for Research M. Jack Ohanian. In addition to the ribbon cutting ceremony (see photo), Browne recognized the accomplishments of the twenty members of the 60 T Magnet Development Team and awarded them the LANL Distinguished Performance Award (see NHMFL Reports, Summer Issue, for more information).

60 T LONG PULSE continued on page 4

Preparing to commission the 60 T Long Pulse Magnet are (left to right) LANL Director John Browne, NSF Science Advisor Karl Erb, and Chancellor Adam Herbert of the Florida State University System.

NHMFL Salutes New Nobel Laureates

Writing the official press release for the third international conference on Physical Phenomena at High Magnetic Fields (PPHMF-III), October 24-27, became an easy task when the Nobel Prize in physics was announced just ten days before the gathering. While we were expecting 200 leading scientists, we were delighted to learn that among the most distinguished guests and presenters would be two of the three new Nobel Prize winners in physics: Horst Störmer (Columbia University) and Robert C. Laughlin (Stanford University). Störmer and the third new Nobel laureate, Daniel Tsui (Princeton University), have been frequent users of the high field magnets in Tallahassee, and Störmer was an early user of the new ultra low temperature, high field facility at the University of Florida in Gainesville.

Robert Schrieffer and Klaus von Klitzing (on the right) congratulate new Nobel Laureates Horst Störmer and Robert Laughlin during opening dinner festivities at the laboratory, as part of the PPHMF-III conference.

The award recognizes research that Tsui and Störmer did together in 1982 at the Francis Bitter National Magnet Laboratory, and that was elaborated on by Laughlin the following year. Only one other Nobel Prize has come out of a magnet laboratory, and that was by Klaus von Klitzing of the Max Planck Institute,

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Supported by the National Science Foundation and the State of Florida

From the
Director's Desk

Congratulations!

As noted on the cover of this issue of NHMFL Reports, the announcement of the 1998 Nobel Prize in physics afforded the laboratory a nice opportunity to recognize the significant accomplishments of Horst Störmer, Daniel Tsui, and Robert Laughlin during the Physical Phenomena at High Magnetic Fields Conference. These new Nobelists have numerous friends and colleagues at the NHMFL, and rather than speak for them, I am pleased to use this space to present their comments and reflections.

Congratulations to the 1998 Nobelists for their discoveries leading to the opening of an exciting new frontier for quantum systems at the extremes of temperature and magnetic field.

Neil Sullivan, UF Physics Chair and NHMFL Co-Principal Investigator

The fractional quantum Hall effect requires the highest fields and lowest temperatures that are practical to use in combination. We can therefore be grateful to Horst, Dan, and their many collaborators and competitors for bringing some pizzazz to high field facilities. Horst has always pushed for improvements to high field facilities with the same energy and creativity with which he approaches his research. Dan Tsui seldom left Princeton to visit the Francis Bitter National Magnet Lab, except when one of his daughters was in college in Cambridge. But he somehow managed to collaborate with both Horst's group and a competing group for several years. Horst was a regular user of the FBNML, spending whole weeks at the lab in the early days and gradually turning the work over to students and postdocs. Both Dan and Horst provided advice in the early days of the NHMFL, for which we are grateful. We also enjoy their continuing visits and interest.

Bruce Brandt, Director NHMFL DC Field Facility

As a graduate student working for Professor Tsui and Professor Störmer, I am impressed that they always find time for their students no matter how busy they are.

Wei Pan, NHMFL

With warmest congratulations on your marvelous accomplishment.

Bob Schrieffer, NHMFL Chief Scientist

At MIT in 1982, when searching for a Ph.D. research topic, I quickly focussed on the recently discovered and very mysterious "fractional quantum Hall effect," observed in experiments requiring the highest magnetic fields available. After meeting with Horst and Dan, it became pretty clear that the next few years were to be both scientifically exciting and personally enjoyable. Those years exceeded expectations on all counts, thanks to the keen intellect, warm personality, and clever wit that Horst and Dan each possess.

In 1983, I picked up a copy of "Physical Review Letters" and, after reading just four pages, joined the rest of the world in suddenly understanding the physics underlying the fractional quantum Hall effect. In the most remarkable scientific paper that I have ever read, Bob Laughlin methodically explains how the collective behavior of electrons in a strong magnetic field gives rise to (smaller) fractional charges, even though the fractional charges are "built" out of integer-charged electrons. It is as if, in building a house out of bricks, one could somehow make the entire finished house to be smaller than a single brick!

The fractional quantum Hall effect is a striking manifestation of the bizarre quantum mechanics which results when huge numbers of particles behave collectively. Together, Horst, Dan and Bob have clearly proven that, in physics, "more is different."

Greg Boebinger, Director, NHMFL Pulsed Field Facility

And speaking on behalf of the laboratory:

Both Drs. Störmer and Tsui are not only great scientists—clearly established by the awarding of the Nobel Prize—but great citizens. Both Drs. Störmer and Tsui have given of their time to help the laboratory during its early years. Dr. Störmer was a member of our first User Committee and also chaired the committee and Dr. Tsui was a member of our Advisory Committee. We are very indebted to them for their leadership and guidance as this laboratory was being created.

Jack Crow, NHMFL Director

From the Chief Scientist's Desk

Conformational Properties of Neuropeptides by NMR

Arthur S. Edison, Department of Biochemistry & Molecular Biology, University of Florida; NHMFL; UF Center for Structural Biology, and University of Florida Brain Institute

In this issue Arthur Edison discusses the chemical complexity of the brain as measured by NMR spectroscopy. Using advanced techniques he has made excellent progress in characterizing the conformation of several free peptides, important constituents of brain function. He makes the exciting proposal that the modulations of the peptide-receptor interaction may lead to signaling in the brain. This is an excellent example of how high magnetic fields can make important advances possible in the biological area.

Robert Schrieffer

The anatomical complexity of the human brain is well appreciated. Over 10 billion neurons are associated through a vast network of chemical and electrical connections. Less well appreciated is the chemical complexity that is associated with the anatomical network. Several hundred small molecules—neurotransmitters or neuropeptides—have been identified in animal nervous systems. Many of these small molecules produce extremely potent and diverse effects.

Neuropeptides exist in three major biochemical states: as precursor proteins, as processed free peptides, and as receptor-bound peptides. My laboratory is using NMR spectroscopy to characterize the conformations of peptides in each of these biochemical states. In this report, we describe our recent advances in the characterization of processed free peptides. By comparing several different neuropeptides (Table 1), we have been able to develop a model that describes how the conformations of non-receptor-bound peptides can modulate their receptor interactions. We propose that these modulated interactions will lead to differential signaling in the brain.

Table 1: FMRFamide-like peptides used in this study

Peptide	Organism	Reference
GFGDEMSMPGVLRFa	Ascaris suum	Edison et al., 1997
SDMPGVLRFa	Ascaris suum	Edison et al., 1997
SMPGVLRFa	Ascaris suum	Edison et al., 1997
AVPGVLRFa	Ascaris suum	Edison et al., 1997
SDIGISEPNFLRFa	Ascaris suum	Cowden & Stretton, 1995
ASGDPNFLRFa	C. elegans	Rosoff et al., 1992
SDPFLRFa	Helix aspersa	Lutz et al., 1992; Price et al., 1990
GDPFLRFa	Helix aspersa	Lutz et al., 1992; Price et al., 1990
GYPFLRFa	H. aspersa Modified	Payza, 1987
pQYPFLRFa	H. aspersa Modified	Payza, 1987

The upper portions of Figure 1 show typical examples of sequential assignments, using the standard procedure developed by Wuthrich (1986). With the sequential assignments, we are able to compare differences in chemical shifts both within and between the subfamilies of similar peptides from Table 1. Peptides within subfamilies are often produced by the same gene and are active in the same cells. One goal is to see what, if any, changes occur in the conserved C-terminal (right hand) part of the peptides as functions of the N-terminal (left hand) end. We found that the "PGVLRF" subfamily was extremely uniform, regardless of the N-terminal substitutions. The "PNFLRF" subfamily was similar, except relatively large changes at the first phenylalanine (F). In contrast, the "PFLRF" subfamily had very large chemical shift changes that depended on the amino acid immediately preceding the proline (P). These qualitative patterns suggested to us that the sequence of aspartic acid-proline (DP) has a large influence on the conformations of these peptides in solution.

