OMINAF Highlights

National Facilities

- **CHESS**
- **CHRNS**
- **IMR – MIP**
- **NHMFL**
- **NNIN**
- **SRC**

MRI

CHESS Highlights

Control of Myosin (Muscles) by Kinases
Zongchao Jia (Queen's, Kingston ON), CA Inst. Of Health, NSERC, DMR-0936384

Automated spin-assisted layer-by-layer assembly of nanocomposites
Hart and Hammond (U. Mich., M.I.T.), CMMI-0800213, DMR-0936384

Portable X-ray Station for Outreach and Education
P. Revesz, K. Spoth (REU) (CHESS), DMR-0225180

Interaction between Supersonic Disintegrating Liquid Jets and Their Shock Waves
Wang and Gruner (Argonne Nat. Lab, Cornell), DOE, CHESS DMR-0936384

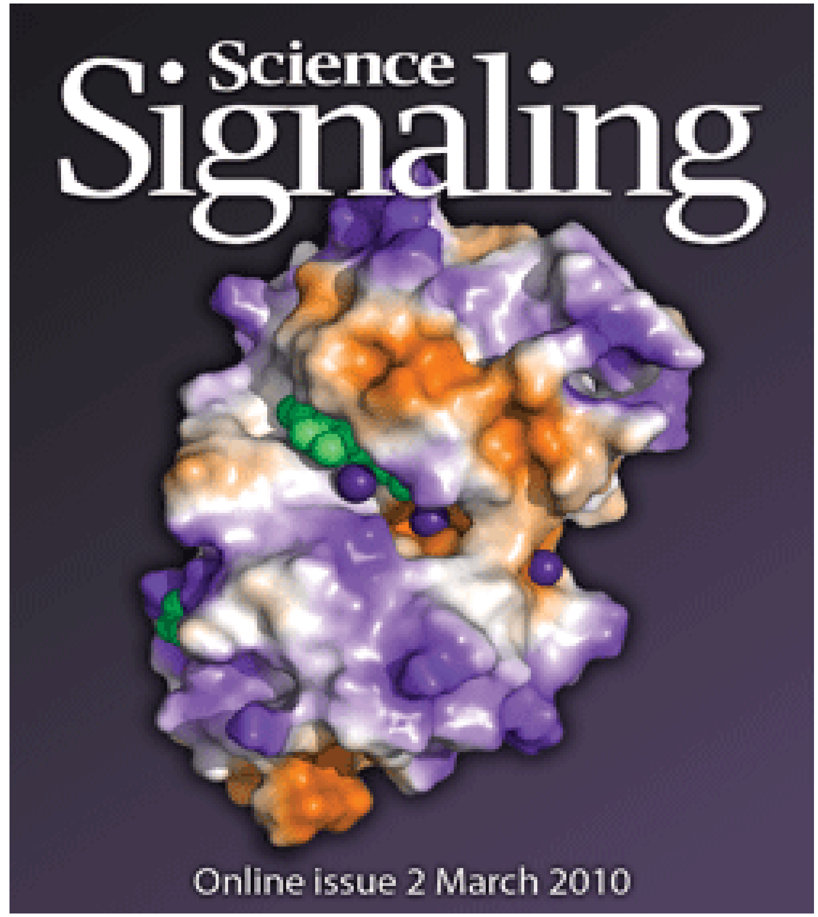
Measurements of Surface Diffusivity and Coarsening during Pulsed Laser Deposition
Ferguson, Brock (Cornell Univ., Ithaca NY), DMR-0705361

Control of Myosin (Muscles) by Kinases

Zongchao Jia (Queen's, Kingston ON), CA Inst. Of Health, NSERC

Intellectual Merit: In order for muscles to generate contractile force, myosin molecules must be assembled into filaments, and the assembly is regulated by proteins called myosin heavy chain kinases (MHCK's). Jia's group used CHESS to get the first detailed look at the structure of several complexes of the MHCK A catalytic domain (A-CAT), providing new insights into the regulatory functions of a-kinases.

"Crystal Structure of the α-kinase Domain of Dictyostelium Myosin Heavy Chain Kinase A"; Q. Ye, S.W. Crawley, Y. Yang, G.P. Côté, and Z. Jia, Science Signaling (2010), Vol. 3, ra17.

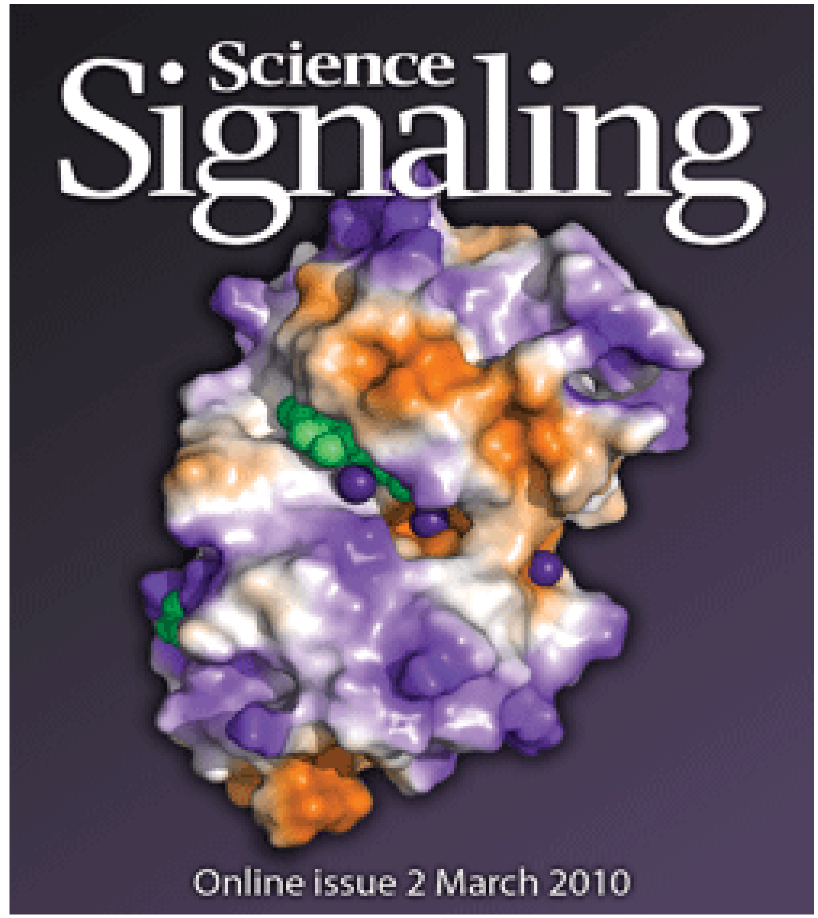


Journal cover image showing the newly determined electrostatic potential surface of A-CAT.

Control of Myosin (Muscles) by Kinases

Zongchao Jia (Queen's, Kingston ON), CA Inst. Of Health, NSERC

Broader Impact: The protein myosin is essential for the contraction of muscles, and is also used by non-muscle cells to move and reshape themselves and is found in all cells in the body. To generate contractile force, myosin molecules must be assembled into filaments, and the assembly is regulated by proteins called myosin heavy chain kinases (MHCK's). Jia's group used CHESS to advance understanding of these critical proteins.



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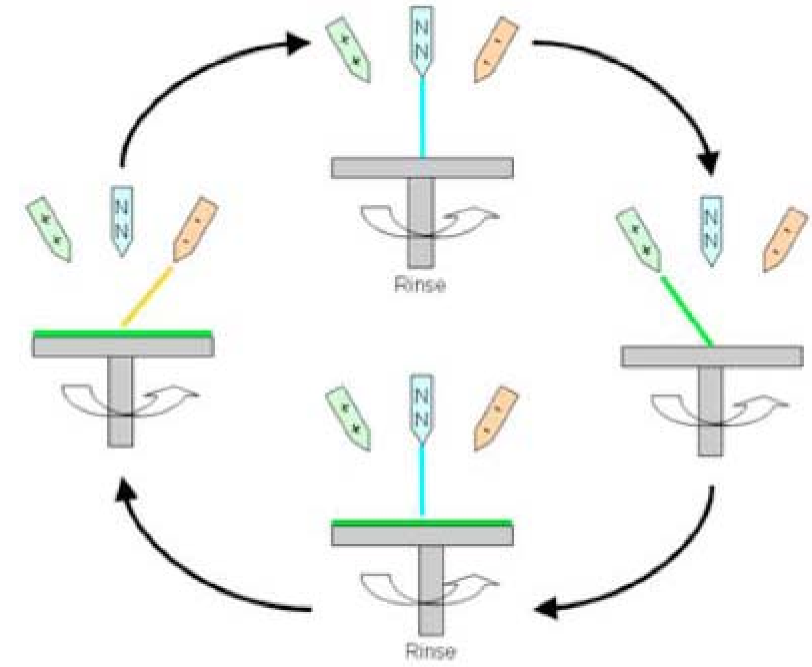
Automated spin-assisted layer-by-layer assembly of nanocomposites

Hart and Hammond (U. Mich., M.I.T.), CMMI-0800213

Intellectual Merit: Collaborating groups of Hart (University of Michigan) and Hammond (M.I.T.) designed and tested a novel desktop system for the automated production of nanostructured thin films via spin-assisted layer-by-layer (spin-LBL) assembly. The utility of this system is demonstrated by fabricating polyvinyl alcohol/clay nanocomposites. Ellipsometry measurements demonstrate that the automated spin-LBL method creates composites with bilayer thicknesses and growth rates comparable to traditional dip-LBL; however, the cycle time of their new spin-LBL method is an order of magnitude faster. Small angle x-ray scattering analysis shows that the clay platelets in spin-LBL nanocomposites are more highly aligned than in dip-LBL composites – thus better ordered structures can result.



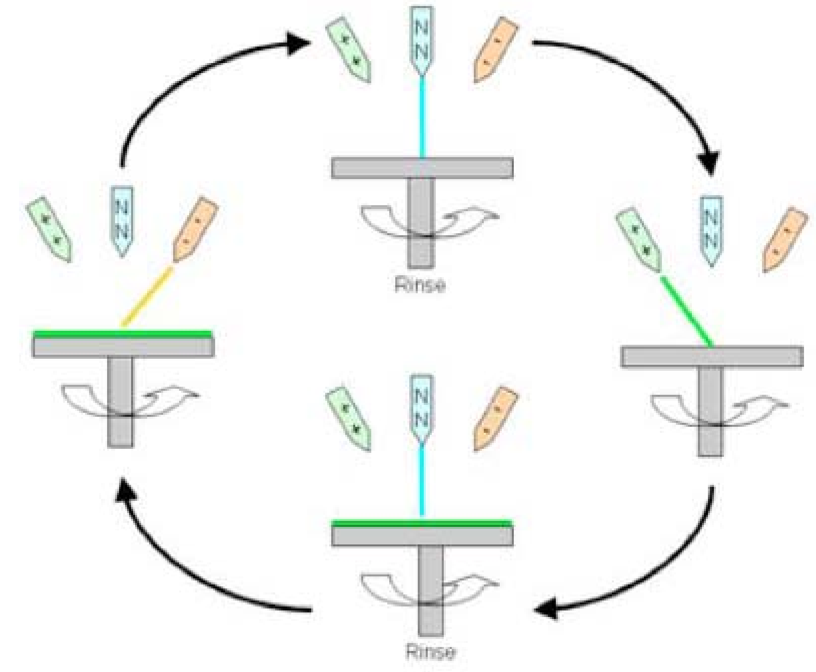
Spin-assisted chemical layer-by-layer deposition of a thin film, wherein alternating compounds are injected onto a rotating substrate.

Steven Vozar, Yeh-Chuin Poh, Thomas Serbowicz, Matthew Bachner, Paul Podsiadlo, Ming Qin, Eric Verploegen, Nicholas Kotov, and A. John Hart, "Automated spin-assisted layer-by-layer assembly of nanocomposites," Review Of Scientific Instruments 80, 023903, 2009.

Automated spin-assisted layer-by-layer assembly of nanocomposites

Hart and Hammond (U. Mich., M.I.T.), CMMI-0800213

Broader Impacts: The layer-by-layer growth process is an important technological tool and has been used to create nanostructured materials for myriad applications including structural composites, filtration membranes, functional coatings, tissue scaffolds, solar cells, and batteries. The automated system invented by these investigators can significantly increase the throughput of laboratory-scale LBL discovery and processing, can enable testing of functional properties of LBL nanocomposites over wafer-scale areas, and can be scaled to larger substrates for commercial production.



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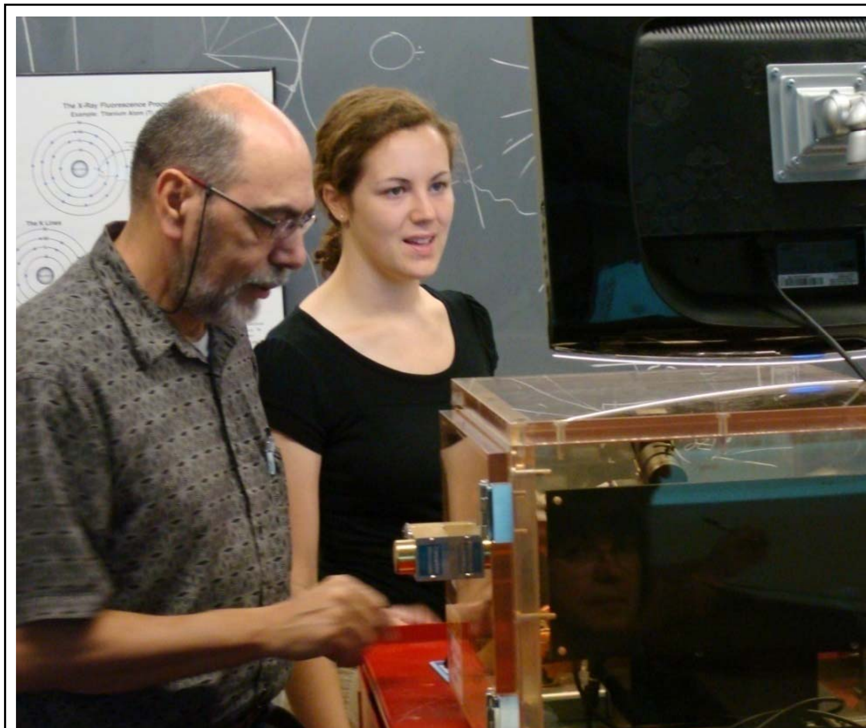
Portable X-ray Station for Outreach and Education

P. Revesz, K. Spoth (REU) (CHESS), DMR-0225180

Broader Impacts: CHESS has developed a mobile station for performing x-ray fluorescence (XRF) measurements for outreach and teaching. XRF is an excellent way to teach introductory x-ray physics because it is a method that is simple to explain and quick to carry out; a sample's composition can be determined within a matter of minutes. To do this, CHESS built a portable, roll-around station that lets students and teachers bring specimens of interest, mount them on a stage they can move with a remote joystick, and create x-ray fluorescence histogram plots. From these plots, students can identify elements present in a sample. The portable XRF unit has been used to test common household items such as cosmetics, jewelry, and small toys to determine if they also contain hazardous elements, such as lead or mercury.

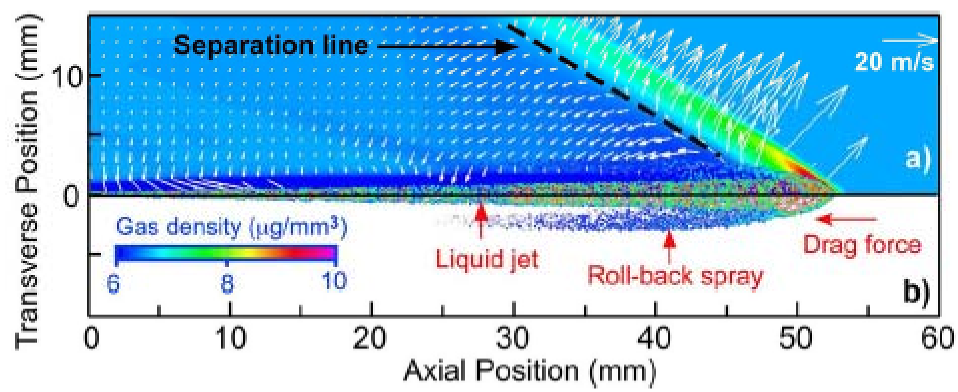


REU student Katherine Spoth uses the XRF station to teach a lesson to visiting high-school teachers. CHESS staff scientist Peter Revesz, above, demonstrates how to lock the door to the shielded enclosure before turning on the x-ray generator.

Interaction between Supersonic Disintegrating Liquid Jets and Their Shock Waves

Wang and Gruner (Argonne Nat. Lab, Cornell), DOE, CHESS

Intellectual Merit: A collaboration of groups led by Wang (Argonne National Laboratory) and Gruner (Cornell) has measured, for the first time, the dynamic behavior of shock waves generated by and interacting with a supersonic and disintegrating-liquid jet. They used ultrafast x-radiography to capture images of the shock waves, and developed a new time-resolved multiphase fluid dynamics simulation method to study the data. The agreement between the simulation and the data implies that the 3-dimensional transient multiphase simulation can be applied to understand the fluid dynamics in many other systems, such as shock-wave induced microbubble jetting, primary breakup modeling, and cavitating flows.



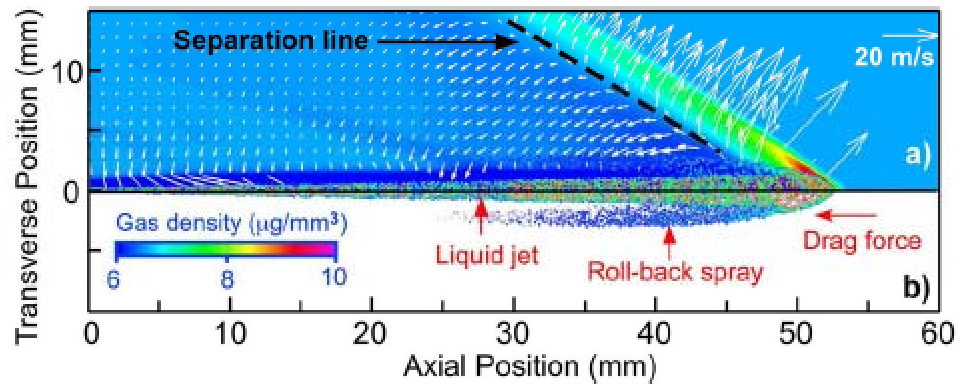
Transient multiphase simulation results on aerodynamic behavior and internal structure of the shock waves superimposed with gas phase velocity vectors and gas density distributions measured by x-radiography.

Kyoung-Su Im, Seong-Kyun Cheong, X. Liu, and Jin Wang, Ming-Chia Lai, Mark W. Tate, Alper Ercan, Matthew J. Renzi, Daniel R. Schuette, and Sol M. Gruner, "Interaction between Supersonic Disintegrating Liquid Jets and Their Shock Waves," PRL 102, 074501 (2009).

Interaction between Supersonic Disintegrating Liquid Jets and Their Shock Waves

Wang and Gruner (Argonne Nat. Lab, Cornell), DOE, CHESS

Broader Impact: This work demonstrated that high-speed x-radiography can be used to capture unique information about transient shock waves in the presence of high-density dispersing and disintegrating supersonic liquid jets. This work addresses a historical dearth in experimental, theoretical, and computational methods needed to improve application of high-pressure and high-speed liquid jets. For instance, in modern diesel engines, shock waves may be common under engine operating conditions. The interactions between the shock waves and the disintegrating fuel jets can ultimately affect the fuel breakup and, thus, the combustion efficiency and emission.



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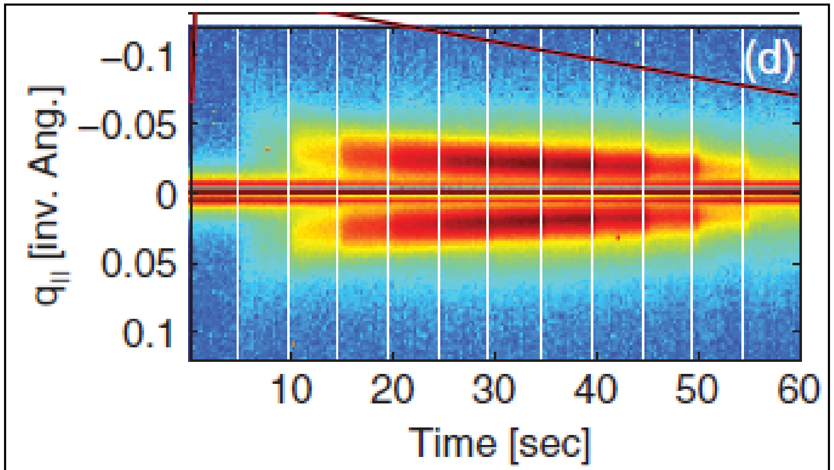
Kyoung-Su Im, Seong-Kyun Cheong, X. Liu, and Jin Wang, Ming-Chia Lai, Mark W. Tate, Alper Ercan, Matthew J. Renzi, Daniel R. Schuette, and Sol M. Gruner, "Interaction between Supersonic Disintegrating Liquid Jets and Their Shock Waves," PRL 102, 074501 (2009).

Measurements of Surface Diffusivity and Coarsening during Pulsed Laser Deposition

Ferguson, Brock (Cornell Univ., Ithaca NY), DMR-0705361

Intellectual Merit:

Pulsed laser deposition is an important method to grow nearly atomically perfect refractory materials. However, the mechanisms promoting smooth growth are not well understood. Using time-resolve x-ray diffraction recorded during the layer-by-layer growth of a strontium titanate, Brock's group (Cornell) and CHESS scientists have been able to test and refine theories about the growth of complex oxide materials using pulsed laser deposition. They were able to see islands nucleating as early as 200 milliseconds after the first laser pulse, and follow the island coarsening subsequently. Their analysis produced independent estimates of the interlayer and intralayer diffusion of mobile species between pulses and placed constraints on several well-known theoretical values.



Diffuse x-ray scattering during the pulsed-laser deposition of $SrTiO_3$. Vertical lines represent the laser pulses (first pulse at 5 s).

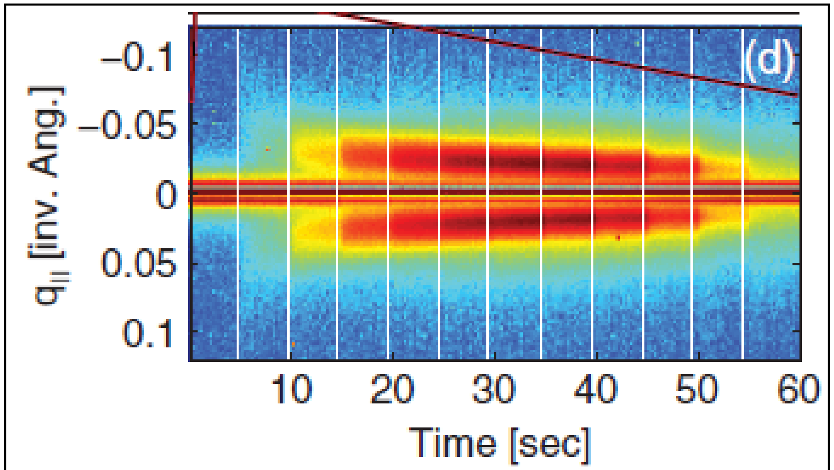
J. D. Ferguson, G. Arikan, D. S. Dale, A. R. Woll, and J. D. Brock, "Measurements of Surface Diffusivity and Coarsening during Pulsed Laser Deposition," PRL 103, 256103 (2009).

Measurements of Surface Diffusivity and Coarsening during Pulsed Laser Deposition

Ferguson, Brock (Cornell Univ., Ithaca NY), DMR-0705361

Broader Impacts:

Growing novel materials has been the foundation of technological advances with magnetic, laser and other high-tech materials. Understanding how these materials grow has been exceptionally difficult because of the strong nonequilibrium nature of these dynamic systems. This work demonstrated how x-ray diffraction is a valuable quantitative tool to study in-situ dynamic phenomena of crystal growth without altering the basic mechanisms (a non-destructive technique). This study was able to distinguish between smoothing mechanisms during complex-oxide growth based on "island breakup," in which an energetic impinging material breaks up existing islands, and "enhanced downhill transport", where material detaches from islands and then becomes mobile.



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CHRNS Highlights: Dan Neumann, NIST, DMR- 0454672

Bilayer membrane dynamics in nonsteroidal anti-inflammatory drugphospholipid adducts

Core-Shell Magnetic Morphology of Structurally Uniform Magnetite Nanoparticles

Electric Field Control of Magnetization in a Multiferroic

Education and Outreach Summer Undergraduate Research Fellowship Program

Building the next generation of neutron scatterers

Testing composition gradients in shear banding flows using in situ neutron transmission profiling

How Does the Stiffness of Lipid Vesicles Change as They Interact with Poreforming Peptides?

Multiple Filling of Voids Improves Thermoelectric Efficiency of Skutterudites

Summer Institute for Middle School Science Teachers

Activities for students and faculty

Record in Neutron Detection: High Intensity Cold Neutron Spectrometer with Multichannel Analyzer

Bilayer membrane dynamics in nonsteroidal anti-inflammatory drug-phospholipid adducts

DMR-0454672
CMMI-0708096

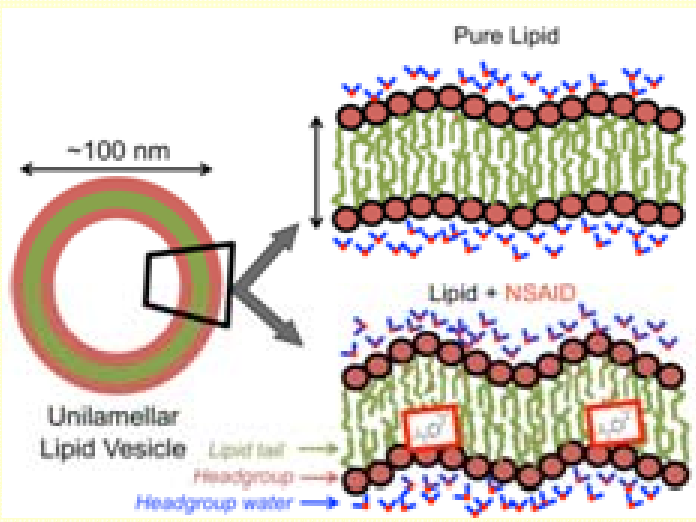
M.B. Boggara[1], Antonio Faraone[2] and Ramanan Krishnamoorti[1]

[1]University of Houston; [2]NIST Center for Neutron Research

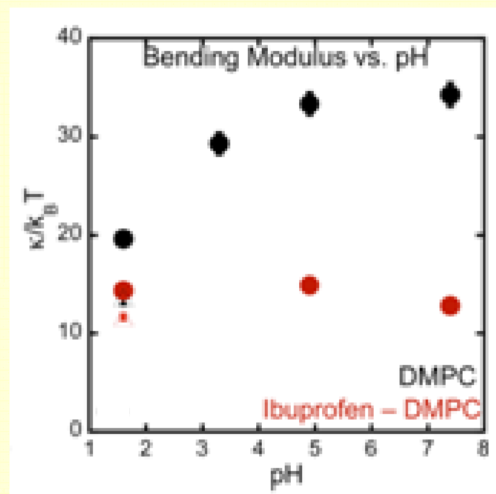
Most drug molecules, such as nonsteroidal anti-inflammatory drugs (NSAIDs), interact with the cell membranes to exert their therapeutic action. Understanding the effect of drugs on the elastic properties of cellular membranes is therefore important: *(a) in understanding specific disease situations* as well as *(b) in developing drug-bilayer adducts for applications such as targeted drug delivery or biosensors.*

Using a combination of NSE along with structural studies based on SANS and MD simulations, we have examined changes in the bending modulus k (a measure of the membrane's elasticity), for DMPC-based membranes, both with pH and with addition of ibuprofen, a popular NSAID. Significantly, we observe effects related to lipid interactions, headgroup hydration, bilayer thinning, and reduced area compression modulus.

This work is an important first step to understand at the molecular level how NSAIDs might be causing ulcers as well as creating lipid-based systems for targeted delivery of such NSAIDs to inflammation sites.



Sketch describing the lipid vesicles used for experiments (left) and the bilayer fluctuations for pure lipid bilayer and bilayer with drugs incorporated (right).



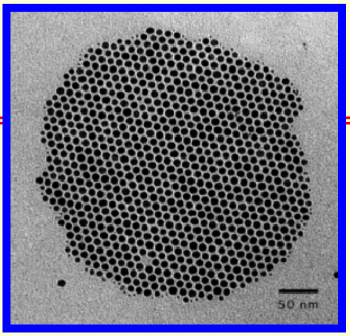
Membrane bending moduli (k) as a function of pH for DMPC and ibuprofen – DMPC (mole ratio 0.31/1) at 30 ˚C (solid circles). Also shown are the data for pH ≈ 1.6 and 37 ˚C (open triangles).

M.B. Boggara, A. Faraone, R. Krishnamoorti , J. Phys. Chem. B, 114, 8061 (2010).

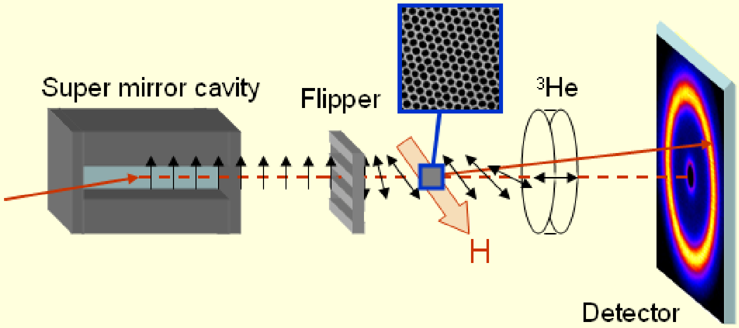
Core-Shell Magnetic Morphology of Structurally Uniform Magnetite Nanoparticles

K.L. Krycka[1], R.A. Booth[2], C.R. Hogg[2], Y. Ijiri[3], J.A. Borchers[1], W.C. Chen[1],4, S.M. Watson[1], M. Laver[5], T.R. Gentile[1], L.R. Dedon[3], S. Harris[3], J.J. Rhyne[6], S.A. Majetich[2]

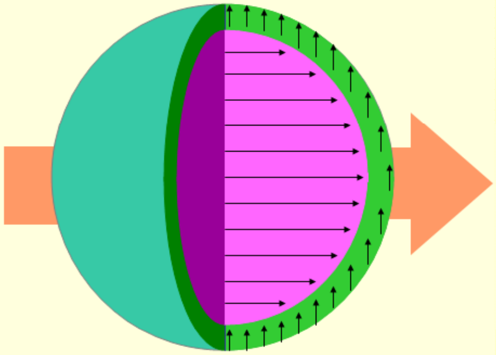
[1]NIST [2]Carnegie Mellon U. [3]Oberlin College [4]U. Maryland [5]PSI Switzerland [6]LANL



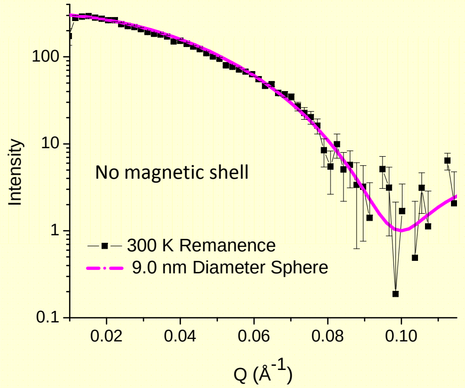
Fe_3O_4 nanoparticles (NPs) are promising candidates for applications from data storage to hyperthermic cancer treatment. Efficacy depends on the interparticle magnetic correlations or "cross-talk." We focus on monodisperse, 9 nm NPs that are close-packed into long-range *3D* crystallites.



Small-angle neutron scattering (SANS) is an ideal probe of both structural and magnetic ordering. Polarization analysis of the neutron spin allows us to uniquely determine the vectorial magnetic morphology.



At nominal saturation (1.25 Tesla, 200 K) polarized SANS reveals that the NPs form an unexpected magnetic morphology with a core that points along the applied field and a 1 nm thick shell canted perpendicular to it. These shells collectively order in clusters of ~10 NPs.



The shell thickness changes with temperature, and it disappears completely when external field and interparticle correlations are removed. This discovery underscores the connection between interparticle correlations and internal magnetic morphology.

DMR-0454672, 0704178,0804779; DE-FG02-08ER40481

K.L. Krycka et al., Phys. Rev. Lett. 104 (2010) 207203

Electric Field Control of Magnetization in a Multiferroic

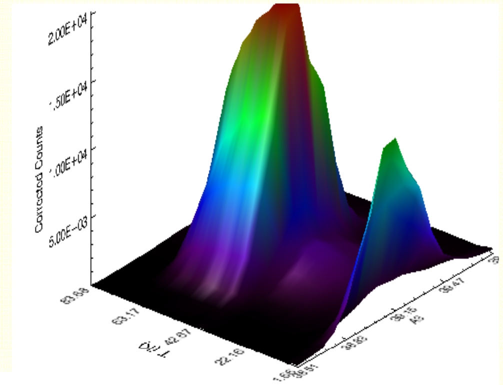
DMR-0454672
DMR-0520471

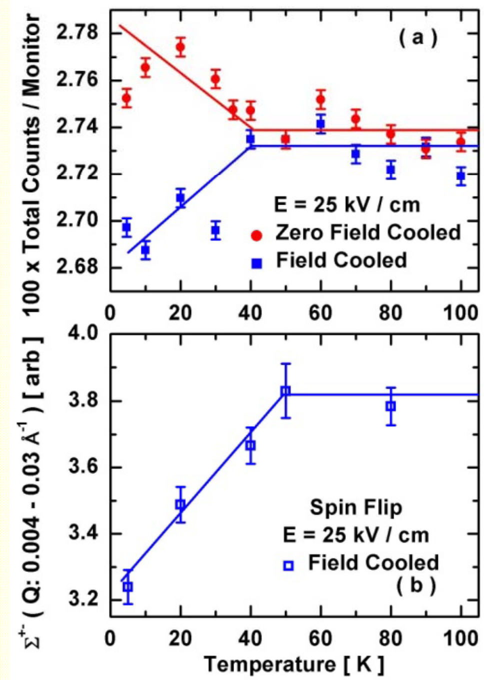
Ben Ueland (NIST), Jeffrey Lynn (NIST), Mark Laver (NIST/U. Maryland), Young Choi (Rutgers U.), Sang-Wook Cheong (Rutgers U.)

Multiferroics are materials that exhibit ferroelectricity and magnetism simultaneously, a very rare combination of properties. Such materials are of great scientific and technological interest because of the potential to control the magnetization electrically rather than with a magnetic field. This would allow new "spintronics" devices, for example, that would directly combine magnetic storage with computer electronics and circumvent the need for hard disks for data storage, dramatically increasing the speed of computer systems.

One such multiferroic material is $HoMnO_3$. Our measurements using neutron scattering found that the ferromagnetism exists in the domain walls rather than in the bulk of the material. Nevertheless, these magnetic domain walls can be controlled by an electric field as shown by the data to the right, providing the proof-of-principle of controlling the magnetism with an electric field. This coupling of the electric field to magnetic domain walls should prove particularly useful in device applications in the form of thin films.

The development of magnetic order and abrupt changes that occur in $HoMnO_3$. Abrupt changes in the ferroelecticity are also found at the same temperatures.





The data in (a) show that the magnetism can be controlled by an applied electric field. The data in (b) uses polarized neutrons to prove that the magnetism is indeed changing with electric field and not some other property of the material.

B. G. Ueland, J. W. Lynn, M. Laver, Y. J. Choi, and S.-W. Cheong, *Phys. Rev. Lett.* 104, 147204 (2010).

CHRNS Center for High Resolution Neutron Scattering NIST

Education and Outreach

DMR-0454672

Summer Undergraduate Research Fellowship Program

CHRNS participates in NIST's Summer Undergraduate Research Fellowship (SURF) program. Students spend 12 weeks working on individual research projects with a NIST advisor. They also participate in group educational and cultural activities.

From left to right:
Rob Dimeo (NCNR), Magdalen Lovell (SUNY Albany), Andrew Baker (Univ. Delaware), Navjot Kaur (City College of NY), Joseph Redman (Middlebury College), Theresa Ginley (Juniata College), Thomas Grant White (Univ. Southern Mississippi), Vikas Bhatia (Univ. of Maryland), William Riedel (Brown University), Dan Neumann (NCNR)

CHRNS Center for High Resolution Neutron Scattering NSF NIST

tion and Outreach

DMR-0454672

Building the next generation of neutron scatterers

2010 CHRNS/NCNR Summer School on Neutron Small Angle Scattering and Reflectometry
May 10-14, 2010

This year we had 90 applications for 36 positions. We had
31 students, 3 postdocs, and 2 professors from 34 different universities in North America:
25 males, 11 females, 5% African Americans, 8% Hispanics.
Guest speakers were Tiffany Santos from Argonne National Laboratory and
Matt Helgeson from MIT.

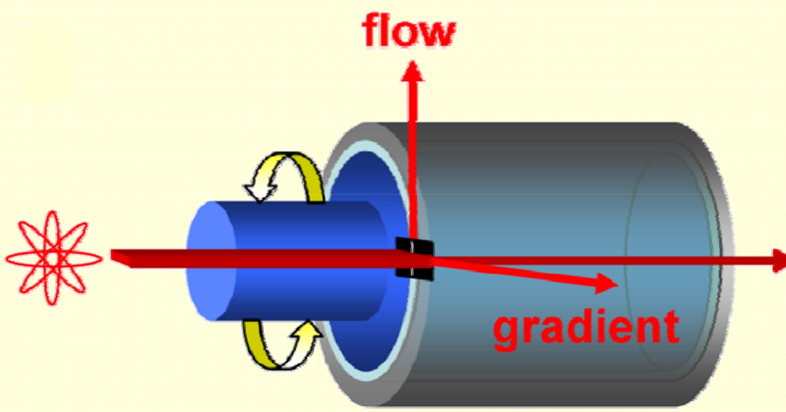
Testing composition gradients in shear banding flows using *in situ* neutron transmission profiling

M.E. Helgeson[1], L. Porcar[2,3], C. Lopez-Barron, N.J. Wagner[1]

[1]MIT, [2]Univ. Delaware, [3]ILL Grenoble

DMR-0454672
& Unilever Res.

Many everyday fluids, including shampoos, body washes, gels, and pastes, exhibit **shear banding** when sheared between surfaces, where the fluid between them spontaneously divides into regions of different shear rate (velocity gradient). Theories for shear banding often assume that these flows are coupled to phase separation within the fluid, and predict concentration differences between shear bands. However, these predictions have never been tested in real fluids.

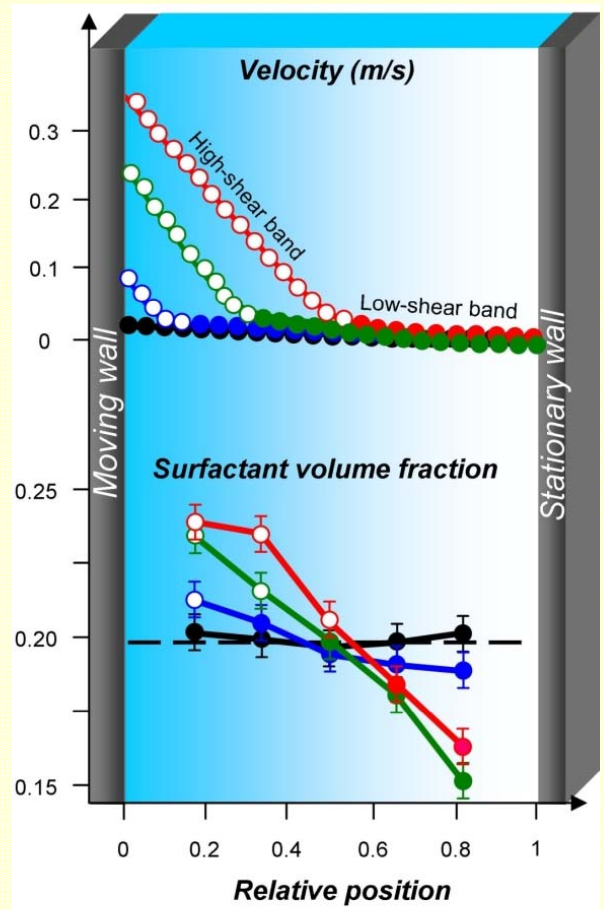


Concentration

$$T \propto \exp(-\phi)$$

Transmission

We have developed a new method, scanning narrow aperture flow-ultra small angle neutron scattering (SNAFUSANS), to test these predictions by measuring the fluid composition profile directly through neutron transmission measurements. Measurements on a model shear banding fluid comprised of surfactant micelles are the first to conclusively show shear banding-induced concentration gradients.