To further characterize the conformations of the peptides, we analyzed the patterns ROESY (Rotating frame Overhauser Effect Spectroscopy: Bothner-By et al., 1984) cross peaks to estimate distances between atoms. The lower portion of Figure 1 shows the ROESY amide to amide regions of two similar peptides, GDPFLRF-NH_2 and GYPFLRF-NH_2. Despite only a single amino acid change, these two peptides give rise to very different spectra. The patterns of peaks in the GDPFLRF-NH_2 spectrum between the first phenylalanine (F) to leucine (L) as well as L to arginine (R) are consistent with the presence of a significant fraction of reverse turn (Dyson et al., 1988).

NEUROPEPTIDES BY NMR continued on page 4

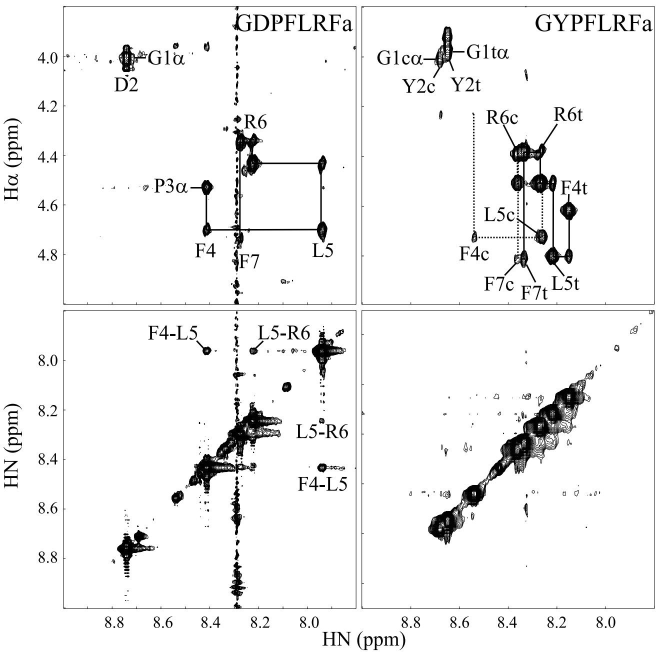

Figure 1. ROESY spectra of GDPFLRF-NH_2 and GYPFLRF-NH_2 neuropeptides. The top panels show the sequential assignments in the "fingerprint" region. The bottom panels show the amide proton region, which is indicative of conformations with compact structures like turns or helices. GDPFLRF-NH_2 has peaks that correspond to a trans DP peptide bond. GYPFLRF-NH_2 has two sets of peaks that correspond to mixtures of cis (c) and trans (t) DP peptide bonds. Not only are the patterns of chemical shifts quite different between these two peptides, but GYPFLRF-NH_2 has none of the amide interactions present in GDPFLRF-NH_2, suggesting that GYPFLRF-NH_2 has a higher population of extended structures in solution.

The details of the turn conformations were further explored with pH titrations. Changes in pH affect the ionization state of some amino acids, including aspartic acid (D) and glutamic acid (E). As seen in Figure 2, the DP-containing peptides (top two panels of Figure 2) have significant interactions between the D and the amino acid following the proline (F in the top and N in the middle). In contrast, the EP-containing peptide (bottom panel of Figure 2) shows very few inter-amino acid interactions. The sequence "DP" is often found in type I reverse turns, and the amino acid side chain of D often interacts with the amide group of the amino acid following the P (Wilmot and Thornton, 1988). By comparing the magnitude of the shift of the shifts of peaks with pH, we estimate that as much as 80% of the DP-containing peptides are in a turn (Bundi & Wüthrich, 1979).

The NMR data show that the DP-containing peptides have significant (e.g. 80%) populations of turns while the YP-containing peptides are predominantly extended with little or no turn. Functional data from previous studies have shown that the DP-containing peptides bind more weakly to receptors than their YP counterparts (Payza, 1987; Payza et al., 1989). Although we are unable to rule out direct differences in interactions with receptors, the functional and conformational data suggest that active concentration of the DP-containing peptides is reduced by an amount similar to the percentage of turn observed by NMR. Thus, we propose that the peptides are capable of "conformational inhibition," a process we have coined to describe how transient conformations of ligands in equilibrium can lower the effective concentration of that ligand for a particular

NEUROPEPTIDES BY NMR continued on page 5

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who also would be attending PPHMF-III. Certainly there was cause for celebration and Conference Chair Bob Schrieffer—himself a Nobel winner in 1972—and conference planners quickly moved to organize the appropriate event.

On the first evening of the conference, Saturday, October 24, conference participants gathered under the "old oak tree" at the laboratory for dinner and for a toast to the new Nobelists. For further comments and reflections on the prize-winning achievements, see From the Director's Desk, page 2.

60 T LONG PULSE continued from page 1

NHMFL co-principal investigators Crow, Parkin, and Sullivan also took the occasion to present NHMFL Distinguished Service Awards to LANL DX Division Director Robert Day and DX-6 Group Leader Richard Boudrie. The NHMFL reserves this award for its most significant supporters and replicas of the awards are on permanent display in the laboratory in Tallahassee. The inscriptions read as follows:

To Bob Day, in recognition of his enthusiastic support of the NHMFL during its formative years. Due to his interest and involvement with the NHMFL, the Pulsed Field Facility at Los Alamos National Laboratory has become a world recognized leader in high field research.

To Richard Boudrie, in recognition of his promotion of the NHMFL and his effective leadership role during the successful construction and testing of the 60 tesla quasi-continuous magnet at Los Alamos National Laboratory. His support and enthusiasm for the NHMFL program was an inspiration to all who worked on the program.

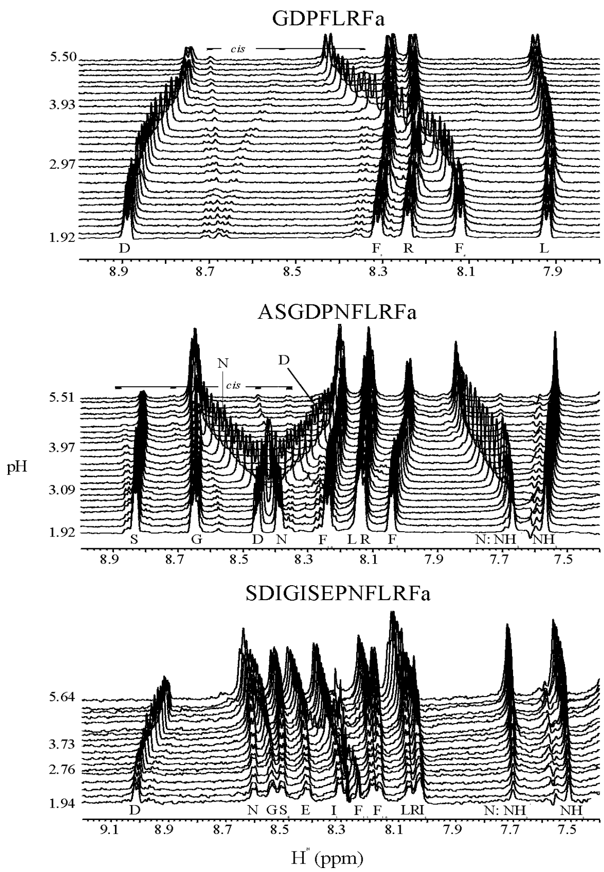

Figure 2. pH titrations of three different neuropeptides, with and without DP in their sequences. The top two series of spectra demonstrate significant interactions between the side chain carboxylates of the aspartic acids (D) and the amino acids following the proline, as evidenced by significant downfield shifts at higher pH. Another naturally occurring neuropeptide, SDIGISEPNFLRF-NH_2, shows very different behavior, despite the fact that glutamic acid (E) is only one carbon longer than aspartic acid. Therefore, the DP-containing peptides (but not the EP peptide) are able to form interactions that strongly suggest that they form high populations of reverse turns in solution.

receptor. The effects of lowered ligand conformations to receptor-bound populations are shown in Figure 3.

Of course, other receptors might exist that would prefer the turn conformation over the extended conformation. If such receptors exist, differential signaling would result. Peptide signaling is very complex and only beginning to be unraveled. The diverse functions produced by many peptides strongly suggest that many mechanisms exist to diversify the activity of peptides. Conformational inhibition might be one of these mechanisms and may be crucial to a detailed understanding of neuropeptide structure-function relations.

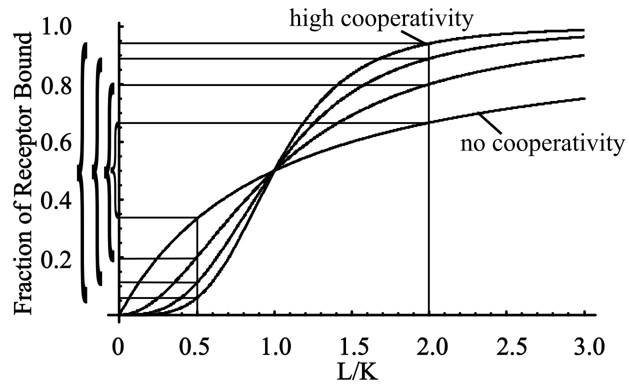

Figure 3. Binding curves showing the effect of lowering the concentration of ligand on the fraction of bound receptors. The horizontal axis is divided by the equilibrium dissociation binding constant. The different curves represent different degrees of binding cooperativity, ranging from none to highly cooperative (Hill coefficient of 4). The vertical lines represent our estimates of the decrease in active ligand concentration resulting from the population of turn in solution for the DP-containing peptides. This change in active ligand concentration will translate into a drop in receptor activation that ranges from about 0.3 (no cooperativity) to nearly 1 (high cooperativity).

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The Magnet Lab Open House

The NHMFL's dedication in October 1994 was the occasion of the first open house of the laboratory. Its success helped area residents and businesses alike get to know the new science and technology center "in the neighborhood" and to begin to understand its potential to enhance education and local, state, and regional economic development.

This year, at the 5th Annual Open House of the NHMFL on October 3rd, we were very pleased to incorporate many of our community partners in science and education, including ODYSSEY Science Center, Sea-to-Sea Program, FSU Chemistry, St. Marks Wildlife Refuge, Gulf Specimen Marine Laboratory, and many others. In addition, we launched the **First Annual NHMFL Youth Science & Art Contest** in partnership with Leon, Wakulla, and Gadsden county schools. These new activities were extremely well received and are likely to be repeated.

Becoming An Annual Community Science Event

NHMFL faculty were not to be outdone by the new groups, however, and presented a myriad of interesting, informative activities that demonstrated the fascinating and sometimes even fun world of science. “A picture is worth a thousand words” so we’ll let the accompanying images show more about the excitement and energy of **NHMFL Open House–1998**.

ATTENTION USERS

Alex H. Lacerda
Pulsed Field Facility User Programs

Gregory S. Boebinger
Pulsed Field Facility Director

Scientific Impact of the NHMFL 60 Tesla Long Pulse Magnet

One of the key features of the new 60 tesla (T) Long Pulse magnet at the NHMFL is the incredible flexibility offered to experimentalists to tailor the magnetic-field pulse shape in response to the demands of the experiment. The magnet can be pulsed every hour and the magnetic-field pulse shape can be changed from pulse to pulse at the wishes of the experimentalist. Pulse shapes already delivered to experiments include "flat-top" pulses in which the magnetic field has been held constant at 60 T for as long as 100 milliseconds (msec), at 50 T for 200 msec, and at 40 T for 500 msec. Smooth magnetic field sweeps from 60 T down to 0 T have been demonstrated to last more than two seconds. More recently, stair-step pulse shapes have been developed for specific heat measurements.

Experiments completed to date already have demonstrated the potential of this magnet to revolutionize research using pulsed magnetic fields. In addition to expected improvements in electron transport and magnetization experiments, optics experiments have been able to record over 1000 low-intensity (less than 500 microwatts illumination) photoluminescence spectra during a single magnetic field pulse, providing a "video" of the spectral evolution in response to the magnetic field. Experiments of this type have been performed on semi-magnetic quantum wells by Scott Crooker, Yongmin Kim, and Florin Munteanu and were the topic of an article in the Summer 1998 Issue of the NHFML Reports. These experiments provide an opportunity to reach the quantum limit of a two-dimensional electron layer in a system containing manganese impurities. The magnetic moments of the manganese impurities are expected to locally polarize the electron spins that play a role in the formation of integer and fractional quantum Hall states.

The first experiments on the 60 T long-pulse magnet by an external user have utilized these same techniques to find evidence of a new excitonic state in the anomalous photoluminescence spectrum observed at high magnetic fields. X. Lee and H.W. Jiang from UCLA collaborated with W.J. Schaff from Cornell and Y. Kim at the NHMFL-LANL to measure the photoluminescence of a high-density GaAs/AlGaAs heterostructure up to 60 T. Due to the high electron density, two subbands of the heterostructure are populated and the Fermi level, E_F , lies just above the second subband. The sample was placed in a helium three refrigerator and held at 400 mK during the pulse. The NHMFL's fast, fiber-optics data acquisition system (developed by Yongmin Kim, Clive Perry, and Scott Crooker) was used to collect the data shown in Figure 1. Magnetotransport data was taken simultaneously on the sample. Due to the proximity of E_F to the second subband, it requires little energy for the equilibrium two-dimensional system to interact strongly with the photo-excited, non-equilibrium electrons and holes. Thus, electrons can be rearranged near the photo-excited holes to form a many-body excitonic state (a Mahan exciton). The data show a good correlation with the calculated dependence

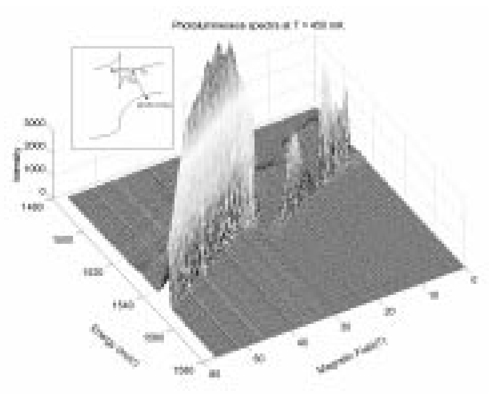


Figure 1. Photoluminescence spectra of the high density (n = $1.3\times10^{12}/cm^2$) GaAs/AlGaAs heterostructure at a bath temperature of 450 mK.