Left: Illustration of the SNAFUSANS shear cell.
Above: (Top) Velocity profiles indicative of shear banding. (Bottom) Concentration profiles measured using SNAFUSANS.

M.E. Helgeson *et al.*, Physical Review Letters 105, 084501 (2010).

How Does the Stiffness of Lipid Vesicles Change as They Interact with Pore-forming Peptides?

DMR-0454672
DMR-0803103

J.-H. Lee,[1] S.-M. Choi,[1] C. Doe,[1] A. Faraone,[2] P.A. Pincus,[3] and S.R. Kline[2]
[1]KAIST; [2]NIST Center for Neutron Research; [3]University of California, Santa Barbara

Antimicrobial peptides are proteins which modify membrane morphology. At low concentrations, individual peptides insert themselves into the lipid bilayers. At a high enough concentration, they group together to form a trans-membrane pore. This research project studied the effect of this process on the membrane's elastic properties.

Neutron Spin Echo (NSE) spectroscopy was used to investigate the elasticity of large, unilamellar vesicle membranes interacting with the pore-forming peptide melittin. NSE measurements revealed three distinct effects on the membrane stiffness as the concentration of melittin was increased. At low melittin concentration the overall effect is a "softening" of the membrane. When the melittin concentration was large enough to form pores, the membrane became slightly more rigid. At even higher concentrations additional pores formed, and the inter-pore interactions within the membrane became significantly more rigid.

These findings have improved current understanding of the elastic behavior and morphological changes of cell membranes induced by protein-membrane interactions.

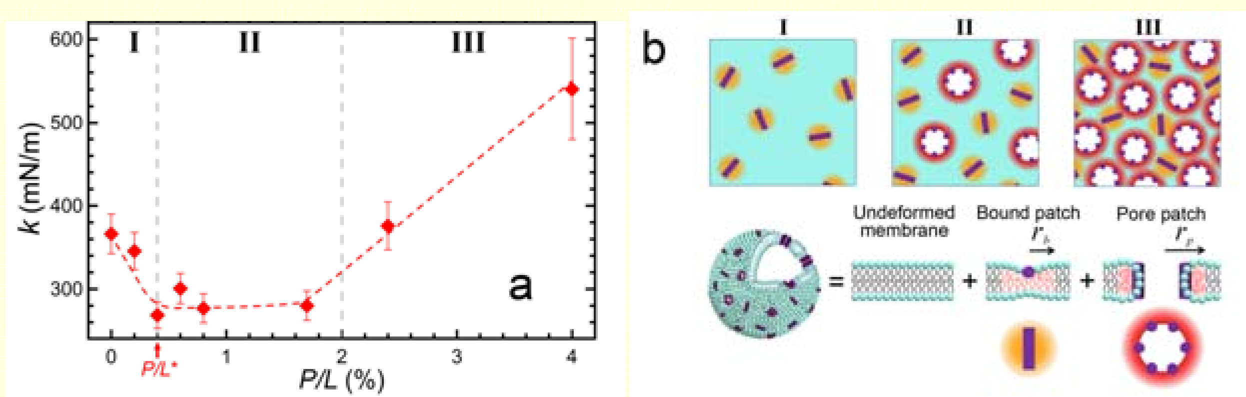


Fig. 1 a) Bilayer compressibility modulus, *k*, (a measure of the elasticity of the membrane) of DOPC/melittin in D2O buffer at different protein to lipid ratios, *P/L*. b) Scaled schematics of the distributions of bound melittin and pores on the membrane at *P/L* = 0.4% (I), 1.7% (II) and 4.0% (III).

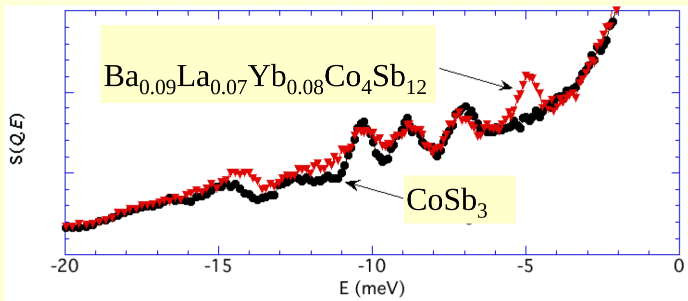
J.-H. Lee, S.-M. Choi, C. Doe, A. Faraone, P.A. Pincus, and S.R. Kline, Phys. Rev. Lett., 105, 038101 (2010).

Multiple Filling of Voids Improves Thermoelectric Efficiency of Skutterudites

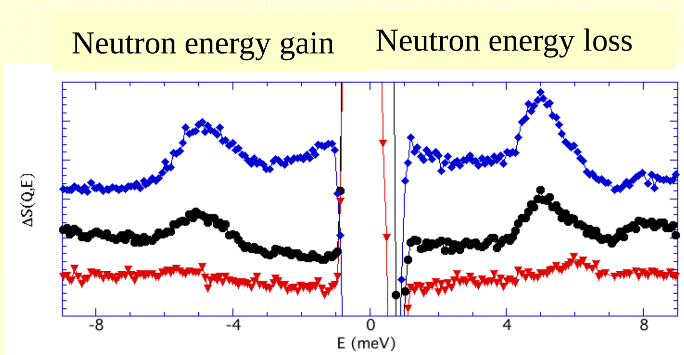
X. Shi[1], Jihui Yang[1], J.R.D. Copley[2], and J.J. Rush[2,3]
[1]GM R&D Center, [2]NIST, [3]U. Maryland

DMR-0454672
DE-FC26-04NT42278

Recent advances in the design of thermoelectric materials have led to increased thermal-to-electrical energy conversion efficiencies (characterized by the dimensionless figure of merit ZT). These increases can result in significant energy savings in generating electricity from waste heat, as for example in the exhaust systems of automobiles. Researchers at GM have synthesized a range of cage-structured compounds with very high values of ZT. These compounds, known as skutterudites, contain atomic sites that are 20% to 25% occupied by guest rare earth elements such as Ytterbium and/or alkaline earth elements such as Barium. In order to further increase ZT we need to improve our understanding of the atomic scale dynamics of these materials, particularly the role of the guest atoms.



Neutron energy gain data for the host and for a partially filled material.



Difference scattering functions, for partially filled skutterudites $Yb_{0.2}Co_4Sb_{12}$ (top), $Ba_{0.09}La_{0.07}Yb_{0.08}Co_4Sb_{12}$ (middle), and $La_{0.2}Co_4Sb_{12}$ (bottom).

Scattering experiments, using the CHRNS Disk Chopper Spectrometer, reveal a rich spectrum of excitations in partially filled skutterudites, including a particularly strong feature associated with Ytterbium atoms rattling within the caged host. The results confirm theoretical predictions of the energies associated with different additives, and support the notion of phonon glass behavior, which allows dilute guest atoms to interact strongly with acoustic phonons thereby greatly reducing thermal conductivity. Steady improvements are observed on adding different types of filler atoms into the skutterudite crystal structure. Furthermore the average ZT value has been improved by a factor of roughly two, making these materials very attractive for power generation applications.

X. Shi, J. Yang, H. Wang, M. Chi, J.R. Salvador, J. Yang, S. Bai, W. Zhang, L. Chen, J.R.D. Copley, J.B. Leão, and J.J. Rush, submitted.

Education and Outreach

DMR-0454672

Summer Institute for Middle School Science Teachers

21 science teachers from Florida and three Maryland counties enjoyed a day of science at the NCNR.

The teachers performed an experiment that they could repeat in their science classes: growing crystals of aluminum potassium sulfate ("alum").

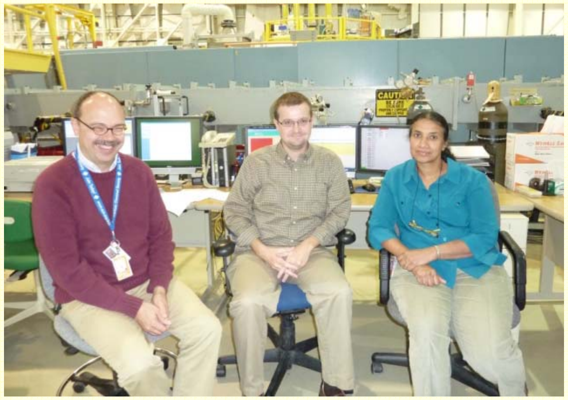
During their tour they were shown the NCNR powder diffractometer, which is used for crystal structure studies.

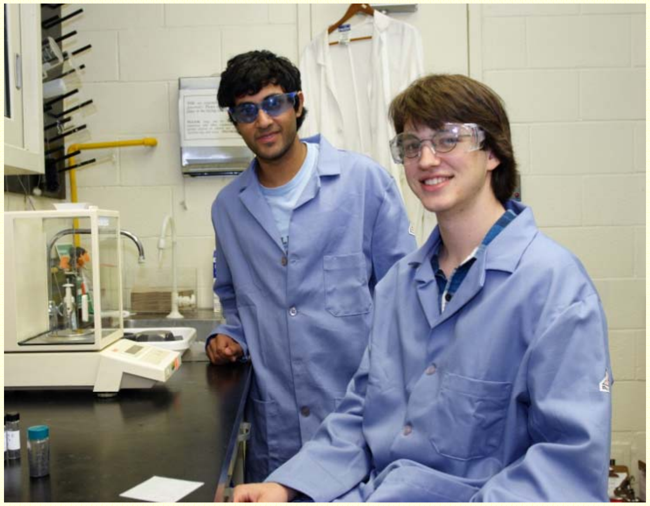
Education and Outreach

Activities for students and faculty

DMR-0454672

Tutorials based on the experiments and lectures presented at the 2009 Summer School were offered to graduate students during the year.





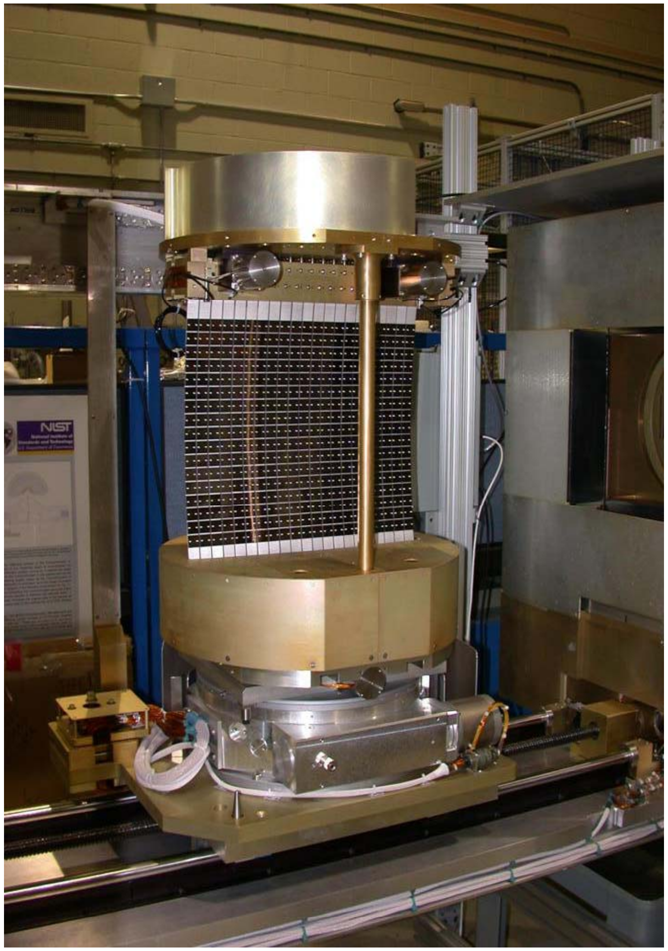
SURF student Vikas Bhatia (left), and SHIP (Summer High School Internship Program) student Jonathan Schear.

(left to right)
Drs. Dan Neumann and Andrew Jackson (NCNR) with Selin Mammen from Seneca Valley High School, who spent 6 weeks during the summer doing research at the NCNR.

Record in Neutron Detection: High Intensity Cold Neutron Spectrometer with Multichannel Analyzer

Collin Broholm, Johns Hopkins *DMR- 0116585*

An NSF-funded instrument at the Center for High Resolution Neutron Scattering now holds the record for producing the world's most intense neutron beam. The instrument, called MACS, produces a beam that exceeds the competition by more than an order of magnitude. Neutrons are an ideal probe of materials at the nanoscale level. However, because neutrons interact weakly with materials, researchers need a very intense beam to study small samples. The instrument was built at Johns Hopkins University with the involvement of graduate and undergraduate students. It comprises 357 graphite platelets that can be oriented to direct neutrons at the sample. With 40 times more neutrons and 20 times better detection capability, MACS will be 100 to 1,000 times more efficient than a conventional spectrometer.



IMR - MIP Highlights

Broader Impacts of CICC Magnet Development, Mark D. Bird (NHMFL)

Neutron characterization of polymer solar cells
Brent T. Fultz, California Institute of Technology, DMR 0520547

Mechanical Design of Cable-in-Conduit Coils, Mark D. Bird (NHMFL)

Design of Cable-in-Conduit Coils

Neutron characterization of polymer solar cells
Brent T. Fultz, California Institute of Technology, DMR 0520547

Characterization of Nb_3Sn Wire, Mark D. Bird (NHMFL)

Testing of Cable-In-Conduit Conductors

Broader Impacts of CICC Magnet Development

Mark D. Bird (National High Magnetic field Laboratory),

Construction of a Series-Connected Hybrid Magnet DMR- 060342

Societal Impact:

Several large superconducting magnets are being built worldwide using the Nb_3Sn Cable-in-Conduit Conductor (CICC) technology. Applications include nuclear fusion (International Thermonuclear Experimental Reactor, European Dipole), neutron scattering and diffraction (Helmholtz Center Berlin, Spallation Neutron Source), condensed matter physics (Nijmegen, The Netherlands; Hefei, China). The NHMFL is leading the way in characterizing Nb_3Sn CICC's conductors and is collaborating with all of these projects to advance the technology.

Education:

Education is an important element of the work and students and post-docs play important roles in developing technology for the SCH. A post-doc, shown far left, played a leading role in designing and testing the 20 kA joints for the SCH outsert. The mechanical engineering graduate student shown below center worked on the analysis of strain in Nb_3Sn conductor.

Involvement in Outreach programs is also an important part of the SCH project. In the summer of 2009 two teachers from local middle schools, shown close left, worked with SCH personnel on Reaction Comparisons of Nb_3Sn Wires Using Image Analysis of Micrographs within the Research Experience for Teachers (RET) program.

Neutron characterization of polymer solar cells

Brent T. Fultz, California Institute of Technology, DMR 0520547

Children at play: searching for symmetry during a Saturday morning session of Adventures in Science.

4-H Adventures in Science (K12)
- Crystals, polymers, magnets

Summer Undergraduate Projects
- In-plane magnetic scattering
- Magnetism in layered materials
- Magnetism calculations in crystals

Conferences
- ACA, ACNS, APS, ICNS

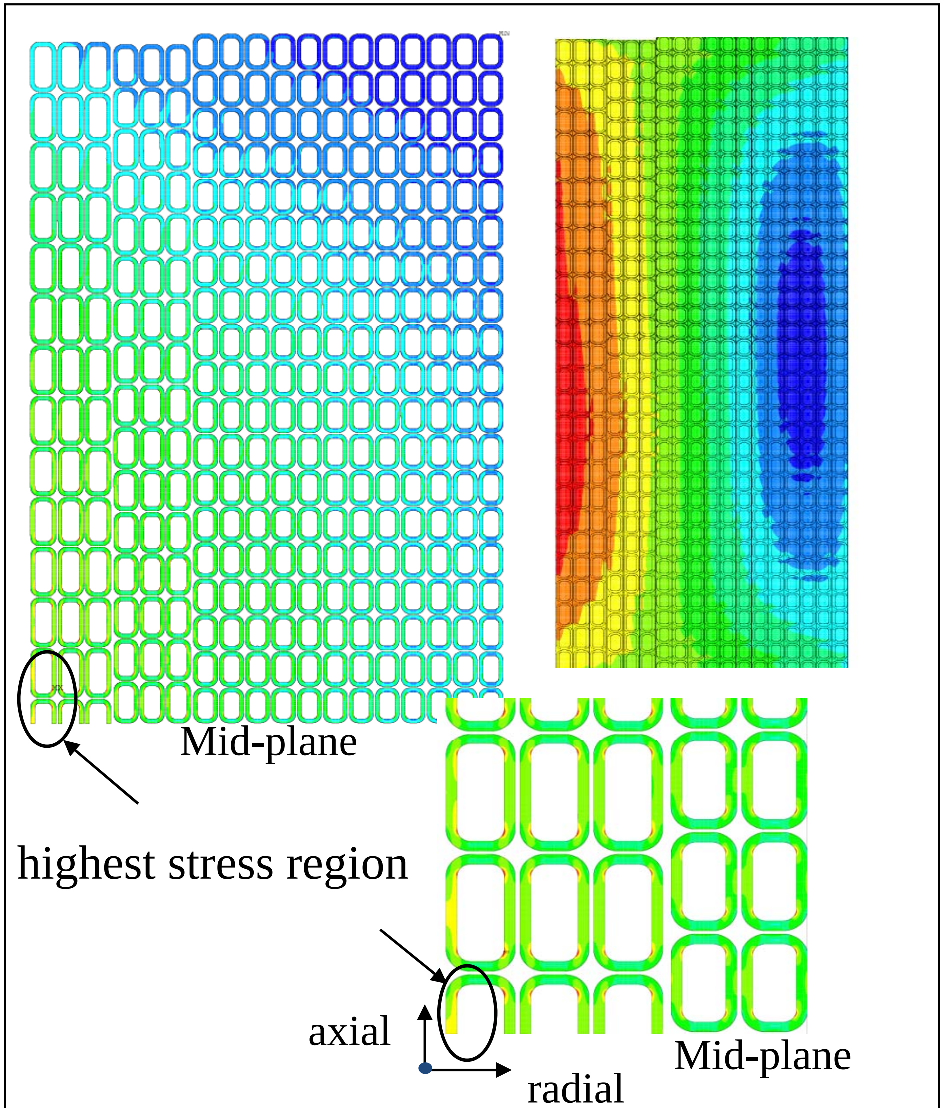
Workshops
- NCNR neutron summer school

Diversity
- 2 offers for FTE positions

Open Source Community Projects
- matplotlib, flot, nexus

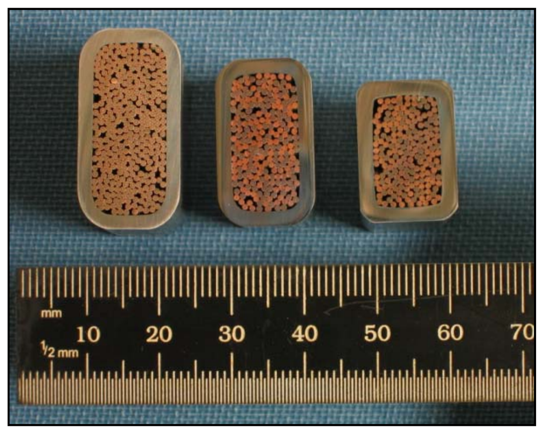
Mechanical Design of Cable-in-Conduit Coils

Mark D. Bird (National High Magnetic field Laboratory),
Construction of a Series-Connected Hybrid Magnet DMR- 060342



A detailed finite element model including all outsert winding components was developed for the stress evaluation in conductor jacket and insulations. All stresses under normal, quench and fault load conditions satisfy their respective design limits. Total axial force from half coil is about 46.5 MN and the highest stress is near the mid-plane of the high field region.

The figures on the left present outsert primary coil Tresca stress distribution of half coil under normal load condition (top left), non-symmetric magnetic field distribution of whole coil under fault load (top right), and a stress detail near coil mid-plane and inner radius. Peak Tresca stress is dominated by a combination of stress due to accumulated axial force near coil mid-plane and coil hoop stress.