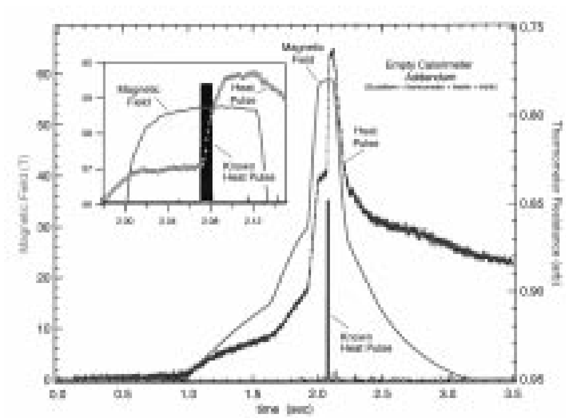


Figure 2. First heat capacity data utilizing the 60 T Long Pulse magnet on a single crystal of a metallic $YbInCu_4$

of the Fermi energy on the magnetic field; however, the most striking feature in the data is the unexpected emission line that appears suddenly at a critical field near 30 T. This magnetic field corresponds to a filling factor of ν=2 for the equilibrium two-dimensional electron system and the new emission line exhibits a giant red-shift in energy (>10 meV). It is believed that the new line is a spin-polarized exciton state that results once the photo-excited holes undergo a phase transition from a free state to a spatially localized bound state (much like the Mott transition). This transition is a consequence of the competition between the built-in repulsive potential of the heterostructure and the attractive potential of the electrons that can occur in high magnetic fields due to the strong reduction of the screening strength in the quantum limit. A manuscript describing this work has been recently submitted to *Physical Review Letters*.

Perhaps the most spectacular experimental achievement to date has been the recently demonstrated capability to make sensitive specific heat measurements in pulsed magnetic fields. While the magnetic field was fixed, experimentalists were able to inject a known amount of energy into a sample and record the temperature rise of the sample—five times during a single magnetic field pulse! Since a changing magnetic field injects uncontrolled amounts of energy into a sample, specific heat measurements were impossible in pulsed magnetic fields prior to the successful commissioning of the 60 T Long Pulse magnet.

The specific heat measurement technique was developed by M. Jaime and R. Movshovich from LANL; W. Beyermann from UC Riverside; and G. Stewart from U Florida using funding from a successful proposal submitted to the NHMFL In-House Research Program. A heat pulse method is used to measure the heat capacity, where a known amount of heat is delivered to the sample using a chip resistor as a heater element. The heat capacity of the sample, C(T), is determined as the ratio of the heat delivered to the sample and the change in its temperature. The flat-top magnetic field pulse allows the heat capacity cell and sample to reach thermal equilibrium before and after the applied heat pulse. Figure 2 shows the data collected during the very first specific heat experiment at 60 T, when successful determination of the addendum heat capacity (of the empty cell consisting of the platform, heater, thermometer and leads) was performed at a temperature of 3.9 K. The known heat pulse is delivered to the cell in the middle of the magnetic field plateau at 59 T. The cell comes to equilibrium before and after the heat pulse, all within the 120 msec of the field plateau at 60 T.

Subsequent experiments were performed on a single crystal of a metallic $YbInCu_4$. This system has a first order valence phase transition at 40 K in zero field, which can be suppressed down to 4 K with field of about 33 T. When thermal relaxation (equilibrium) time of the cell is much smaller than the duration of the flat-top plateau, a sequence of heat pulses can be delivered to the sample to measure a series of C(T) data at fixed magnetic field during a single magnetic field pulse, as illustrated in Figure 3(a) for the field of 20 T. Data at B=0 T and 20 T taken in 0.5 seconds using this technique are shown in Figure 3(b). The zero field data is in excellent agreement with previously available data using conventional techniques. The magnitude of the cubic term due to phonons is field-independent as expected.

There is another way to increase the data acquisition rate during a specific heat experiment: A series of plateaus at different magnetic fields can be produced within a single pulse. As shown in Figure 4, a pulse designed to have four plateaus at 25, 30, 35, and 40 T, each 130 msec long, was produced by the 60 T Long Pulse magnet team led by J. Schillig. At each of the magnetic field plateaus the heat capacity measurement of $YbInCu_4$ was performed. Note that as the field was changed between 30 and 35 T through the first order phase boundary, the temperature of the sample is observed to go down on the up-sweep, and up on the down-sweep, due to magneto-caloric effect. These features are very sharp, and allow direct determination of the phase diagram of $YbInCu_4$.

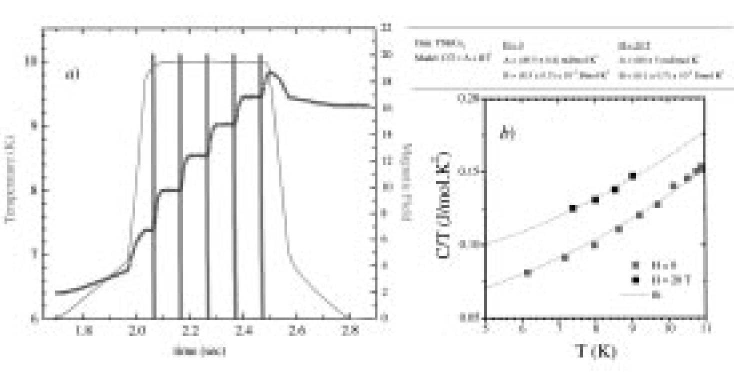


Figure 3 (a). Sequence of heat pulses during a 20 T flat top pulse.
Figure 3 (b). C/T vs. T at 0 and 20 T of $YbInCu_4$

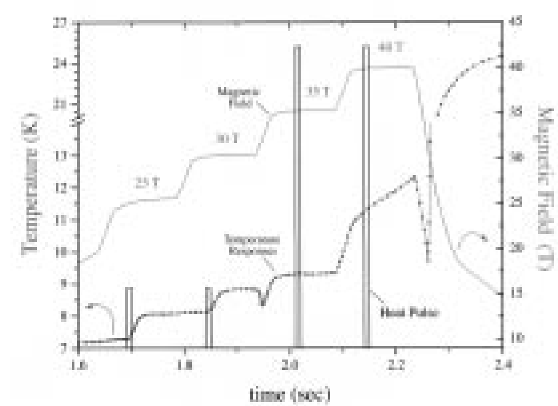


Figure 4. The magnetic field plateaus are at 25, 30, 35 and 40 T, each 130 msec long. The heat pulses are measured in temperature vs. time. The data is $YbInCu_4$ temperature responses.

People in the News

The NHMFL is enormously pleased to report that **Director Jack Crow** and **Deputy Director Hans Schneider-Muntau** were recently elected as Fellows of the American Association for the Advancement of Science. AAAS is among the oldest societies in America, having been founded in Philadelphia in 1848. Many of today's most prestigious and influential scientific societies, including the American Chemical Society (1876) and the American Anthropological Association (1902), have their historical origins in AAAS.

Crow was cited "For fundamental contributions in studies of superconducting materials, and for his leadership as founder and director of the NSF National High Magnetic Field Laboratory."

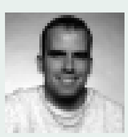
Schneider-Muntau was cited "For original and record-setting design and construction of many of the world's highest-field and highest-performance magnets for research in physics, chemistry, and biology."

Andrew Rinzler is a new Assistant Professor of Physics at the University of Florida. Rinzler is a condensed matter experimentalist specializing in nanoscale structures and is an expert on electron field emission studies of nanotubes. He joins the NHMFL extended family at UF after working as a postdoctoral associate for Nobel Laureate Richard Smalley at Rice University. Rinzler is currently building a new laboratory in the new physics building at UF.

Justin Schwartz, Associate Professor of Mechanical Engineering at Florida State University and head of the MST-HTS group at the NHMFL, won the 1998 Roger W. Boom Award given by the Cryogenic Society of America. This award, named for a distinguished University of Wisconsin–Madison professor, recognizes young scientists who "show promise for making significant contributions to the fields of cryogenic engineering and applied superconductivity." Schwartz was selected for his work within a university/laboratory setting and in collaboration with industry. His activities have focused on the development of high temperature superconductors for high field systems including NMR, MagLev, and energy storage technologies.

Stone D.-H. Shi, a member of Alan Marshall's ICR-MS group at the NHMFL, was selected to receive the Society for Applied Spectroscopy 1998 Graduate Student Award for "outstanding research in the field of spectroscopy." This national award was presented at the 1998 Federation of Analytical Chemistry and Spectroscopy Societies meeting in Austin, Texas, on October 13. Official announcements will appear in upcoming issues of Applied Spectroscopy and Analytical Chemistry.

The recent research activities of Shi, ICR-MS Instrumentation Director Christopher L. Hendrickson, and Professor Marshall will appear as a paper entitled "Sulfur atoms in a protein counted by weighing" in the Proceedings of the National Academy of Sciences [95, 11532 (1998)], and as a "concentrate" in Chemical and Engineering News [70, 702A (Nov. 1, 1998)]. These results also appeared in the Spring 1998 Issue of NHMFL Reports.



Other members of the NHMFL ICR program are receiving similar recognitions: A recent issue of the American Chemical Society journal, Analytical Chemistry, included a short feature on the recent development by FSU Ph.D. students, **Ryan Rodgers** and **Forest M. White** (now a postdoc at the University of Virginia), and NHMFL machinist, **Dan McIntosh**, of an FT-ICR instrument dedicated to analysis of complex volatile mixtures, such as petroleum distillates. This feature is the twelfth such nationally distributed article on the NHMFL's ICR Program in the last five years. Marshall recently applauded the graduate students, postdoctoral fellows, and staff of the ICR Program for their creativity and hard work in producing the fine research that has triggered these recognitions.

Optimizing High-Strength Conductors

F. Heringhaus, NHMFL, Institut für Metallkunde und Metallphysik, RWTH Aachen, and Degussa AG, Hanau, Germany (as of Fall 1998)
H.-J. Schneider-Muntau, NHMFL
G. Gottstein, Institut für Metallkunde und Metallphysik, RWTH Aachen

For many applications, materials are needed that satisfy a defined set of properties. These combinations of properties are typically not found within one material or alloy, and composites are required. Among composites are those that comply with the rule-of-mixtures (ROM), i.e., they linearly combine the properties of their constituents, and those that disagree with the ROM. For high strength conductors, as applied in high-field Bitter and pulse magnets, this disagreement provides the potential for new achievements in combinations of high mechanical strength and high electrical conductivity.

Two almost classical examples for these so-called microcomposites are Cu-Nb and Cu-Ag. Upon solidification, both typically reveal two-phase microstructures, consisting of pure Nb embedded in a practically pure Cu matrix (Fig. 1) respectively a combination of proeutectic, Cu-rich dendrites and eutectic Ag-Cu (Fig. 2). During plastic deformation, this structure refines and the density of internal interfaces increases accordingly. The observed deviations from the ROM are due to the influence of the internal interfaces, which may be strongly different for different properties. From the dependence of each property on the characteristic microstructural parameter, the optimal microstructural state for the desired combination of properties can be determined. The following requirements apply: First, the appropriate microstructural parameter needs to be such that it can be varied and adjusted to specification. As for Cu-Nb and Cu-Ag composites, this can be achieved through plastic deformation. Second, the microstructural parameter needs to be quantifiable. For this, both scanning (compare Fig. 1 and 2) and transmission (compare Fig. 3 and 4) electron microscopy are invaluable tools. Third, an analytic expression needs to be found that describes the development of the property, P, as a function of the microstructural parameter. Fourth, as a normalization factor, in order to account for the microstructural effects only, the ROM value for the property needs to be known. This can be achieved by simultaneously processing and investigating pure Cu, Nb, and Ag wires.

With $\tilde{P}$ being the normalized property, the optimal microstructure (MS) can then be found at the minimum of a cost function, C(MS), (Eq. 1) that accounts for the relative importance of the different properties for a given application. For an equal-weight

Figure 1. Nb dendrites (light) embedded in Cu matrix. SEM micrograph.

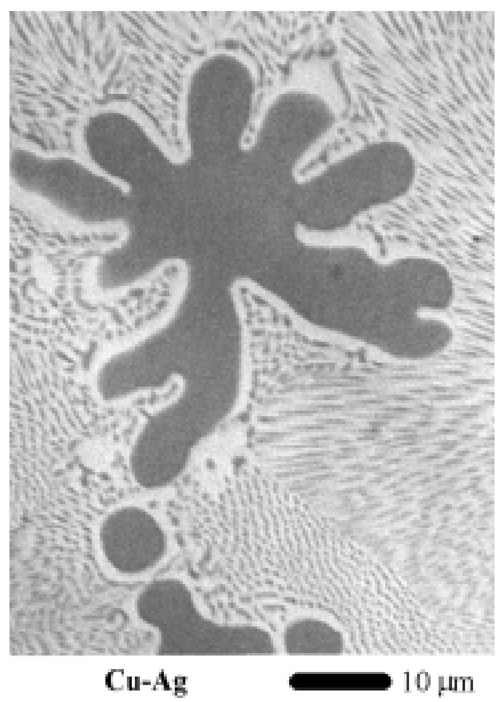


Figure 2. Proeutectic, Cu-rich dendrites (dark) embedded in eutectic Ag-Cu. SEM micrograph.

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Figure 3. Nb filaments (arrows) in Cu matrix.[3] TEM micrograph.

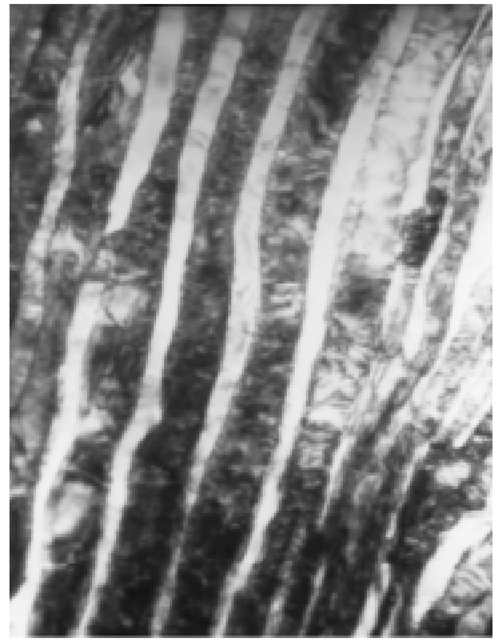


Figure 4. Ag (dark) and Cu lamellae. TEM micrograph.

combination of high ultimate tensile strength and low electrical resistivity of eutectic Ag-Cu at 77 K, the optimum lamella thickness is 16 nm (compare Fig. 5 at 0,0). The cost function can be solved for an unlimited number of combinations of n properties. The parameter, k_{ij}, represents the desired ratio of the derivatives of the properties i and j, and m_{ij} represents the weight factor given to this combination. These parameters allow for the consideration of design preferences or application-dependent restrictions. Non-trivial solutions for more than one combination of properties, i.e., more than two properties, will lead to a minimum of C(MS) greater than zero. The value of C_{min} can then be viewed as quantifying the inherent contradictions in the desired properties.[1,2] This is the reason for which the optimal lamella thickness increases with any increase in the weight factor of a combination of properties (Fig. 5). Furthermore, this increase is the stronger the more contradictory the properties of this combination are. With the data currently available, this optimization can be carried out for a number of mechanical, electrical, and thermal properties of Cu-20%Nb and eutectic Ag-Cu. Further experiments on the proeutectic, Cu-rich phase need to be carried out to complete the spectrum of available data on Cu-Nb and Cu-Ag micro-composites.