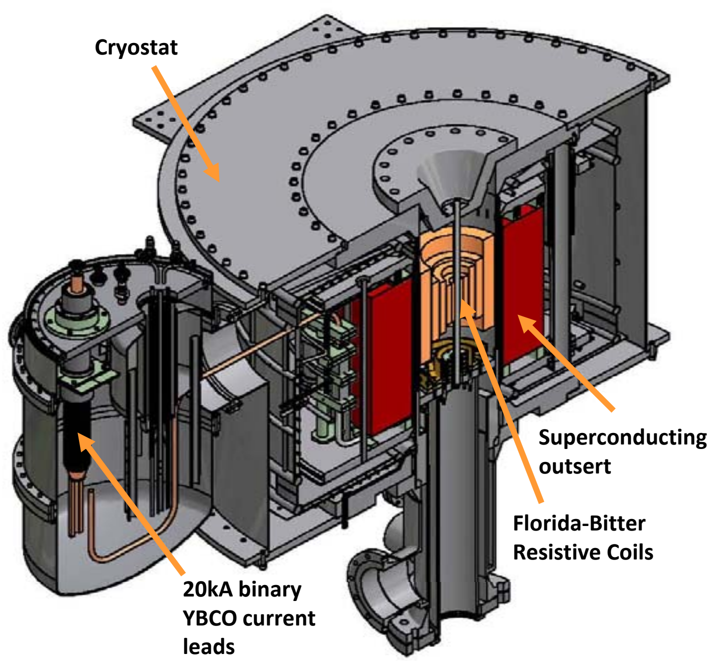


HF, MF, and LF CICCs (from left to right)

Y. Zhai, I.R. Dixon, M.D. Bird, *IEEE Trans. On Appl. Supercond.*, vol. 19, no. 3, June 2009, pp. 1608 – 1611.

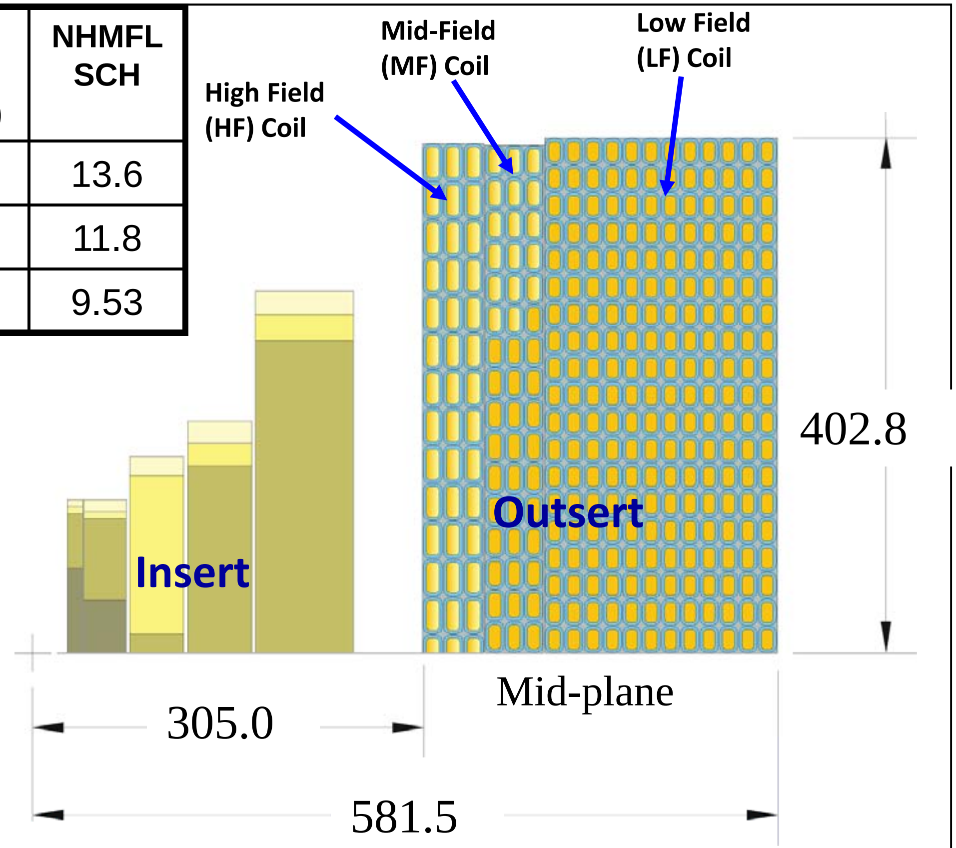
Design of Cable-in-Conduit Coils

The SCH superconducting outsert has been redesigned with an iron shield instead of an active shield coil. In this configuration not only is instrumentation shielded from the magnet, but the experiment is shielded from magnets nearby. The magnet is under construction.



NHMFL SCH magnet system cross-sectional view

Outsert Peak Field (T)	NHMFL SCH
HF	13.6
MF	11.8
LF	9.53

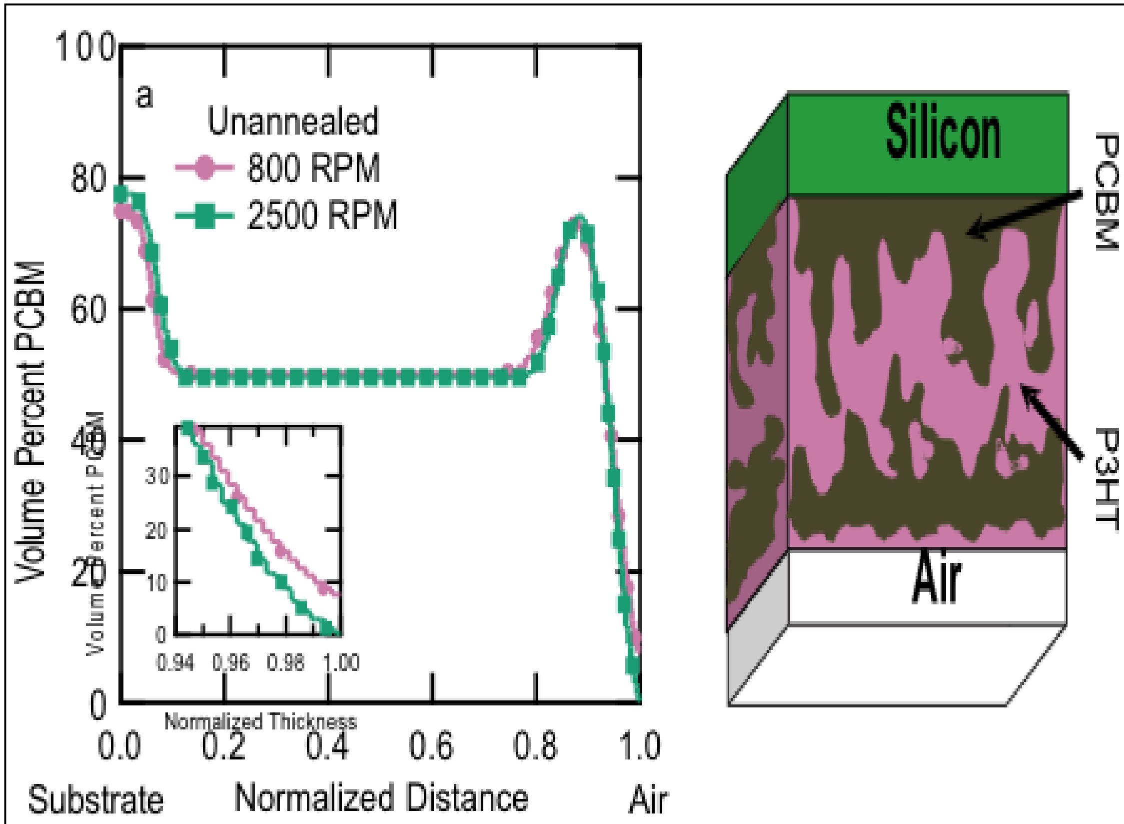


The new cross section of the SCH superconducting outsert (right) with the 12MW Florida-Bitter insert coils (left). Only half coils are presented due to symmetry. The number of layers (and turns/layer) in the HF, MF, and LF coils is changed. The CICC inner structure is improved, also.

Neutron characterization of polymer solar cells

Brent T. Fultz, California Institute of Technology, DMR 0520547

Cheap, light, flexible solar cells can be made from a conducting polymer (P3HT) doped with nanoparticles (PCBM). PCBM extracts photogenerated electrons from the polymer matrix, so cell efficiency depends critically on PCBM distribution. This distribution is difficult to measure with techniques such as XRD or TEM, which cannot effectively distinguish between P3HT and PCBM. Using neutrons and DANSE reflectometry software, researchers have discovered that PCBM gathers preferentially at the interfaces. Modifying fabrication methods may lead to improvements in cell efficiency.



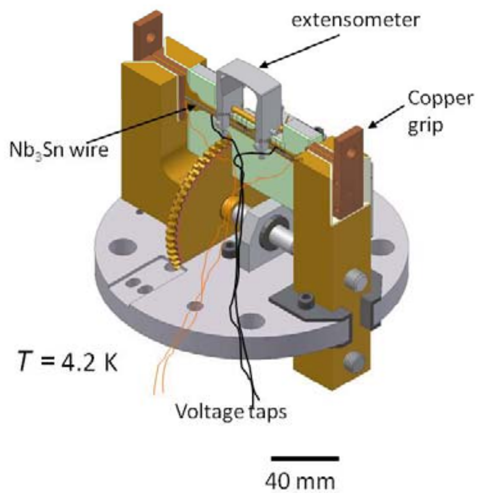
Ratio of phenyl-C61-butyric acid methyl ester (PCBM) to poly-3-hexylthiophene (P3HT) in a spin coated OPVC.

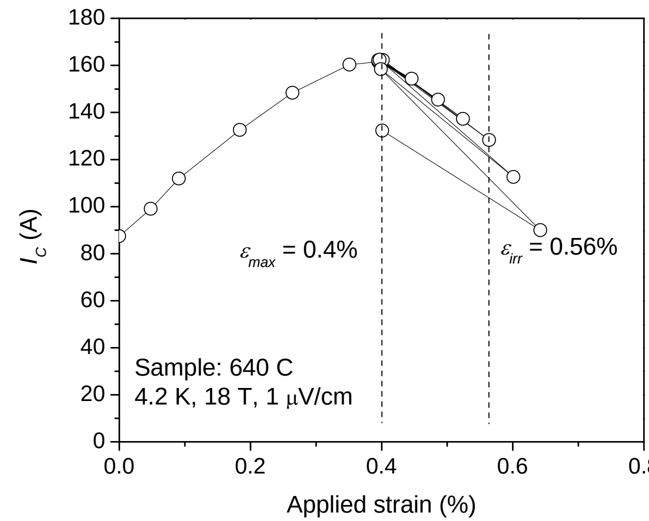
Characterization of Nb_3Sn Wire

Mark D. Bird (National High Magnetic field Laboratory),

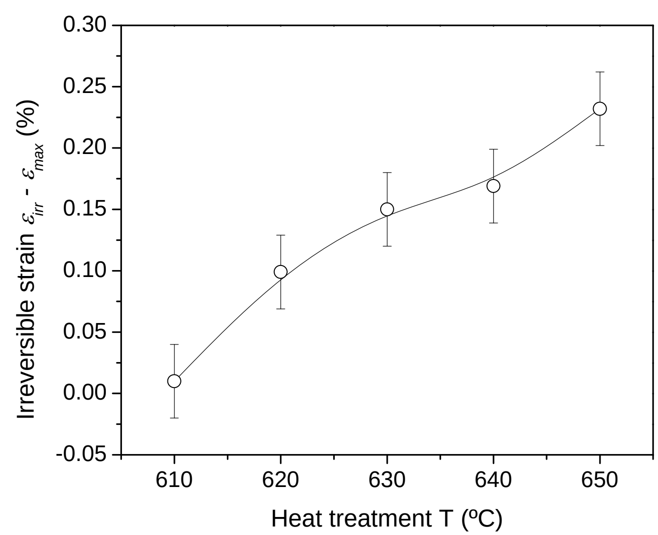
Construction of a Series-Connected Hybrid Magnet DMR- 060342

Characterization of critical properties of Nb_3Sn wires used in the SCH is crucial to both the magnet design and quality assurance of procured wires. In particular, the critical current I_c of the Nb_3Sn is very sensitive to thermal and electromagnetic strain.





We use a unique apparatus developed in-house to accurately measure Nb_3Sn wire I_c versus strain taking advantage of a large bore high field magnet at the NHMFL. The irreversible strain limit ε_{irr}, above which Nb_3Sn wire is permanently damaged, is an indicator of wire strain tolerance. We measured ε_{irr} of Nb_3Sn wires heat treated at different temperatures. We found that ε_{irr} increases with heat treatment temperature. This is the first experiment on heat treatment temperature dependence of ε_{irr}. This finding made significant contribution to the understanding of I_c strain behavior of Nb_3Sn wires.



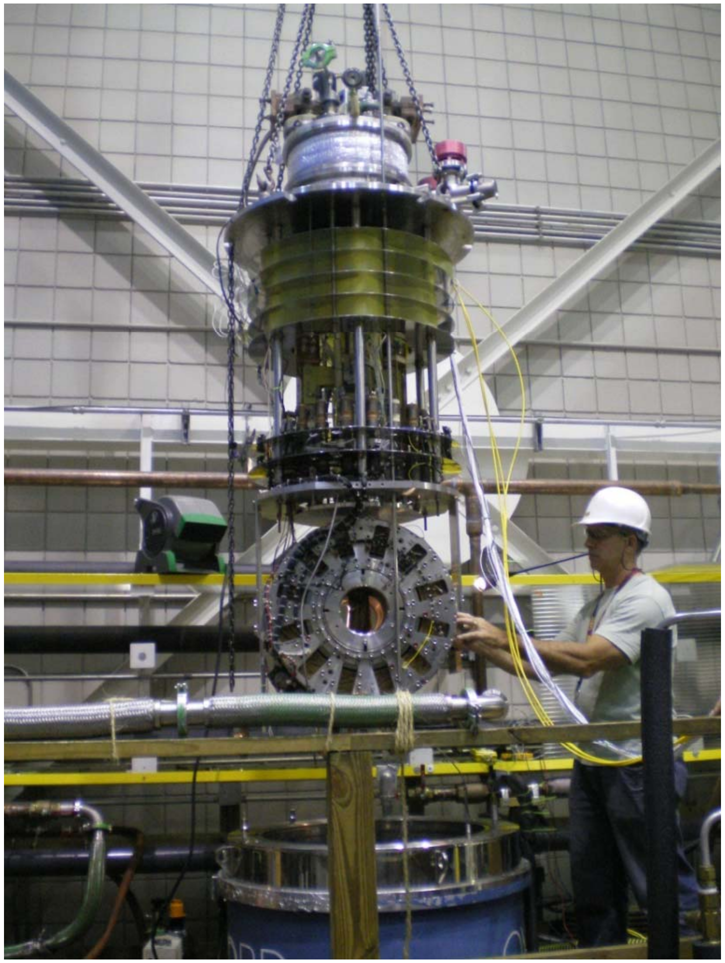
J. Lu, K. Han, R.P. Walsh, I.R. Dixon, A. Ferrera, B. Seeber, *IEEE trans. Appl. Supercond.*, **19**, 2615 (2009).

Testing of Cable-In-Conduit Conductors

The test campaign of candidate Cable-In-Conduit Conductors (CICC's) for use in the Series Connected Hybrids is complete. Six sub-size and three full-size cables of different designs have been tested under realistic conditions. This required the creation of a facility with unique capabilities at the NHMFL.

Transverse load cycling did not cause significant degradation and their current-carrying capacity as a function of temperature, magnetic field and axial strain is acceptable and can be modeled accurately.

This allowed the CICC specification to be finalized, the coil design to be finalized and conductor fabrication for the Series Connected Hybrids is now underway.



Above: A CICC sample mounted through a superconducting magnet is being lowered into its cryostat in preparation of a test

I.R. Dixon, M.D. Bird, A. Bonito-Oliva, K.R. Cantrell, J. Lu, G.E. Miller, P.D. Noyes, R.P. Walsh, H.W. Weijers, *IEEE Trans. On Appl. Supercond.*, vol. 19, no. 3, June 2009, pp. 1462 – 1465.

I.R. Dixon, M.D. Bird, P. Bruzzone, A.V. Gavrilin, J. Lu, B. Stepanov, H.W. Weijers, *IEEE Trans. On Appl. Supercond.*, vol. 19, no. 3, June 2009, pp. 2466 – 2469.

Partly funded by Helmholtz Center Berlin

NHMFL Highlights Gregory S. Boebinger, NHMFL, DMR-0654118

Overcoming Frustration in Magnetism

Gregory S. Boebinger, National High Magnetic Field Laboratory

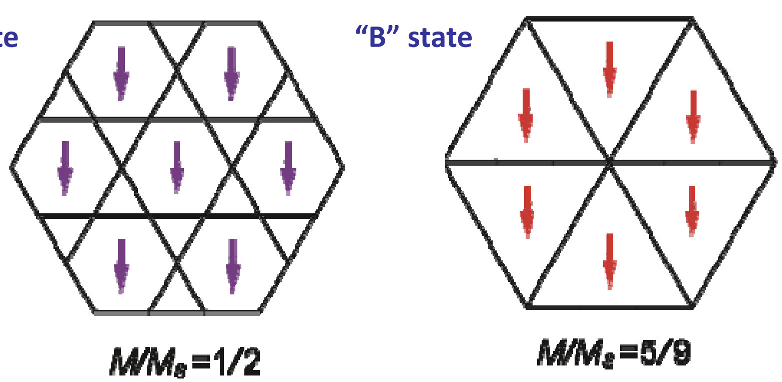
DMR-Award 0654118

DC Field Facility User Program

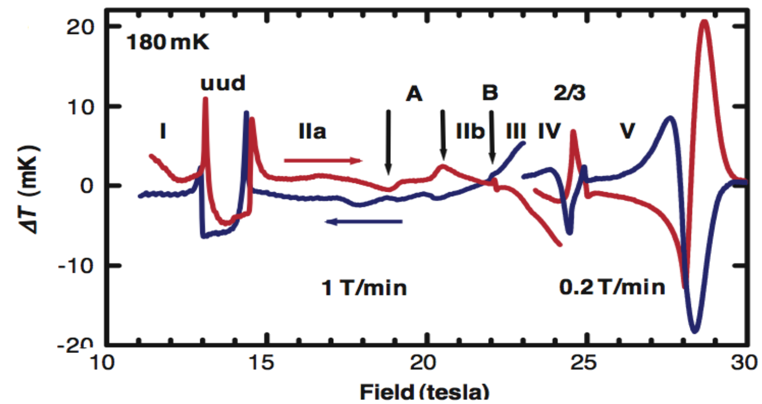
Frustrated triangular antiferromagnets are like three curmudgeons on election day who can't decide how to vote: they are inclined to disagree with everyone around them but they can't all simultaneously disagree with each other.

In these materials, the arrangement of the magnetic moments are known to produce a plateau at 1/3 of the maximum magnetization. Recent magnetic and thermal measurements have provided evidence for other stable arrangements of spins at higher fractions that were not expected.

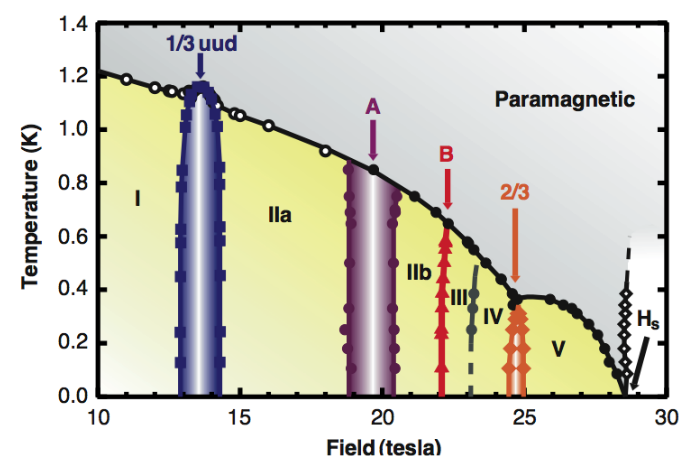
"A" state "B" state



Proposed spin arrangements for the new "A" and "B" states discovered at ~ 20 T (left) and ~22 T (right)



Thermodynamic transitions in high fields



Phase diagram at high field, low temperature showing new states.

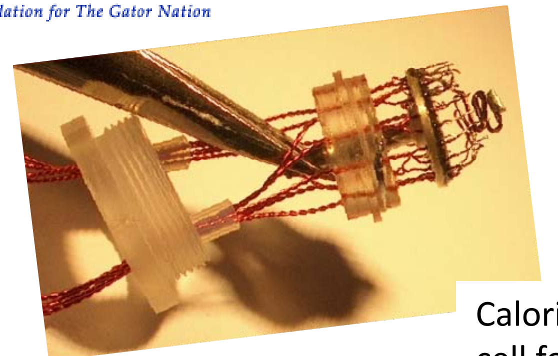
N. A. Fortune, S. T. Hannahs, Y. Yoshida, T. E. Sherline, T. Ono, H. Tanaka, and Y. Takano, *Phys. Rev. Lett*. **102**, 257201 (2009)

Overcoming Frustration in Magnetism

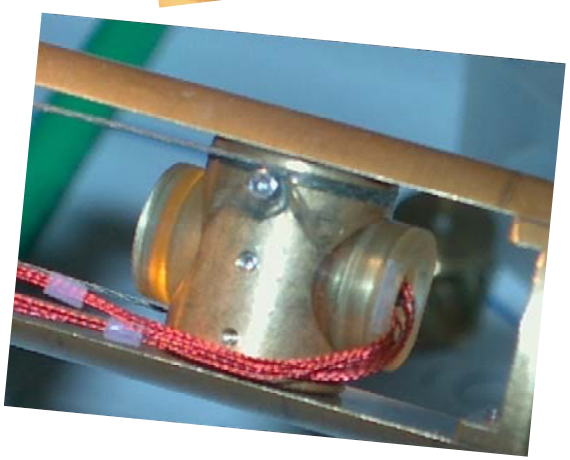
Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

DC Field Facility User Program



Calorimetry cell for measuring heat capacity



Calorimetry cell in mechanical rotator designed for millikelvin temperatures

This work was enabled by the development of unique instrumentation: a rotating calorimeter that operates at millikelvin temperatures. Developed as a Magnet Lab collaboration with Smith College, a liberal arts college for women, this instrument has made a whole new class of measurements on low-dimensional magnetic systems accessible to the users of the NHMFL.

The project trained students at all levels: from introducing undergraduates to data collection and analysis, to graduate students and postdocs who have gone on to other research institutions in the United States and Europe.

This work was international in its conception bringing samples from Japan, techniques from NHMFL in Tallahassee, and expertise from UF and Smith College.

Quantum Oscillations and Superconductivity

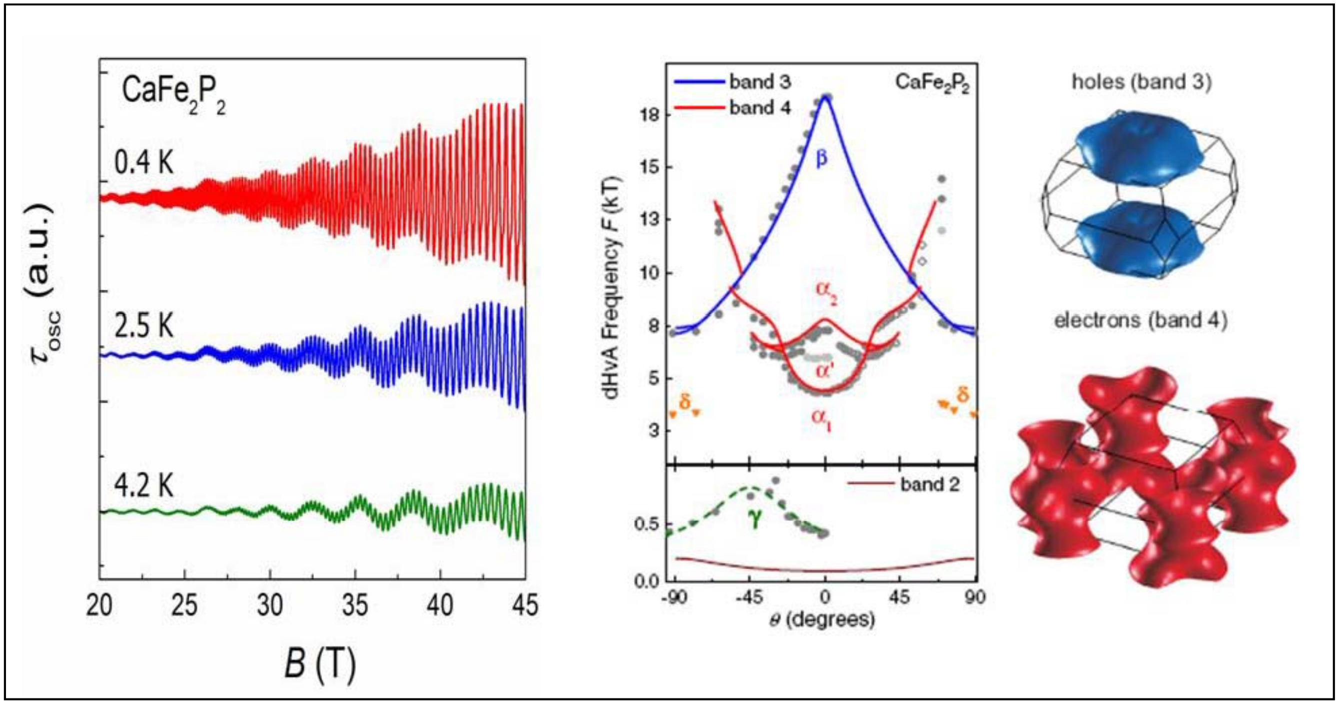
Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

DC Field User Facility User Program

Recently a new class of superconductors was discovered that exhibits high temperature superconductivity, the “pnictide” superconductors. High magnetic fields reveal quantum oscillations that provide unique information about the electronic properties of a material.

Researchers from Bristol University (UK), Stanford University, and the Magnet Lab have found that the *non-superconducting* compound $CaFe_2P_2$ has an electronic structure with key differences from the closely related *superconducting* compound $SrFe_2P_2$ and other superconducting pnictides. The difference is that the nonsuperconducting compound has a smaller ratio of atomic spacing along its *c* axis than along its *a* axis (c/a). This causes the electronic structure to be much more three dimensional in character than related superconducting compounds and provides important clues about the nature of high-temperature super-conductivity in the pnictides.



Coldea, A.I.; Andrew, C.M.; Analytis, J.G.; McDonald, R.D;. Bangura, A.F.; Chu, J.-H; Fisher, I.R. and Carrington, A., *Phys. Rev. Lett.*, 103, 026404 (2009)

Quantum Oscillations and Superconductivity

Gregory S. Boebinger, National High Magnetic Field Laboratory

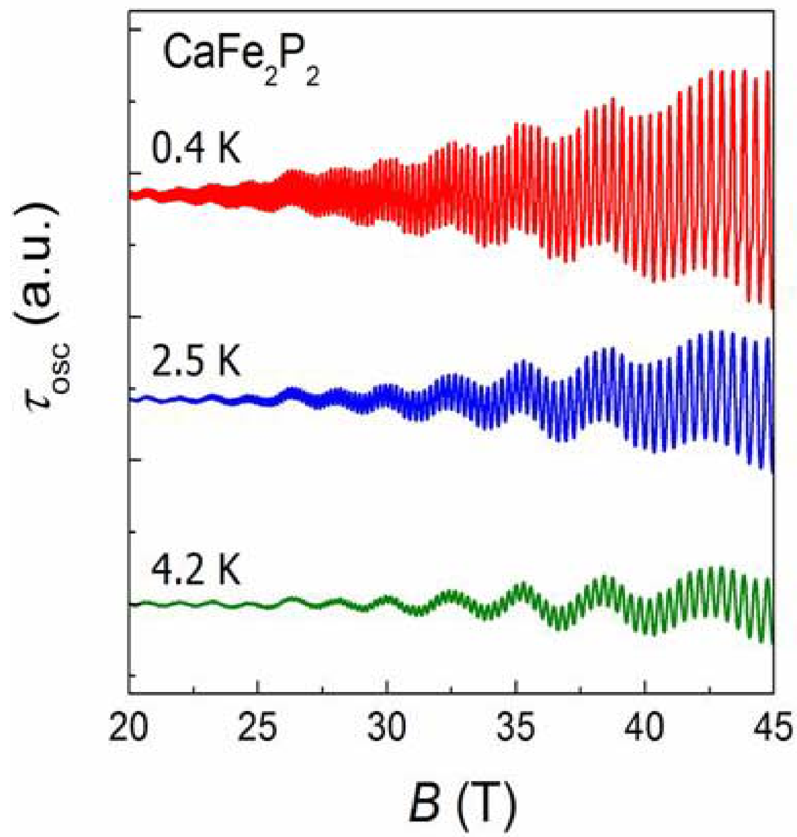
DMR-Award 0654118

DC Field User Facility User Program

Dr. Amalia Coldea
University of Bristol (UK)

The leader of this research collaboration among Bristol, Stanford and the Magnet Lab was Dr. Amalia Coldea at the University of Bristol. Samples were grown at Stanford University while high field measurements were performed in the DC Field Facility of the NHMFL in Tallahassee, FL.

This international collaboration combines the strengths of many different programs to advance our understanding of high-temperature superconductivity.



Coldea, A.I.; Andrew, C.M.; Analytis, J.G.; McDonald, R.D;. Bangura, A.F.; Chu, J.-H; Fisher, I.R. and Carrington, A.,
***Phys. Rev. Lett.,* 103, 026404 (2009)**

Toward Graphene Electronics

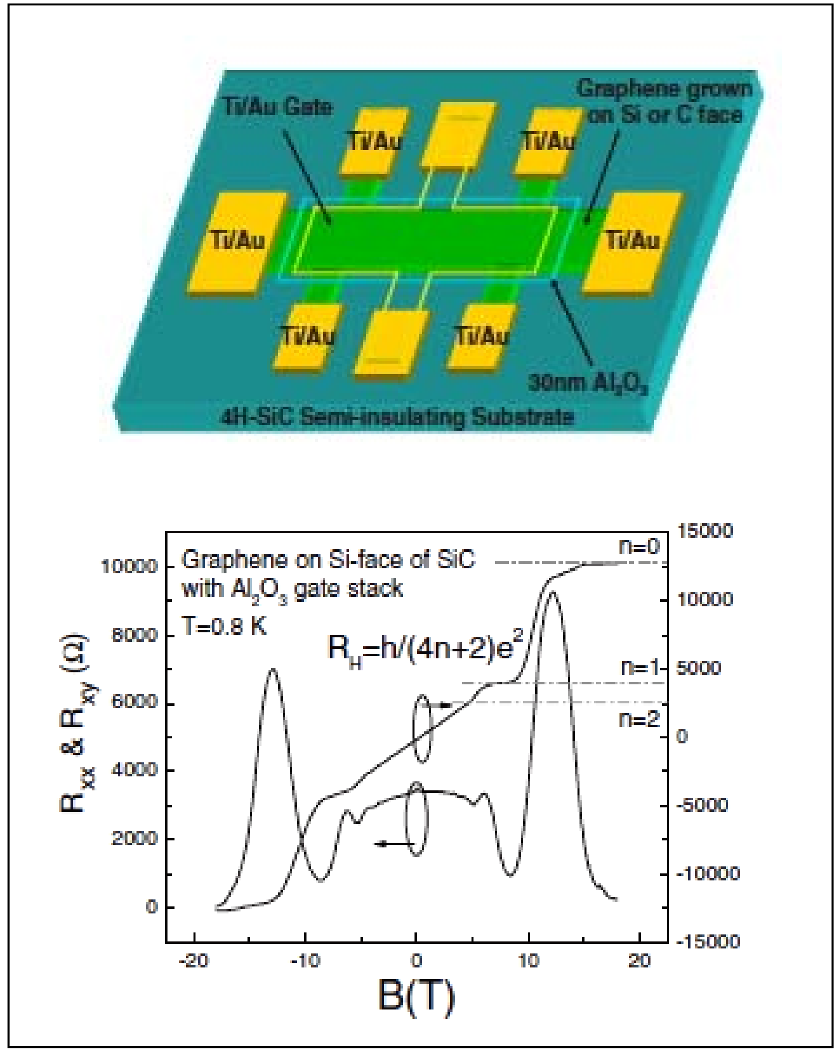
Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

DC Field Facility User Program

Graphene, a single layer of carbon atoms arranged in a 2-D hexagaonal lattice, is providing exciting new results in both scientific and technical arenas. Researchers at Purdue University and the Magnet Lab have measured the quantum Hall effect in a monolayer of graphene on a Silicon Carbide substrate with an integral gate.

The fact that one can observe the quantum Hall effect points to the high quality of this two-dimensional electron gas and indicates that graphene grown and processed in such a way has a real potential for use in "real-world" semiconducting devices.



T. Shen, J.J. Gu, M. Xu, Y. Q. Wu, M.L. Bolen, M.A. Capano, L.W. Engel and P. D. Ye,
Appl. Phys. Lett., **95**, 172105 (2009).

Toward Graphene Electronics

Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

DC Field Facility User Program

Fabrication facility for graphene devices at Purdue University.

The fact that one can fabricate a monolayer of carbon atoms on a substrate with a gate electrode on top and have a high enough quality device to observe the Quantum Hall Effect demonstrates that graphene has a real potential to become the technology that will allow the semiconductor industry to continue to provide faster and smaller high performance devices.

As silicon technology moves toward quantum mechanical limits, graphene has been predicted to be the technology that will overcome those limits.

These results clearly show that graphene has moved past the earliest samples cleaved with scotch tape to become a robust technology compatible with modern semiconductor mass production technology.

Researching Educational Outreach Effectiveness

Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

Center for Integrating Research & Learning

The Magnet Lab continues to expand its educational outreach *and to do research on the effectiveness of that outreach:*

- **Increased outreach to Title I and under-served schools** for the 2009-2010 academic year. Total number of students reached: ~8,000-10,000

- 2010 Research Experiences for Undergraduates (REU) program hosted 21 students
- 2010 Research Experiences for Teachers (RET) program hosted 14 teachers; 6 of these teachers are from Title I schools

- **Secured funding** for the *SciGirls Program*, a partnership with Public Television to encourage mid-high girls to pursue STEM careers.

- **Published paper on *"Research Experiences for Teachers (RET): Motivation, Expectation, and Changes to Teaching Practices due to Professional Program Involvement."*** Pop, M. M., Dixon, P., & Grove, C. *Journal of Elementary Science Education 21(2),* 127-148 (2010).
- Presented research on the effectiveness of RET and *SciGirls* programs at national education conferences

Justin Mincey of Bethune-Cookman University (an HBCU institution) conducts engineering research with Yan Xin

The REU's at the Magnet Lab's FSU branch represented 17 universities and worked with 19 science mentors

Partnerships Encourage STEM Careers

Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

Center for Integrating Research & Learning

Camp encourages girls to pursue science careers

By Kate Schofield
DEMOCRAT WRITER

Choosing 32 girls was never this hard.

From July 19 to 30, SciGirls held its fifth year of camp.

The camp started in 2006 and was created to address the issue of a large a drop in the number of girls interested in science as they entered middle school. It's run by a partnership between WFSU and the National High Magnetic Field Laboratory.

"Our goal is to engage girls' interest in science," said Kim Kelling-Engstrom, director of educational services at WFSU-TV. "The girls get to meet women in science fields. They go on field trips and see interesting things."

The camp's hands-on activities make the program memorable for participants.

"We get them involved in real research opportunities," said Pat Dixon, director of the Center for Integrating Research and Learning at the Mag Lab.

KATE SCHOFIELD/Democrat

A group of SciGirls listen to science project presentations at the National High Magnetic Field Laboratory.

Online TALLAHASSEE.COM

Miami and Georgia," Kelling-Engstrom said.

Center for Integrating Research and Learning partnerships help the Magnet Lab reach diverse audiences to promote career choices in Science, Technology, Engineering and Mathematics. Public Television's enthusiastic partnership with the Magnet Lab has enabled CIRL to offer *SciGirls* to middle and high school girls interested in science. CIRL partnering with ERC FREEDM, the FSU Center for Advanced Power Systems, North Carolina State University, and Arizona State University facilitates Renewable Energy Camps and Young Scholars programs.

Community partners Barnes & Noble, Chik-Fil-A and WFSU-TV help the Magnet Lab reach early readers and engage children and their families in the excitement of science. Through partnerships with area schools, school districts and academic departments, CIRL assists teachers in gaining science content and STEM skills to reach thousands of students over their entire careers.

Bismuth Qubits in Silicon

Gregory S. Boebinger, National High Magnetic Field Laboratory

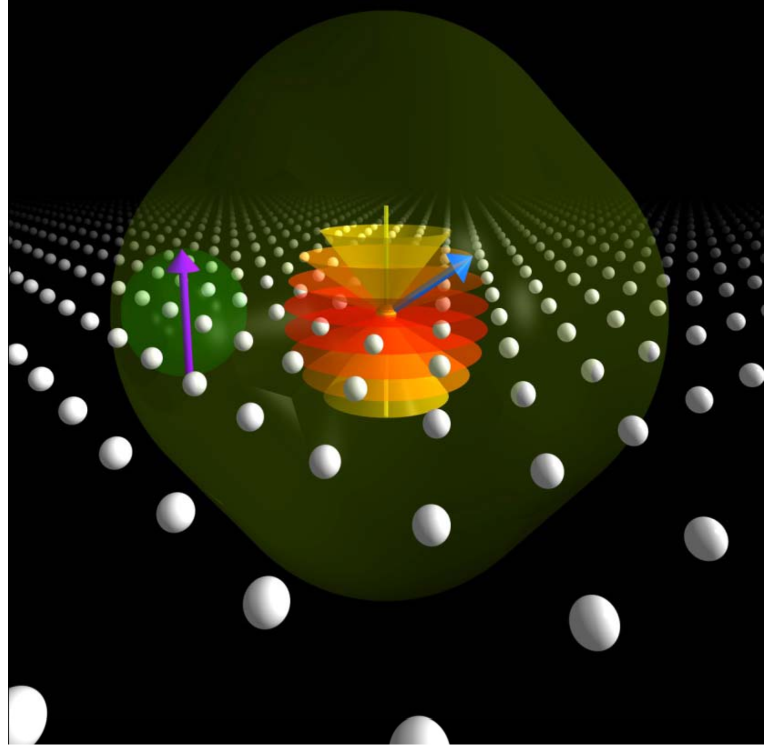
DMR-Award 0654118

Electron Magnetic Resonance (EMR) User Program

Taking full advantage of quantum mechanics would allow future computers to solve problems that would take longer than the lifetime of the universe on a normal computer.

Scientists from the London Centre for Nanotechnology (LCN) at University College London (UCL) and the Magnet Lab used pulsed electron magnetic resonance to demonstrate the initialization, manipulation, and storage of quantum information using bismuth atoms in silicon. Bismuth is the heaviest stable atom and features a large nuclear 9/2 'spin' (blue arrow) that serves as a tiny compass needle that can point in one of ten states (red and yellow cones). This would allow a bismuth atom to store much more quantum information than the much-more-studied phosphorus atom. Phosphorus has only 1/2 spin that therefore can point in only two directions.

A bismuth atom in one slice of a silicon crystal. The purple arrow is the electron spin while the blue arrow is the nuclear spin. Artwork by Manuel Vögtli (LCN).



These findings are reported in Nature Materials as an Advance Online Publication:

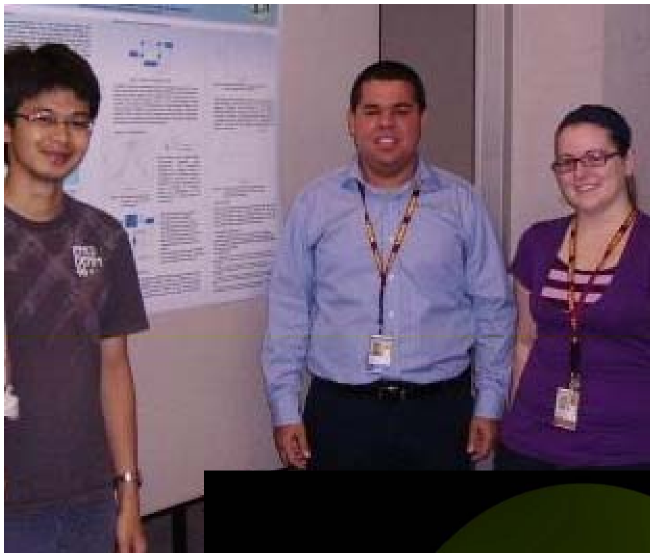
G.W. Morley, M. Warner, A.M. Stoneham, P.T. Greenland, J. van Tol, C.W.M. Kay and G. Aeppli, *Nature Materials* doi:10.1038/nmat2828 (15th August 2010)

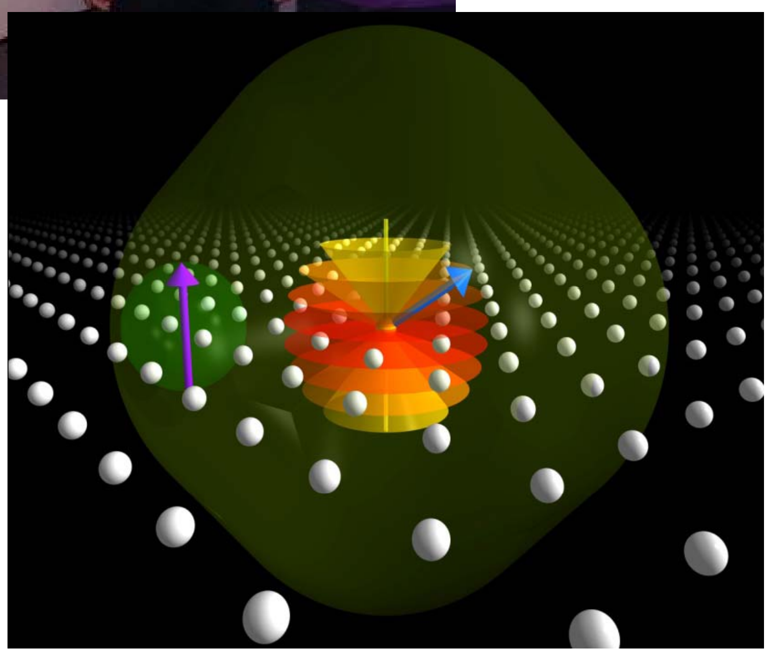
Student Research Experiences and Diversity

Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

Electron Magnetic Resonance (EMR) User Program





In addition to full-time Florida State University (FSU) graduate students affiliated with the NHMFL EMR group, a diverse group of young scientists participated in the quantum computing research program through summer research experiences. These included two students from the University of Puerto Rico-Mayaguez: Yarilyn Cedeño-Mattei, a graduate student in the Dept. of Chemistry and Chemistry of Materials, and an REU student Luis Medina (Dept. of Chemical Engineering).