$$C(MS) = \sum_{\substack{i=1 \\ j>i}}^{n-1} \left[m_{ij}{}^{*} \left(\frac{d\tilde{P}_i}{d\tilde{P}_j} - k_{ij} \right)^2 \right] \qquad (1)$$

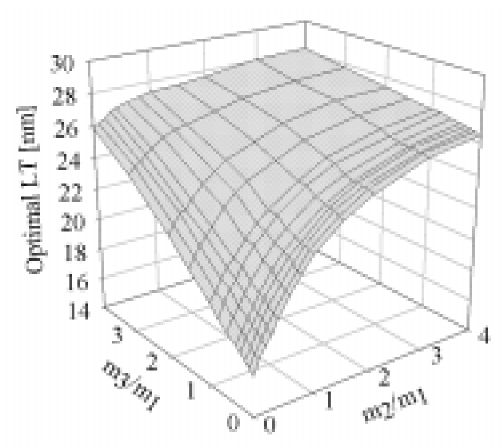


Figure 5. Optimal lamella thickness (LT) of eutectic Ag-Cu for combinations of ultimate tensile strength, electrical resistivity, and thermal resistivity at 77 K as a function of the relative weight of their respective ratios. All k_{ij} are unity. The weight factors are m_1 for a combination of UTS and electrical resistivity, m_2 for UTS and thermal resistivity, and m_3 for electrical resistivity and thermal resistivity.[1,2]

References:

1 Heringhaus, F., et al., Advances in Cryogenic Engineering, in press.
2 Heringhaus, F., Dissertation, 1998, RWTH Aachen, Germany.
3 Hangen, U., Master's thesis, 1994, RWTH Aachen, Germany.

Conference and Workshop Activity

As months go, October 1998 will surely be recorded as one of the busiest months in the history of the laboratory. It started with the 5th Annual NHMFL Open House—which attracted over 3,100 visitors—and ended with the semi-annual gathering of NHMFL Users Committee and back-to-back major international conferences. We view the conferences, in particular, as exceptionally important opportunities to build the user community, expand and enrich the science and technology dialogue, and develop new partnerships with the private sector.

VIII^th International Conference on Megagauss Magnetic Field Generation and Related Topics

October 18-23, 1998
NHMFL, Tallahassee

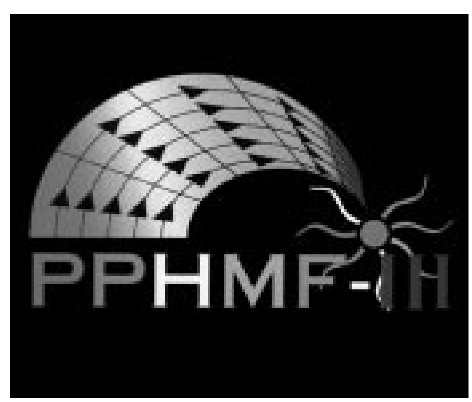
Over 175 scientists from Russia, the United States, and other countries met to discuss the generation of ultra-high magnetic fields and their peaceful applications at this five-day conference. The conference chair was NHMFL Deputy Director Hans Schneider-Muntau, who was recently elected to the American Association for the Advancement of Science. Also attending was the vice president of the Russian Academy of Science, Professor V. Fortov, who previously served as the Russian Minister for Research and Science.

The opening presentation, "From Swords to Plowshares: The U.S./Russian Collaboration in High Energy Density Physics Using Pulsed Power," was given by Steve Younger, a program director at Los Alamos National Laboratory in New Mexico and a distinguished leader in high field research. Younger is the founder and director of the Center for International Security Affairs, which coordinates with Russia, China, and other countries on cooperative programs focused on defense conversion and nuclear material control. He discussed the importance and scientific potential of the conversion of cold war military assets to non-defense applications, and remarked that "since 1992, the nuclear weapons laboratories of the United States and Russia have been working together in fundamental research related to pulsed power and high energy density science. This collaboration...has enabled scientists formerly engaged in weapons activities to redirect their attention to peaceful pursuits of wide benefit to the technical community."

The Megagauss conference series initiated the first scientific exchanges between the research centers at Los Alamos and Arzamas 16 in Russia and resulted in the Dirac Series of ultra-high field experiments that were conducted at Los Alamos in 1996 and 1997. More information on these experiments may be found in the Summer 1998 Issue of NHMFL Reports. Conference proceedings will be published; contact Jo Ann Palmer (850-644-1933, palmerj@magnet.fsu.edu, fax 850-644-8350) for more information.

Physical Phenomena at High Magnetic Fields (PPHMF-III)

October 24-27, 1998
NHMFL, Tallahassee



Megagauss VIII and PPHMF-III were planned back-to-back intentionally because many of the interesting science and research developments in these areas overlap. Approximately 30 participants took advantage of this opportunity and attended all or part of both conferences.

CONFERENCES continued on page 14

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Among the over 200 PPHMF-III participants were two of the three new Nobel Prize winners in physics, Horst Störmer (Columbia University) and Robert C. Laughlin (Stanford University). (See pages 1 and 2 for further details.)

The conference chairman was NHMFL Chief Scientist Robert Schrieffer—himself a Nobel winner in 1972—and a fourth Nobel laureate, Klaus von Klitzing of the Max Planck Institute in Stuttgart, Germany, chaired one of the sessions. The conference was first hosted by the NHMFL in 1991 and has become a major scientific event, as it brings together experts to assess ongoing research, new directions for science and technology, and the uses of high magnetic fields in both basic and applied research.

Proceedings of the conference will be published; contact Mary Layne (850-644-3203, layne@magnet.fsu.edu, fax 850-644-5038) for more information.

BF Goodrich Meeting

February 1999
NHMFL, Tallahassee

Over 50 corporate executives who lead NMR research departments will meet in Tallahassee at the NHMFL for their annual meeting. The group is interested in touring the laboratory and learning more about the research underway. Senior scientists from the NHMFL's Center for Interdisciplinary Magnetic Resonance will present a series of talks to the corporate representatives.

Second North American FT-ICR Mass Spectrometry Conference

March 18-20, 1999
U.S. Grant Hotel
San Diego, California

Planning continues on this conference, which will be held at a lovely hotel in downtown San Diego. The conference will include invited oral and poster presentations (all plenary), as well as contributed posters. All oral and poster abstracts should be submitted by February 1, 1999. A website is being developed; look for more information on the Internet http://www.magnet.fsu.edu/whatsnew or contact Jo Ann Palmer (850-644-1933, palmerj@magnet.fsu.edu, fax 850-644-8350).

16th International Conference on Magnet Technology (MT-16)

September 26-October 1, 1999
Leon County Civic Center
NHMFL, Tallahassee

This conference will bring together approximately 500 scientists, engineers, and experts from around the world to focus on the latest developments in technology, operation, applications of research and industrial magnets, and magnet materials. The first announcement has been released; the second announcement is due out in January, 1999. The abstract deadline is June 15, 1999; the early registration deadline (with payment) is August 15, 1999. Information is available on the web (http://www.magnet.fsu.edu/whatsnew) or by contacting Jo Ann Palmer (850-644-1933, mt@magnet.fsu.edu, fax 850-644-8350).