In addition, Victoria Crawford, an FSU undergraduate WIMSE (Woman in Math, Science and Engineering) student, worked on the development of techniques for performing EPR under high pressures.

Microscopic Dynamics in "Supersolid" Helium

Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

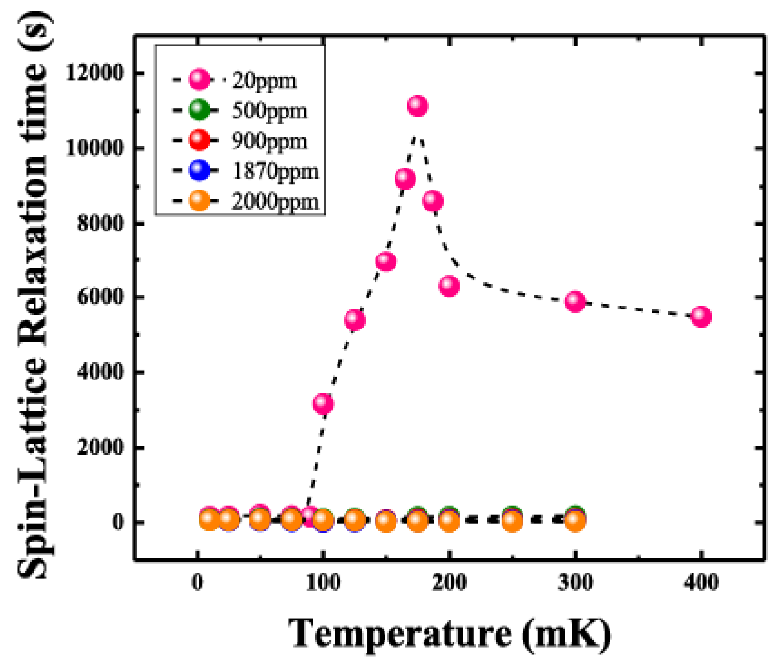
High B/T User Program / Microkelvin Laboratory

A 'supersolid' is a bizarre prediction of quantum mechanics with parallels to superconductivity and superfluidity. However, unlike its better known cousins, there is active debate whether a supersolid can really exist. In order to probe this possibility, users of the Magnet Lab's ultralow temperature facility measured the NMR relaxation rates of ^3He impurities in solid ^4He near the so-called supersolid phase transition of ^4He. This is the region where evidence of a supersolid has been reported.

These experiments are unique because NMR can measure microscopic quantum tunneling directly and thus probe the fundamental ground state better than traditional macroscopic rotation experiments.

A peak in the spin-lattice relaxation time is accompanied by a drop in the spin-spin relaxation times, pointing to a rapid change in the microscopic quantum dynamics near the supersolid transition.

Measurements of the nuclear spin-lattice relaxation time, T_1, down to 22 mK in carefully annealed samples of solid ^4He, shown for five different ^3He impurity concentrations. A sharp peak in T_1 is observed at the same temperature where macroscopic superflow is reported.



Kim, S.S.[1]; Huan, C.[1]; Yin, L.[1]; Xia, J.S.[1]; Candela, D.[2] and Sullivan, N.S.[1], *NMR Studies of ^{3}He Impurities in ^{4}He in the Proposed Supersolid Phase, Journal of Low Temperature Physics* 158, 584 (2010).

[1]NHMFL; [2]U. Mass., Hasbrouck Laboratory

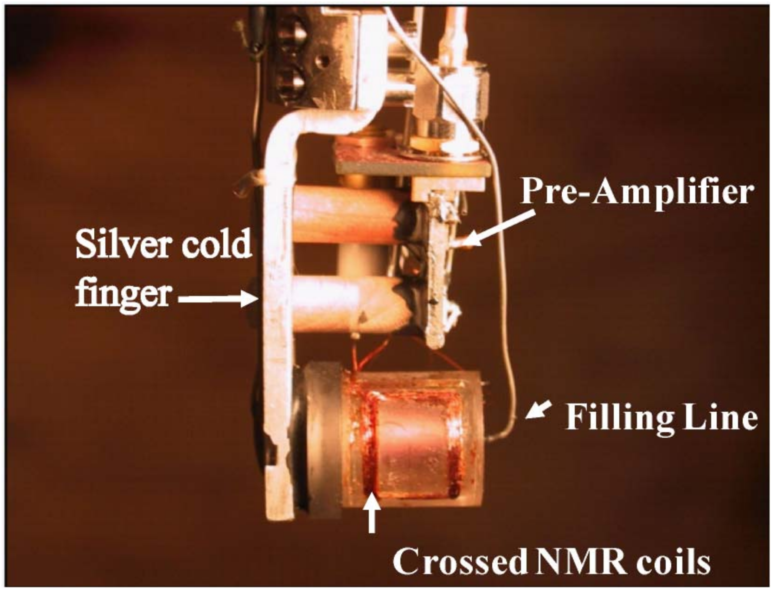
Microscopic Dynamics in “Supersolid” Helium

Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

High B/T User Program / Microkelvin Laboratory

UF UNIVERSITY of FLORIDA



NMR crossed coils and pre-amplifier shown in relation to the silver cold finger extending from the low temperature refrigerator. The nested coils are only weakly coupled to the cold finger and can float to T ~ 0.5K while the sample is maintained at T ~ 0.02K.

Huan, C.; Kim, S. S. *et al., Journal of Low Temperature Physics* **158**, 692 (2010).

In order to observe the weak signals from the small number of ^{3}He atoms (only 16 to 30 atoms for every 1,000,000 ordinary helium atoms), Magnet Lab scientists designed a unique low temperature amplifier and a nested crossed-coil configuration that could operate in an applied magnetic field down to millikelvin temperatures.

The preamplifier used a high electron mobility transistor oriented so that the plane of the chip was parallel to the applied field, an important design feature to avoid having the intense magnetic field interfere with the operation of the transistor. The operating point of the transistor could be adjusted externally by changing the gate bias, just as with ordinary transistors.

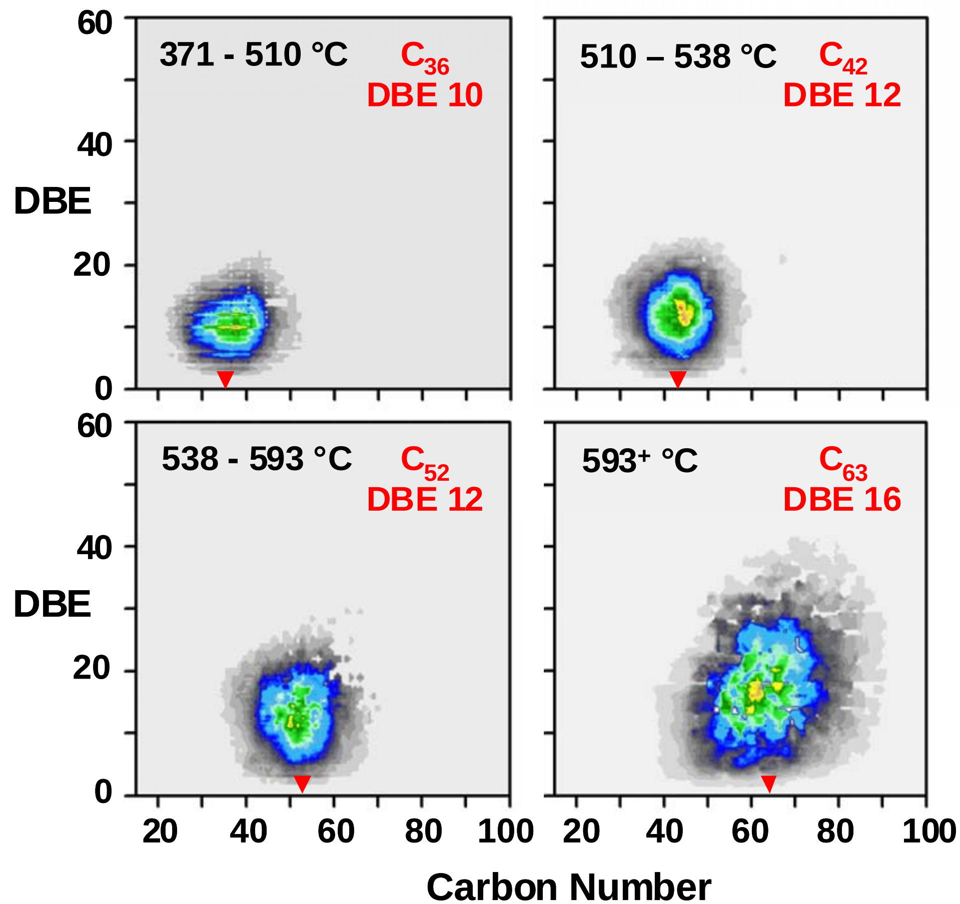
The overall noise temperature was extremely low, approximately 0.8K at 2MHz.

Molecular Basis for Petroleum Distillation

Gregory S. Boebinger, National High Magnetic Field Laboratory
DMR-Award 0654118
Ion Cyclotron Resonance User Program

Petroleum crude oil refining produces various distillation products: naphtha, gasoline, jet fuel, kerosene, lube oil, etc. "Petroleomics", the complete and detailed chemical analysis of petroleum, has been enabled by applying the highest magnetic field to Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry.

FT-ICR can sort the components of distillation products according to the number of Hydrogen, Carbon, Nitrogen, Oxygen and Sulfur atoms in each molecule. Or, as in the figure here, they can be sorted by the number of carbon atoms and "double bond equivalents (DBE = number of carbon rings plus double bonds). Note that the higher molecular weight components distill at higher temperature.



Number of molecules containing only carbon and hydrogen in a given petroleum distillation product, plotted versus number of carbon atoms and double bond equivalents (see text)

McKenna, A. M.; Purcell, J. M.; Rodgers, R. P.; Marshall, A. G. *Energy & Fuels* 2010, *24*, 2929-2938.

McKenna, A. M.; Blakney, G. T.; Xian, F.; Glaser, P. B.; Rodgers, R. P.; Marshall, A. G. *Energy & Fuels* 2010, *24*, 2939-2946.

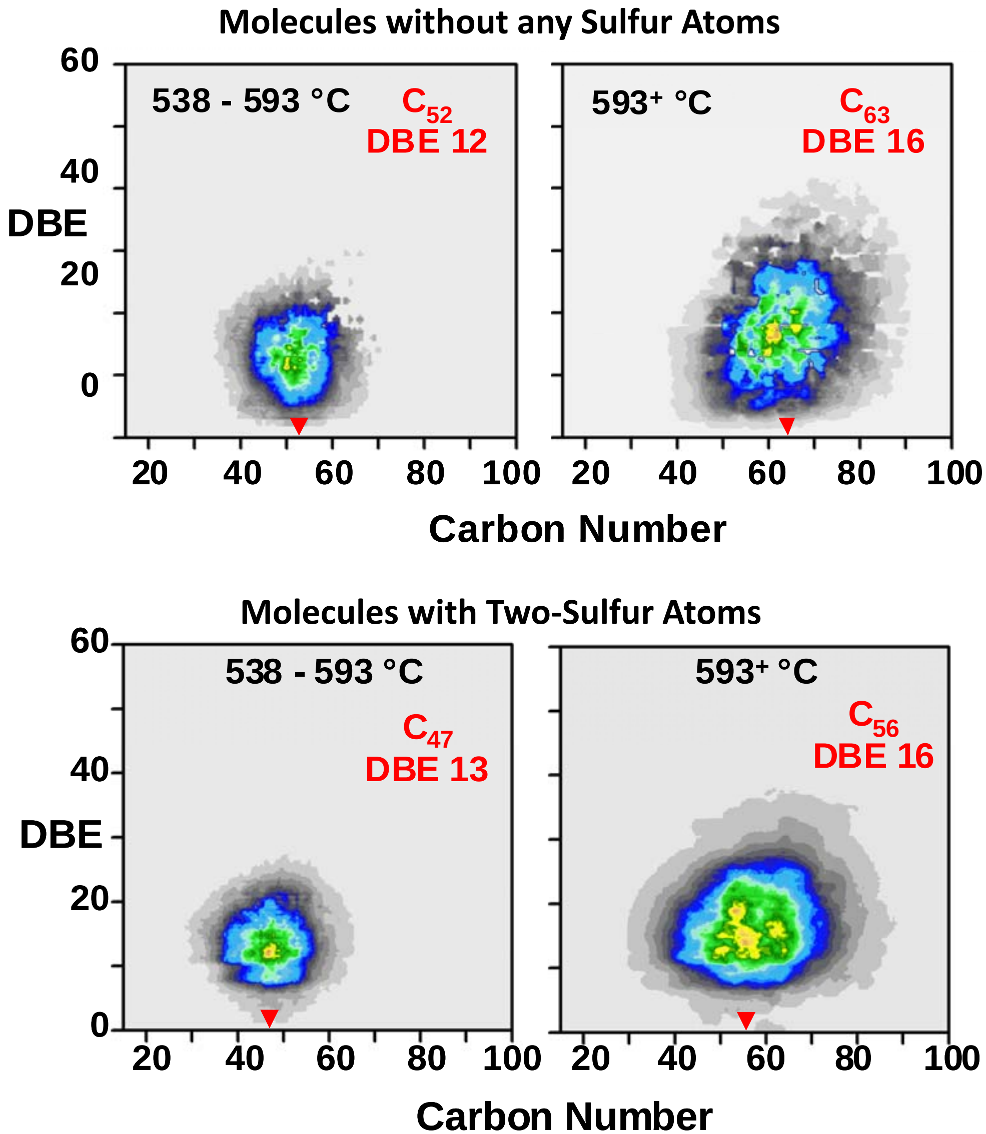
This research is also supported by Shell Global Solutions, Houston, TX.

Molecular Basis for Petroleum Distillation

Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

Ion Cyclotron Resonance User Program



Petroleomics at high magnetic field reveals that the addition of each Nitrogen, Oxygen or Sulfur atom to a hydrocarbon molecule in petroleum requires removal of two or three carbons to produce the same boiling point: compare the red arrows for molecules with only carbon and hydrogen (top panels) to those for molecules with carbons, hydrogens and two sulfurs (bottom panels).

Thus, one can predict the (economically important) distillation profile for a crude oil, based on its detailed chemical composition--one of the first uses of "petroleomics" to predict the properties and behavior of crude oil. We are applying the same approach to predict deposits, corrosion, and formation of oil/water emulsions, and to monitor oil spills.

Design and Fabrication of a Split User Magnet

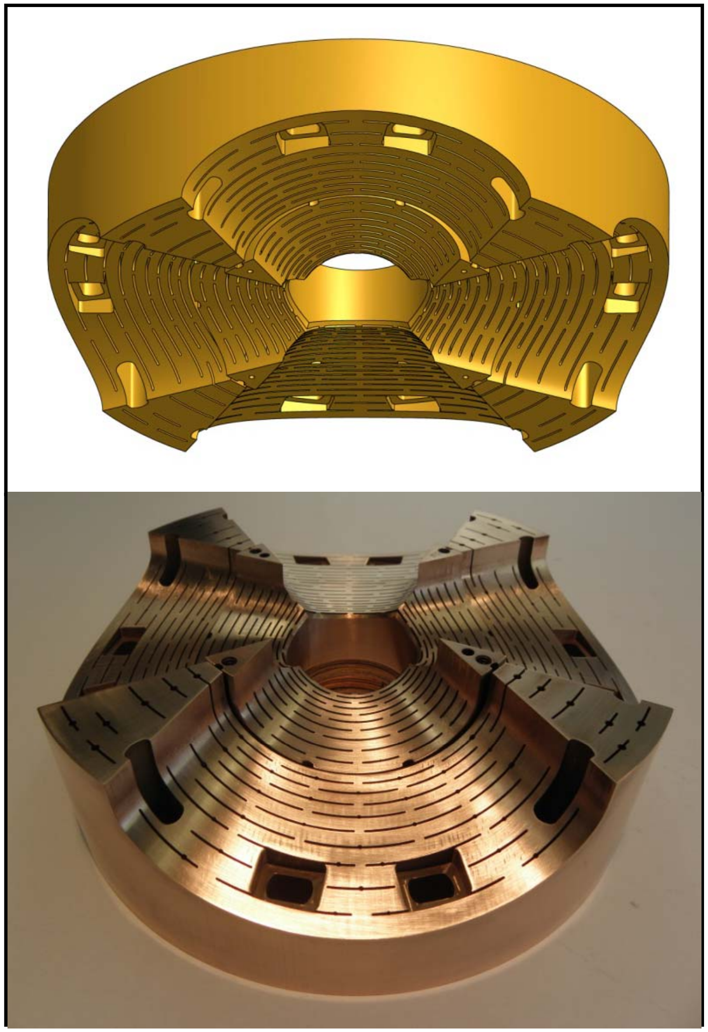
Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

Magnet Science and Technology Program

The NHMFL has completed the design and started fabrication of a high-field split resistive magnet for use in photon-scattering experiments. The magnet includes four large scattering ports of elliptical shape at the mid-plane. Such a magnet configuration results in unique design challenges being especially severe for the windings in the mid-plane region of the innermost coils. Consequently, the NHMFL incorporated its newly developed technology - called the split Florida-Helix (U.S patent #7,609,139) - into the design.

The user magnet, to be operated at the Magnet Lab's DC Facility in Tallahassee, will consist of 5 resistive coils providing a flux-density of at least 25 T at the center of the user space. All coils employ axial current grading for field optimization and stress management. Advanced finite element analysis (FEA) served as the essential tool guiding the design optimization of the overall system and the various components. Fabrication of the Split user magnet is well underway for commissioning in the Magnet Lab's user program in the coming year.