30th Southeastern Magnetic Resonance Conference (SEMRC)

October 1999
NHMFL, Tallahassee

Planning is underway for this conference, which will feature invited and contributed papers and posters in NMR, MRI, EPR, and ICR. Topics will include time-resolved and multidimensional spectroscopies, high magnetic fields, and applications of magnetic resonance technologies in materials science, physics, chemistry, biology, and medicine. For further information e-mail semrc@magnet.fsu.edu or fax 850-644-8350.

EMR Workshop in Washington, D.C.

The NHMFL, Pacific Northwest National Laboratory, and the Albert Einstein College of Medicine sponsored an important new workshop, **High Frequency Electron Magnetic Resonance: Scientific Opportunities and Challenges,** in Washington D.C., on September 17-18. The workshop was by invitation only and fifty scientists from academia and national laboratories, along with representatives of the several U.S. funding agencies, participated in the meeting.

This workshop explored the changing face of science in the next two decades and discussed the unique contributions that HFEMR can make in solving significant scientific and societal problems. Talks by six outstanding scientists on the key issues in their disciplines sparked extended discussions in parallel working groups. The working groups identified how the unique capabilities of HFEMR can best address these scientific issues and what direction HFEMR must take to meet future needs in the broad areas of structural and functional biology; chemistry and biophysics; and materials science and physics.

NATIONAL MAGNETIC RESONANCE COLLABORATORIUM

A Report by the Committee for HIGH FIELD NMR: A NEW MILLENNIUM RESOURCE

The next generation of high field NMR magnets along with advances in spectrometer hardware and spectroscopy experiments have the potential to revolutionize NMR spectroscopy once again. This technology is likely to be in the hands of relatively few scientists unless a new approach for distributing the hardware is developed. A report that addresses this challenge, developed by a group of NMR spectroscopists following a meeting in Washington, D.C. this past January, has been written and submitted to the National Science Foundation, the National Institutes of Health, and the Department of Energy for their consideration. This report recommends the establishment of a National Magnetic Resonance Collaboratorium (NMRC) comprising ten Sectors or NMR facilities with next generation NMR spectrometers. The NMRC, a virtual laboratory or "center without walls," would network collaborations among sites and the nation's scientific communities. Below is a description of the science drivers for high resolution NMR spectroscopy at high fields. These drivers are described in the context of four scientific frontiers selected to illustrate a wide range of scientific challenges: Beyond the Genome, Gene Regulation, Neuroscience, and New Materials.

Scientific Agenda

Beyond the Genome. By the year 2005, 100,000 amino acid sequences representing the proteins of the human genome will be known. This is just one of several genomes currently being sequenced. Each protein performs one or more specific functions, often accomplished via complex mechanisms, and the best approach to modifying function (as important for laboratory bench chemistry as for medicine) is understanding the mechanisms. Describing complex mechanisms and reaction kinetics requires a detailed knowledge of structure, dynamics, and chemical properties. Structure prediction methods based on sequence homology will lead to low resolution structural models for many of the protein sequences. It is anticipated, however, that 3,000 to 10,000 experimental structures will need to be determined to identify all of the structural families in the human proteome. The dynamic properties of individual proteins and their chemical properties (activities) will be more difficult to predict. Although NMR is playing an increasingly important role in such characterizations the rate of NMR data collection and analysis must accelerate to meet the challenges. New instrumentation and methodology will lead to better structures and more accurate descriptions of dynamics and chemical properties of proteins; they also will extend the NMR approach to larger and more interesting proteins and nucleic acids, potentially doubling the current size limit. Indeed,

MILLENNIUM continued on page 16

Committee for
High Field NMR: A New Millennium Resource

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Peter E. Wright, Scripps Research Institute

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at field strengths in the vicinity of 25 to 30 T (1.1 to 1.3 GHz) the spectral quality may become virtually independent of the molecular weight, allowing for spectroscopic studies of much larger proteins. NMR is already the technique of choice for experimentally defining molecular dynamics. The magnetic fields recommended for support in this report will substantially extend field dependent studies.

Gene Regulation. Tremendously complicated molecular machinery is involved in gene regulation and other cellular activities. Understanding regulatory processes is key to developing methods to regain control of aberrant processes, to treat disease, and to manipulate cells for new functions in biotechnology. Biochemical activities are regulated by ligand and protein binding processes that result in changed conformation, dynamics, or stability. Macromolecular complexes consisting of RNA, DNA, and proteins constitute molecular machines. The structural and dynamic characterization of these molecular complexes is an essential part of understanding their activity and interconnectivity. While domain structures rather than intact proteins can be used in studies of complex formation, the NMR molecular weight limit for structure determination is easily exceeded when a structural picture of the whole system is desired. Higher fields, new probe technology, novel isotope labeling strategies, and data collection protocols will dramatically expand the range of molecular structure that can be approached by solution NMR. Indeed, not only is there potential at high fields for the molecular weight limit to dissipate, but signal averaging time decreases in proportion to the B_o^3 and spectral resolution improves in proportion to B_o^3.

Neuroscience. The human brain has 30 x 10^9 synapses that are tightly regulated. Communications across these synapses are primarily regulated by membrane proteins. In fact, 30% of the human genome represents membrane and membrane-associated proteins for which there is a paucity of structural and dynamic information. Without this knowledge, we have been unable to obtain a functional understanding of synapses at the atomic level. Membranes form a spectacular two-dimensional array of molecular activities that is very different from the three-dimensional world of mobile water soluble proteins. The heterogeneity of the membrane environment, however, has prevented routine crystallization required for x-ray crystallography and the formation of isotropic solutions needed for solution NMR analysis. Solid-state NMR, which has no correlation time limit or crystallization requirement, thus is arguably the most promising approach for high resolution structural and dynamic characterizations of these proteins. A recent high resolution polypeptide structure in a lipid environment and recent spectra of uniformly labeled membrane proteins clearly demonstrate this potential for solid state NMR. Other heterogeneous structures such as ß-amyloid, the putative cause of Alzheimer's disease also has been studied by solid state NMR. The prospects of greatly improved sensitivity and resolution discussed above are critical for the continued advances in solid-state NMR investigations of the structure and dynamics of macromolecules in heterogeneous environments. Novel tools from molecular biology and emerging developments in NMR instrumentation and methodology combine to poise the field at a stage where new knowledge and understanding about membrane proteins are ready to be harvested.

New Materials. The development of new materials is limited less by synthetic chemistry than by our current ability to characterize the structure, molecular dynamics, chemical kinetics, and reactivity of products. A unique feature of NMR is its ability to characterize samples in various condensed matter states, from liquids to mesophases (such as liquid crystals and biological membranes) to solids. New materials of interest include, structural composites, coatings, and catalysts, and each presents great challenges for their characterization. For NMR, sensitivity is, once again, of paramount importance. Surface, rather than bulk samples, by definition, will provide fewer nuclei to be observed, but recent developments in the methods of dynamic nuclear polarization and optically pumped polarization transfer promise greatly enhanced NMR sensitivity from surfaces. Today, precise control and manipulation of material architecture on the atomic scale are fundamentally important. Lessons learned from biological systems and manipulation of biological systems to produce materials of interest are active arenas for research. Despite much effort, such synthetic and semisynthetic materials are typically heterogeneous in nature, and NMR is virtually the only high resolution tool that can be used when sample heterogeneity is significant. Even natural materials such as the remarkably strong and flexible fibers of silk, are heterogeneous, and although silk was recognized early on as being predominantly ß-sheet the details of its structure and its functional ramifications are only now being elucidated by solid state NMR. High fields not only yield improved sensitivity and resolution, but changes in relaxation times, isolation of spin interactions and improved acoustic properties of NMR probes will permit the detection of spectra unobtainable at lower fields.