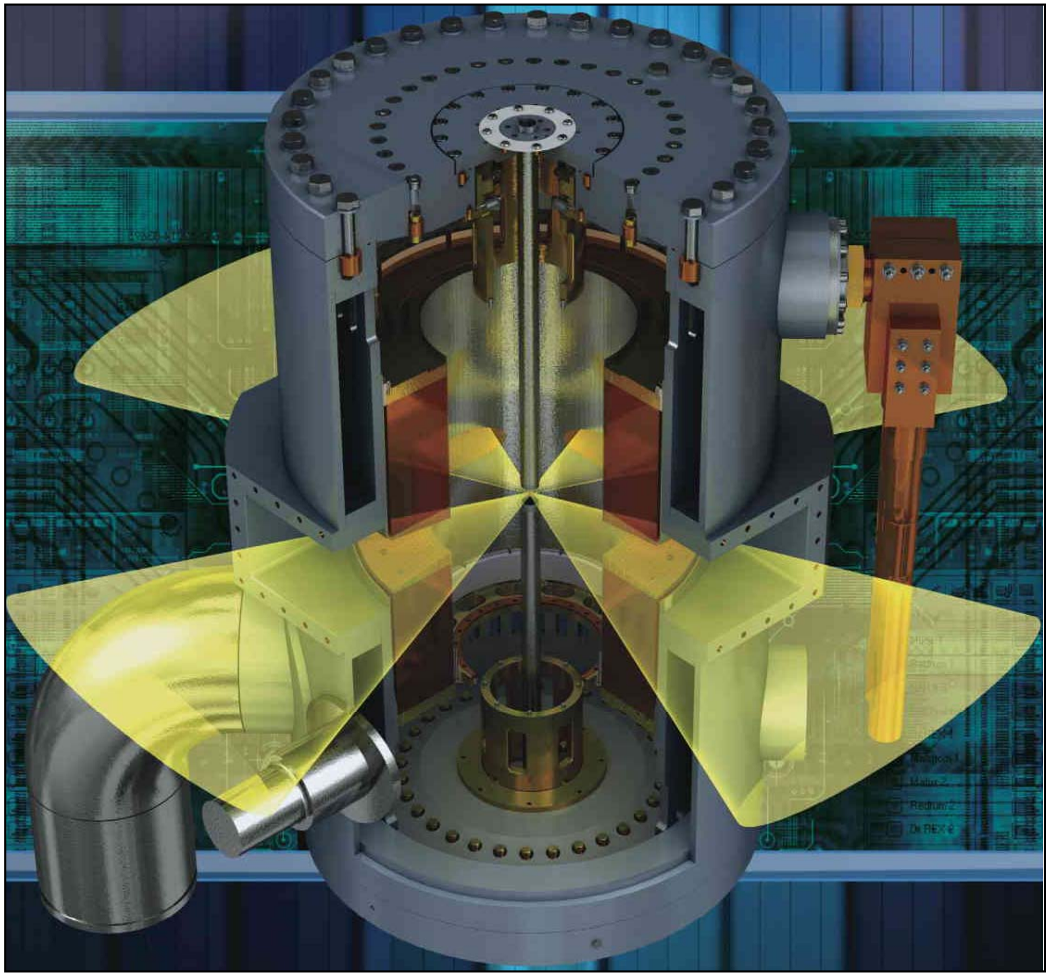
CAD-Model (top) and actual Florida-Helix magnet parts (bottom) of the innermost coils.

The New 25T Split Magnet

Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

Magnet Science and Technology Program



CAD Model of the Split User Magnet illustrated in cut view including light cones available for light scattering experiments.

When completed in the coming year, the Split Magnet will permit optical experiments that have not been possible in other resistive magnets at the Magnet Lab.

Magnet Lab users will soon will have the ability to develop and perform high-resolution Raman experiments, non-linear spectroscopies (such as second harmonic generation), and a greater variety of time-resolved experiments (such as 4-wave mixing and THz Time-Domain Spectro-scopy).

These new optical techniques will allow Magnet Lab users to create versatile optical probes for novel field-induced states that complement other techniques already performed in the Magnet Lab's user program.

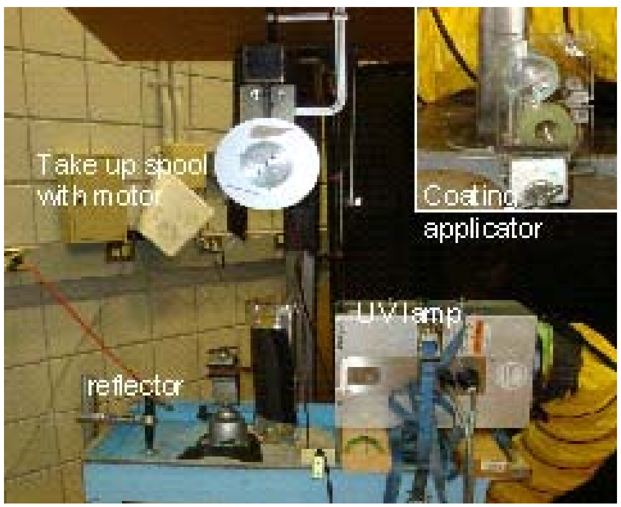
Magnet Technology Research for Undergraduates

Gregory S. Boebinger, National High Magnetic Field Laboratory

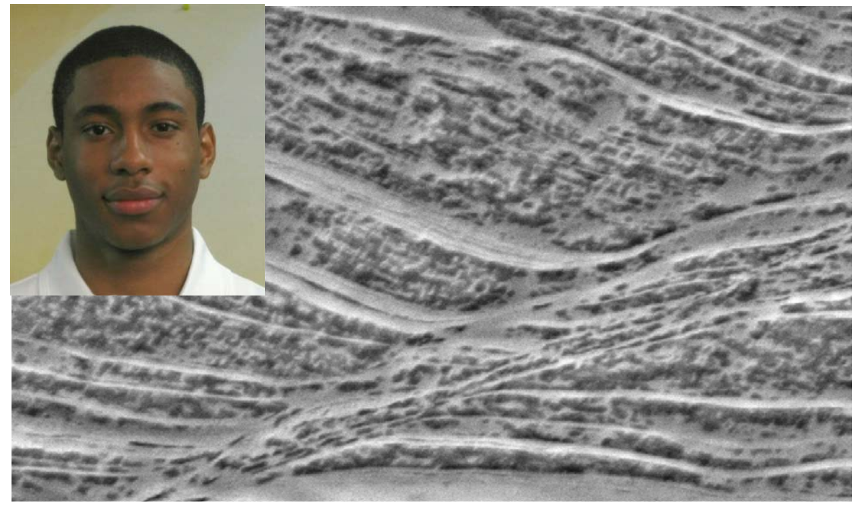
DMR-Award 0654118

Magnet Science and Technology Program

Conductor materials and insulations have a wide range of applications, not just in high field magnets. Research and education in these areas can have particularly broad impact. Scientists and engineers in the NHMFL's Magnet Science and Technology Division hosted three REU students to work on various projects that benefit both the students and research programs at the Magnet Lab.



Rana K. Mohamed from Ohio Wesleyan University studied ultraviolet-cured wire insulations using the equipment shown above. Under the mentorship of Dr. Jun Lu, Ms. Mohamed developed an efficient approach to removing insulation using organic solvents for the purpose of making necessary conductor splice joints during magnet fabrication.



The high resolution scanning electron microcopy image was taken by undergraduate Michael Cole from Georgia Tech (above). It shows nanostructured Cu-Ag obtained by a special deformation approach to high-strength conductors.

Michael Cole and Justin Mincey (left) from Bethune-Cookman University in Daytona Beach, FL worked on YBCO superconductors and high strength nanostructured Cu-Ag conductors. They were mentored by Drs. Ke Han and Yan Xin respectively.

Research Experience for K 12 Students and Teachers

Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

Magnet Science and Technology Program

Research on materials engineering is combined with K-12 outreach programs and the Magnet Lab's Research Experiences for Teachers (RET) program.

Twelve-year-old Joseph Portillo (right) and 13-year-old Olivia Merkhofer studied the ductility of O rings that are used both in the magnet facilities for the NHMFL activities and in the shuttle programs for NASA.

They were mentored by NHMFL researchers Bob Walsh and Vince Toplosky.

The students are funded in part by the annual Middle School Mentorship Program. This program is a partnership of the Magnet Lab and the School of Arts and Sciences (SAS) in Tallahassee.

Emily Morris is a 4th grade teacher from West Elementary School, Arcadia, FL and Steve Kufrovich is a science teacher from Maitland Middle school, Orlando, FL. Their research goal is to identify twin bands in materials using electron backscatter diffraction patterns and orientation imaging microscopy (OIM), both techniques to determine crystallographic orientation in polycrystalline materials. Working with Bob Goddard and Ke Han at the NHMFL, they were able to separate regular random distributed grains from twin bands, as shown by the green color in the image below. Using this method, nanoscale bands may even be distinguished from a regular grain boundary.

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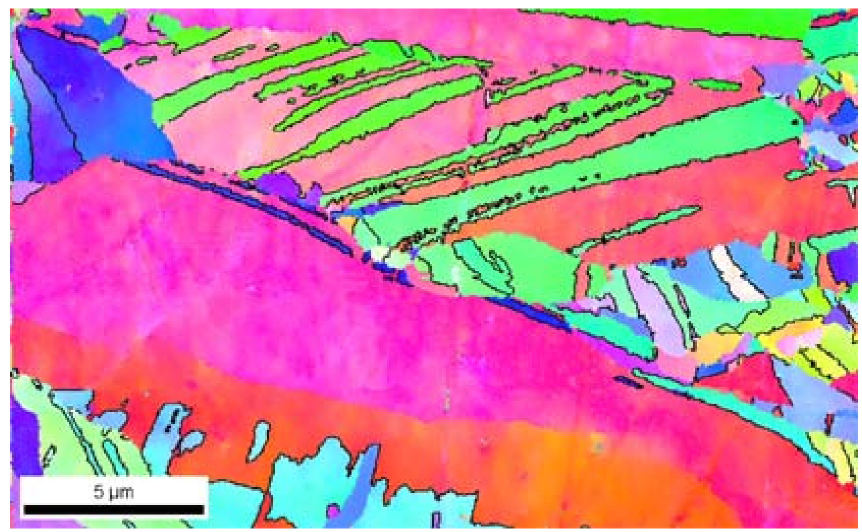


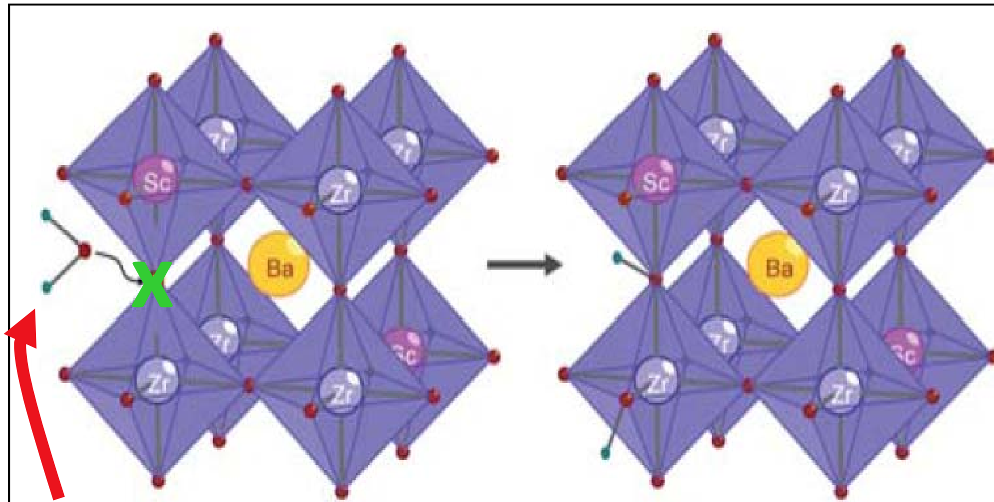
High-Field NMR Study of Solid Oxide Fuel Cell

Gregory S. Boebinger, National High Magnetic Field Laboratory
DMR-Award 0654118
NMR User Program, FSU, Tallahassee

A Solid Oxide Fuel Cell (SOFC) is an electrochemical conversion device that produces electricity directly from oxidizing a fuel. Advantages of this class of fuel cells include high efficiency, long-term stability, fuel flexibility, low emissions, and relatively low cost.

The largest disadvantage is that the operating temperature is typically very high, resulting in long start-up times and problems with mechanical and chemical compatibility at elevated temperatures.

The Professor Clare Grey group at SUNY Stony Brook and Cambridge UK uses high field NMR to study protonic conduction pathways in scandium-substituted $BaZrO_3$ perovskite-type materials which show the best results as conductor in SOFC at lower operating temperatures.



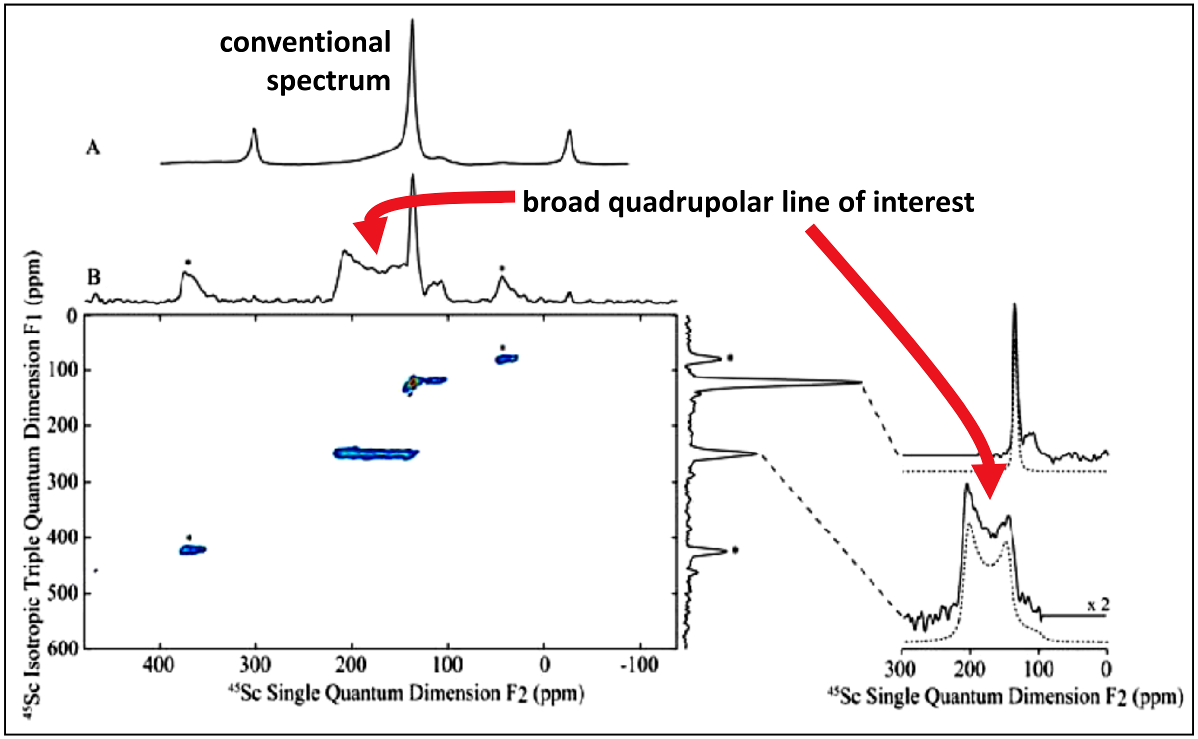
Hydration of the $BaZr_{1-x}Sc_xO_{3-x/2}$ crystal structure occurs when a water molecule (red arrow) attacks an oxygen vacancy (green 'X'). This compound is a leading candidate for solid oxide fuel cells. Yellow, blue, pink, red and green atoms respectively represent barium, zirconium, scandium, oxygen and hydrogen atoms.

This work supported in part by NSF/DMR-0804737, and the New York State Foundation for Science, Technology and Innovation via a NYSTAR award.

High-Field NMR Study of Solid Oxide Fuel Cell

Gregory S. Boebinger, National High Magnetic Field Laboratory
DMR-Award 0654118
NMR User Program, FSU, Tallahassee

• High-field (20T) NMR spectra taken at the NHMFL of scandium-substituted $BaZrO_3$ Scandium (^{45}Sc) multiple quantum magic-angle spinning (MQMAS) with Cq-selective spin-echo suppresses the bulk 6-coordinate Sc site, revealing the 5-coordinate Sc site associated with the oxygen vacancy responsible for the anionic conductance required for fuel cells to operate.



• The two-dimensional MQMAS resolves completely the broad and complex quadrupolar line shape (red arrows in figure) of the 5-coordinate Sc site for extracting electric-field-gradient and chemical shift parameters that are compared with quantum chemical calculations and known parameters to gain a detailed knowledge of the chemical processes in solid oxide fuel cells

This work supported in part by NSF/DMR-0804737, and the New York State Foundation for Science, Technology and Innovation via a NYSTAR award.

L. Buannic, F. Blanc, I, Hung, Z. Gan, C. Grey, *J. Materials Chemistry,* 20, 6322-6332 (2010)

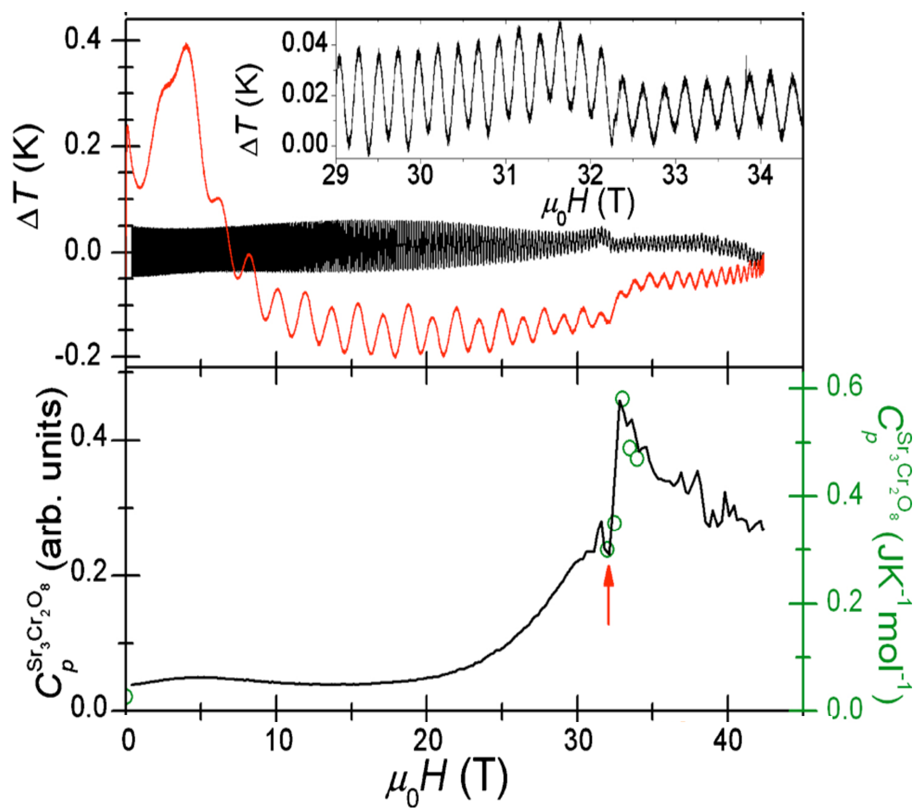
Modulation Calorimetry in Pulsed Magnetic Fields

Gregory S. Boebinger, National High Magnetic Field Laboratory
DMR-Award 0654118
Pulsed Field Facility User Program, LANL

Measuring specific heat in a rapidly pulsed magnetic field was thought to be virtually impossible; however Magnet Lab scientists recently demonstrated a rapid temperature modulation technique for heat capacity and magnetocaloric measurements of small samples in pulsed magnetic fields. Ruthenium oxide thermometry enabled precision as good as 4 mK at T = 2 K. NHMFL scientists tested the method up to $\mu_0 H$ = 50 T, but it can be extended to even higher magnetic fields.

The power of this new technique is demonstrated on the spin-dimer compound $Sr_3Cr_2O_8$ whose phase diagram was able to be completely mapped to record high magnetic fields.

Modulation calorimetry was recently made available to NHMFL users to obtain the phase diagram of heavy fermion compounds in the Ce-115 family.



(Top) Temperature oscillations in the sample recorded as a function of magnetic field to 45 T in a 250 msec long magnetic field pulse. (Bottom) Specific heat calculated from the inverse amplitude of the temperature oscillations above.

Y. Kohama, C. Marcenat., T. Klein, M. Jaime, *Rev. Sci. Instrum.* (2010) in the press.

A.A. Aczel, Y. Kohama, C. Marcenat, F. Weickert, M. Jaime, O.E. Ayala-Valenzuela, R.D. McDonald, S.D. Selesnic, H.A. Dabkowska, G.M. Luke, G.M., *Phys. Rev. Lett.,* 103, 207203 (2009).