For more information on the NMRC, contact Tim Cross, 850-644-0917, cross@magnet.fsu.edu.

NHMFL Partner EURUS Recognized as Entrepreneurial Business & Technology Leader

The NHMFL established its first on-site partnership with EURUS Technologies in 1996 following a magnet technology conference held at the laboratory. They relocated to Tallahassee in March, 1997, and the partnership has been strengthened by their close proximity to the laboratory. We are extremely pleased to share news of their recent awards, as reported to us by General Manager John Romans.

1998 has represented an exciting year of successful research and recognition for EURUS Technologies, Inc. and its subsidiary Plastronic, Inc. In addition to completing two federally sponsored Small Business Innovative Research (SBIR) grants, and receiving three new research grants, EURUS has been nominated for the 1998 Governor's Business Leadership Award and Technology Business of the Year by the State of Florida. In addition, Plastronic, Inc., has been selected as a winner of the 1998 Emerging Technology Award, presented by the Ohio Department of Development and the Thomas Edison Program.

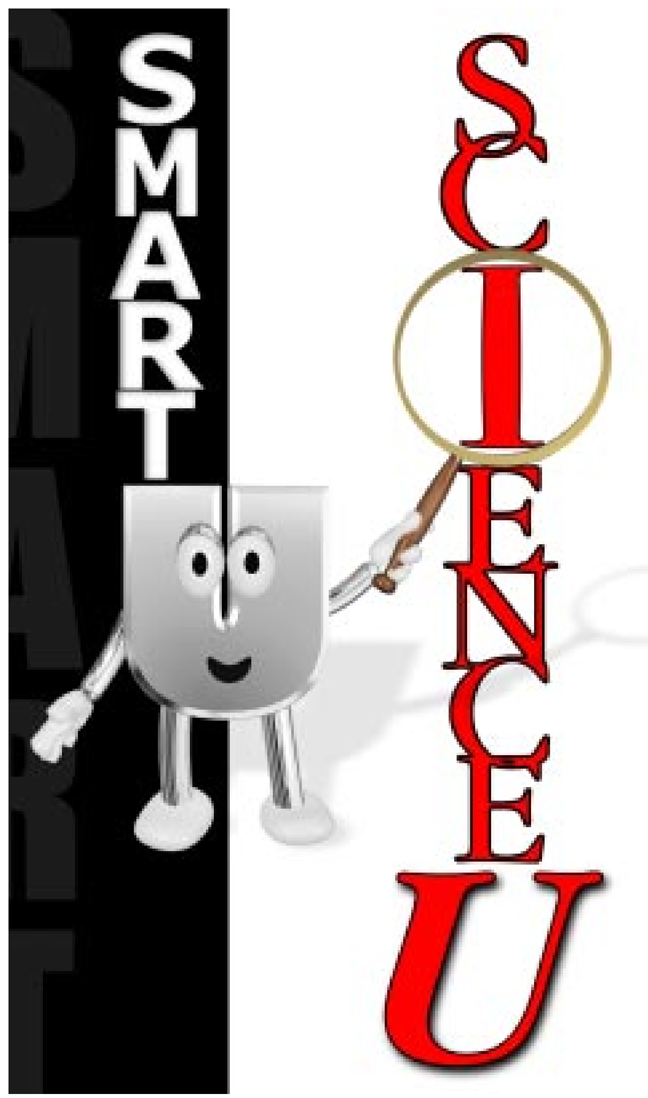
The Governor's Business Leadership Award recognizes outstanding economic contributions made by Florida businesses while the Emerging Technology Award recognizes companies in Ohio that are successfully developing and advancing innovative technologies. Plastronic, Inc. is one of six companies that was honored with the 1998 Emerging Technology Award by Governor George Voinovich at the annual Edison Award reception held September 17 at the Great Lakes Science Center in Cleveland, Ohio.

"Special congratulations go out to Mike Tomsic, President of Plastronic, and the rest of the EURUS team for their ongoing efforts to maintain our position as the low cost leader in HTS wire," commented Lyn Adams, President and CEO of EURUS. "We are honored to be recognized for the present and future economic impact of this revolutionary technology and the systems it will enable in the deregulating electric power industry."

For further information about EURUS, contact John Romans, 800-850-1135, fax 850-574-1800, Jromans@TeamEURUS.com.

NHMFL Joins Statewide Campaign Against Tobacco Use

The State of Florida, through the Department of Health's Office of Tobacco Control, recently awarded $1.6 million to the National High Magnetic Field Laboratory at Florida State University to produce a science education program on tobacco use prevention. **Science U** was kicked off on November 10, 1998, with a statewide Virtual Town Hall Meeting, and will culminate with the distribution in March, 1999, of new science curriculum materials to 1,475 elementary schools in Florida.



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***TOBACCO* continued from page 17**

NHMFL Director of Education Programs Sam Spiegel spoke recently on the importance of this new initiative and its potential to affect change: "Tobacco use is the most preventable cause of disease and premature death today, and people begin to use it very early in life. This situation demands solutions that integrate state, federal, business, school, and institutional resources to address the problem by providing programs that change the way students and teachers deal with tobacco prevention. To this end, we are extremely proud to be developing Science U and hope to see it expanded nationwide at some time in the future."

Funding for the program comes as a result of state's lawsuit against the tobacco companies earlier this year. The $13 billion settlement, to be paid over 25 years, included an additional $200 million for the establishment of an anti-tobacco pilot program. In April of this year, the results of Florida's first Youth Tobacco Survey conducted by the Florida Pilot Program noted that more than 35 percent of the state's high school and nearly one-quarter of the state's middle-school students use some form of tobacco. Partly as a result of these findings, the comprehensive new learning resource Science U is being focused toward 4th and 5th grade students and teachers. By arming this age group with information, skills, and resources—presented in various multimedia formats—the program aims to reduce the use of tobacco products as the students move through the middle school years.

Science U is being developed by the NHMFL's Center for Integrating Research and Learning in partnership with Training Solutions Interactive, Inc. It is a multidisciplinary, multisensory science resource that will include the Virtual Town Hall, web-based resources, interactive CD-ROM, an electronically published student and teacher guidebook, hands-on activities, and teacher training. Through these various media, students will be

able to explore and understand (1) the harmful effects of tobacco on their bodies through scientific analysis and investigation, (2) strategies for handling peer pressure to use tobacco, and (3) the role that advertising plays in promoting addiction.

For example, students using the CD-ROM will have opportunities to create a virtual image of themselves (a “virtual you”) through which they can observe the potential effects of tobacco use over time. The student will be able to place a digital image of his or her face onto the virtual body and select physical attributes such as skin tone. Once the virtual self is created, the student can operate an MRI system and view images of his or her lungs based on tobacco use. The student also can image the brain and other vital organs, noting the effects of tobacco use. Additionally, students will see changes in physical ability, like lung capacity, that result from smoking.

Science U was introduced at a statewide Virtual Town Hall Meeting on November 10. This telecast was beamed via satellite to schools, regional science centers, and local colleges and universities from the laboratory at Florida State University. The program began with a 45-minute broadcast where expert panel members, celebrity guests, and local students discussed issues of tobacco use from a scientific orientation. Students from across the state joined the discussion with local groups and through the website (http://smartu.fsu.edu). The expert panel included Dr. Jeffery Wigand, former V.P. of Research and Development for Brown & Williamson Tobacco Company. Wigand achieved national prominence in 1995 when he became the tobacco industry’s highest ranking former executive to address public health and smoking issues during an interview on 60 Minutes and in a legal deposition. Celebrity guests included, among others, Florida Governor Lawton Chiles, UF Football Coach Steve Spurrier, NSYNC, and Gabrielle Resse.

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