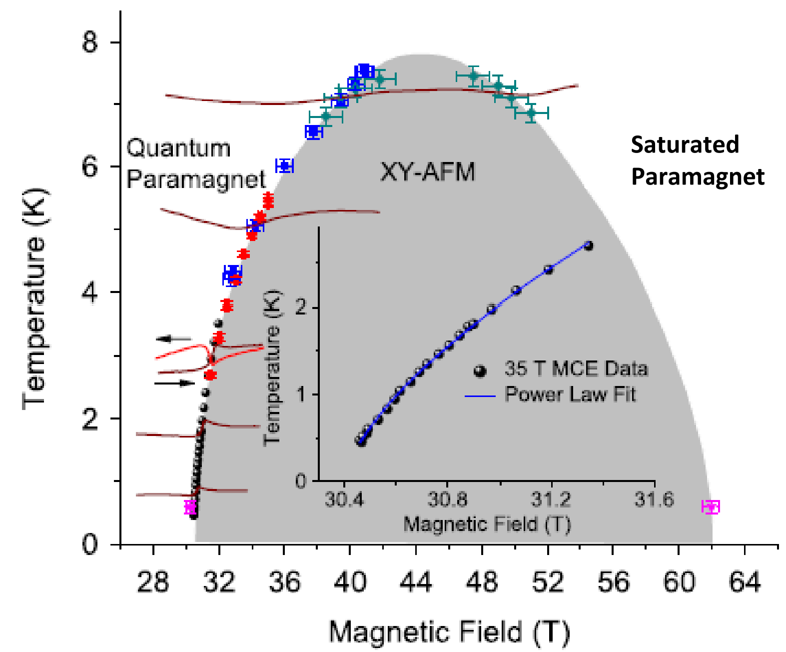
Modulation Calorimetry in Pulsed Magnetic Fields

Gregory S. Boebinger, National High Magnetic Field Laboratory
DMR-Award 0654118
Pulsed Field Facility User Program, LANL

The new modulation calorimetry developed by NHMFL scientists was used to measure the first available single crystals of the spin dimer system $Sr_3Cr_2O_8$. Magnetization, heat capacity, and magnetocaloric data up to 65 T reveal magnetic order between applied fields of $\mu_0 H_{c1}$ = 30.4 T and $\mu_0 H_{c2}$ = 62 T.

The experiments strongly suggest that $Sr_3Cr_2O_8$ is a new realization of a Bose-Einstein condensation of magnetic triplons. This field-induced BEC order (shaded region in figure) persists up to T_{max} = 8K at the optimal field of $\mu_0 H_{max}$ = 44T, the highest temperature for any quantum magnet where the upper critical field H_{c2} is experimentally accessible.

These techniques are now available to NHMFL users for modulation calorimetry experiments in DC magnets to 45T and pulsed magnets to 60T.



$Sr_3Cr_2O_8$ phase diagram with the magnetically ordered phase shaded as a guide to the eye. The new data are the blue and green points near the apex of the ordered phase, an important region beyond the reach of DC magnet techniques. The inset shows the fit to data near Hc1 to a power law $T_c = [H_c(0)-H_c(T)]^{3/2}$, a signature of Bose-Einstein condensation of magnons.

Y. Kohama, C. Marcenat., T. Klein, M. Jaime, *Rev. Sci. Instrum.* (2010) in the press.

A.A. Aczel, Y. Kohama, C. Marcenat, F. Weickert, M. Jaime, O.E. Ayala-Valenzuela, R.D. McDonald, S.D. Selesnic, H.A. Dabkowska, G.M. Luke, G.M., *Phys. Rev. Lett.,* 103, 207203 (2009).

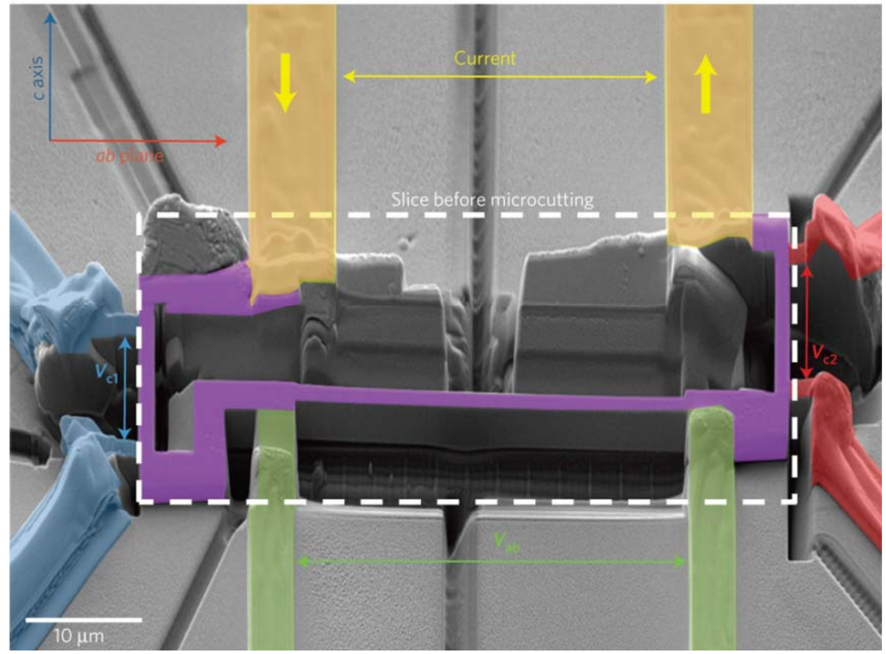
Critical Fields and Currents in SmFeAs(O,F) Microdevices

Gregory S. Boebinger, National High Magnetic Field Laboratory
DMR-Award 0654118
Pulsed Field Facility User Program, LANL

Recent discovery of new high temperature superconducting materials, iron pnictides, made exploring their potential for applications one of the foremost research goals of a collaboration among researchers from the ETH in Zurich, Switzerland and the NHMFL Pulsed Field Facility. They have developed a new approach to determine critical magnetic fields and supercurrents in micron dimension pnictide single crystals, where superconductivity is the strongest and the limits of the material can be best observed.

By using focused ion beam (FIB) techniques, they shaped microscopic crystals few square microns in cross section and attached micron-sized contacts to successfully conduct transport measurements in pulsed magnets.

P. J. W. Moll, R. Puzniak, F. Balakirev, K. Rogacki, J. Karpinski, N. D. Zhigadlo, B. Batlogg, *Nature Materials* **9**, 628–633 (2010)



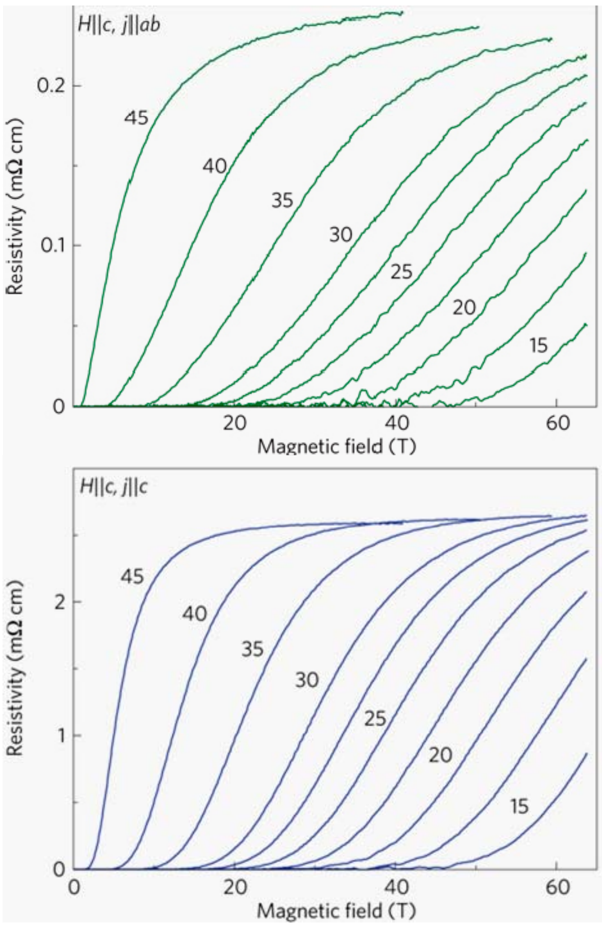
Focused ion beam etching was used to cut $SmFeAsO_{0.7}F_{0.25}$ crystals into micro bridges (purple) for transport measurements along several crystallographic directions at once. The electrical current enters and leaves the sample via the yellow contacts. Voltages are measured using the blue, green and red contacts. The dashed box is roughly 0.025mm x 0.055mm in size.

Critical Fields and Currents in SmFeAs(O,F) Microdevices

Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

Pulsed Field Facility User Program, LANL



Magnetoresistance of $SmFeAsO_{0.7}F_{0.25}$ in pulsed fields up to 65 T at various temperatures for electrical currents perpendicular (top) and along (bottom) the *c* axis.

The exquisite control of the focus ion beam allows one to cut a sample structure that is optimized for the simultaneous measurement of *c*-axis and *ab*-plane resistivity. This enables researchers to address questions of electronic anisotropy in the so-called 1111 pnictides for the first time. Remarkably, the field scale of the resistive transition is found to be essentially independent of the current direction. This is an important prerequisite for possible practical application of these materials in superconducting wires, as the super-current in a polycrystalline wire is always limited by the least favorably oriented crystallites.

Another crucial parameter, the magnetic field up to which dissipation-free current transport can be maintained, is found to be extremely high at the relatively high temperature of 40K, exceeding 30T for magnetic field along the *c* axis and 50T for magnetic field perpendicular to the *c* axis.

P. J. W. Moll, R. Puzniak, F. Balakirev, K. Rogacki, J. Karpinski, N. D. Zhigadlo, B. Batlogg, *Nature Materials* **9**, 628–633 (2010)

Cuprate Quantum Oscillations up to 85 Teslas

Gregory S. Boebinger, National High Magnetic Field Laboratory

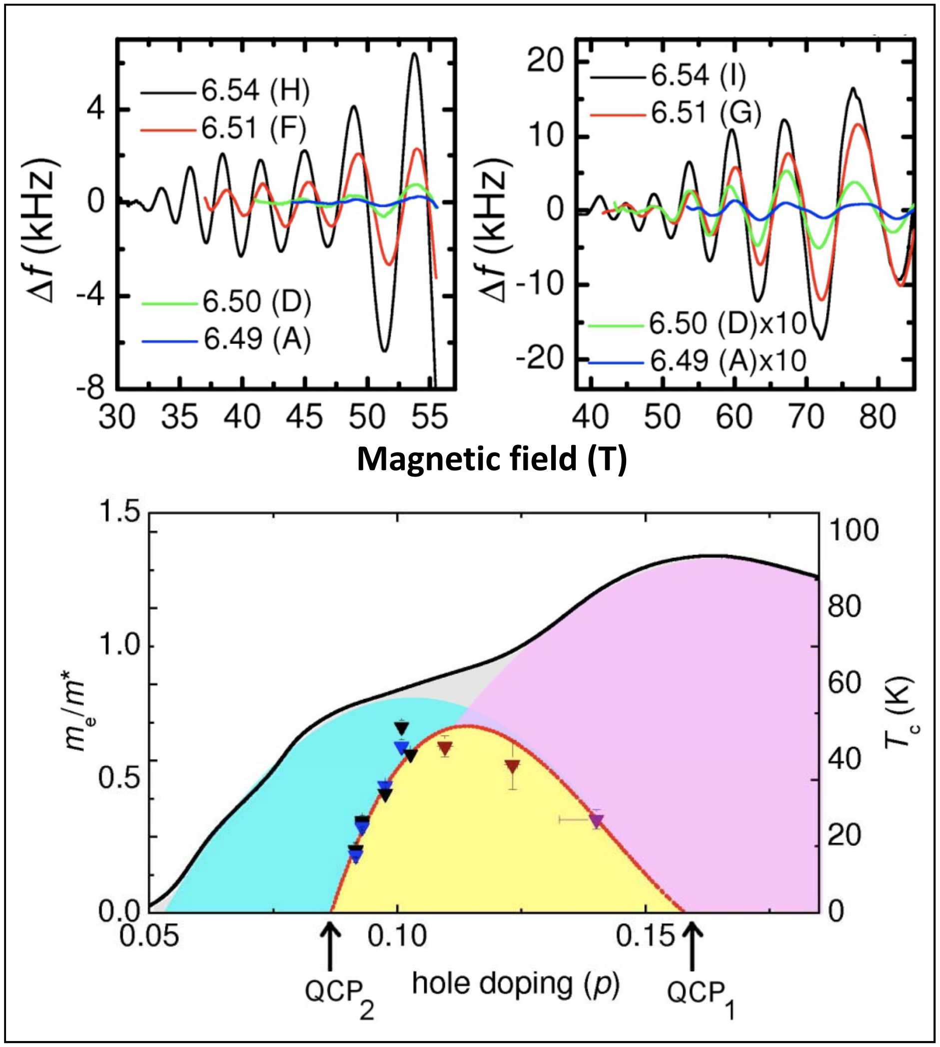
DMR-Award 0654118

Pulsed Field Facility User Program, LANL

The 85 T multi-shot (MS) magnet is a world-unique and indispensable tool for studying magnetic quantum oscillations (QO) on high-temperature cuprate superconductors.

The 85T MS magnet recently enabled a detailed doping dependent study of QO data (top figures) for compositions of YBCO from $YBa_2Cu_3O_{6.49}$ to $YBa_2Cu_3O_{6.69}$ [1,2]. The oxygen concentration is given for each sample in the figures.

The high magnetic fields allow disordered samples to still exhibit QOs *and* give a very large magnetic field window over which the QO's are observed. This enables researchers to resolve multiple QO frequencies in a sample [2]. The QO data also allow doping-dependent trends - for example, in effective mass *m** (lower figure) - to be tracked in detail for the first time over a large range of the phase diagram [1,2].



[1] S.E. Sebastian, N. Harrison, M.M. Altarawneh, C.H. Mielke, R. Liang, D.A. Bonn, W.A. Hardy and G.G. Lonzarich PNAS 107 (14) 6175-6179 (2010).

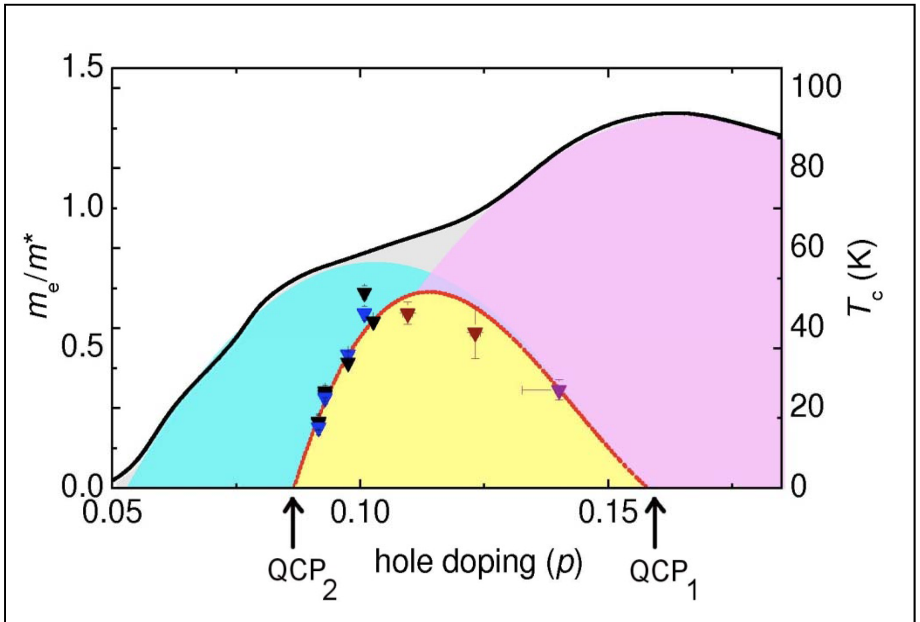
[2] J.Singleton, C. de la Cruz, R. D. McDonald, S. Li, M. Altarawneh, P. Goddard, I. Franke, D. Rickel, C. H. Mielke, X. Yao and P. Dai, Phys. Rev. Lett. 104, 086403 (2010).

Cuprate Quantum Oscillations up to 85 Teslas

Gregory S. Boebinger, National High Magnetic Field Laboratory

DMR-Award 0654118

Pulsed Field Facility User Program, LANL



The 85 T pulsed magnet at the Magnet Lab offers a unique platform for probing the phase diagram of high-temperature superconductors. In YBCO, experiments at 85 T reveal a dramatic upturn in the effective mass *m** at lower hole doping [1]. Plotted at left is the inferred collapse in the inverse mass m_e/m^* (or Fermi temperature) approaching the metal-insulator crossover at a quantum critical point QCP_2 — the very first thermodynamic evidence for a global divergent susceptibility beneath the superconducting dome.

The experiments also extended the hole doping range further towards optimal doping [2]— linking up with previous 85 T data on $YBa_2Cu_4O_8$ (also taken at the NHMFL and published in 2008). The doping dependence of the effective mass strongly suggests a second quantum critical point (QCP_1) close to optimal doping [1,2]. There are therefore likely to be two thermodynamic quantum critical points beneath the high-temperature superconducting dome, suggestive of the possible involvement of quantum criticality in two superconducting subdomes (blue and pink in the figure).

[1] S.E. Sebastian, N. Harrison, M.M. Altarawneh, C.H. Mielke, R. Liang, D.A. Bonn, W.A. Hardy and G.G. Lonzarich PNAS 107 (14) 6175-6179 (2010).
[2] J.Singleton, C. de la Cruz, R. D. McDonald, S. Li, M. Altarawneh, P. Goddard, I. Franke, D. Rickel, C. H. Mielke, X. Yao and P. Dai, Phys. Rev. Lett. 104, 086403 (2010).

NNIN Highlights

Nano-Optical Superlenses with Negative-Index Metamaterials
Sandip Tiwari, Cornell University, ECCS - 0335765

Cantilevers with Integrated Mesoscopic Samples
Sandip Tiwari, Cornell University, ECCS - 0335765

Hydrodynamic Metamaterials: Nanofabricated Arrays to Steer, Refract and Focus Streams of Biomaterials
Sandip Tiwari, Cornell University, ECCS - 0335765

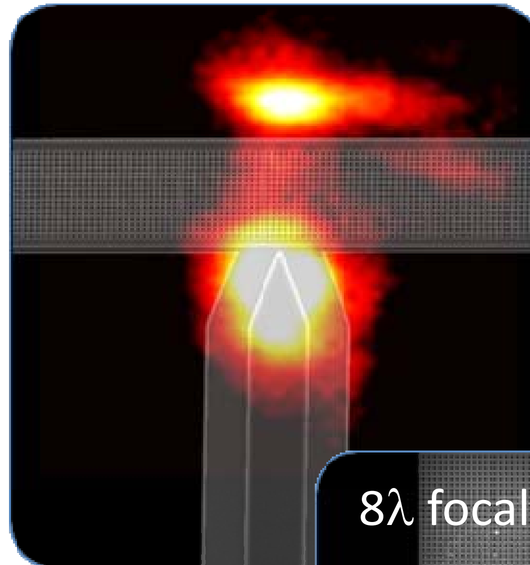
Probing Vortex Dynamics in Superconductors with Nanoscale Weak-Pinning Channels
Sandip Tiwari, Cornell University, ECCS - 0335765

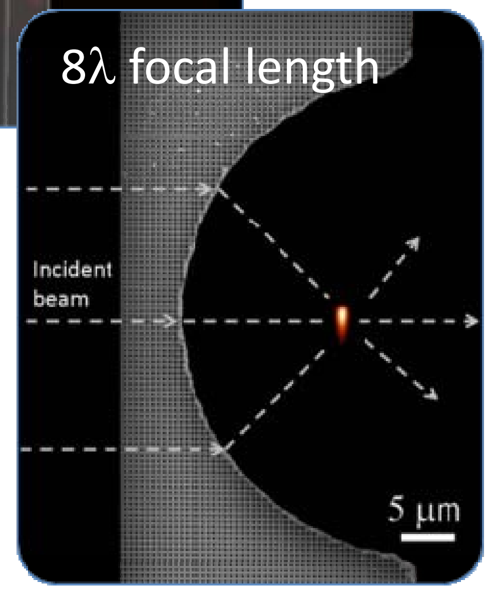
Nano-Optical Superlenses with Negative-Index Metamaterials

Sandip Tiwari, Cornell University, ECCS - 0335765

We have demonstrated experimentally the imaging at 1.55 μm wavelength by a generalized photonic crystal superlens (Fig. 1) nanofabricated in InGaAsP/InP heterostructure. By designing a suitable lens surface termination, an image spot size of $0.12\lambda^2$ was achieved, demonstrating superlens imaging with sub-wavelength resolution well below the diffraction limit ($0.5\lambda^2$).

http://sagar.physics.neu.edu





We have created a new nano-optical microlens that focuses infrared light at telecommunication frequencies. The two-dimensional metamaterial microlens, which uses the negative refractive index, was created by nano-engineering a photonic-crystal substrate into a multi-layered semiconducting wafer. The focusing power of this microlens sets a world record for one of the shortest focal lengths ever achieved, focusing the infrared beam to a spot just 12 microns away from the surface— at the limit of diffraction laws. In addition, the location of the focused light image was very sharp with little blurring. This represents a significant advance in light imaging technology and has the potential to lead to innovations in high density imaging systems.

Nano-Optical Microlens with Ultra-Short Focal Length using Negative Refraction

Y. Huang, Northeastern Unviersity.
Work performed at Harvard CNS facility

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Nanoscale Science, Engineering & Technology

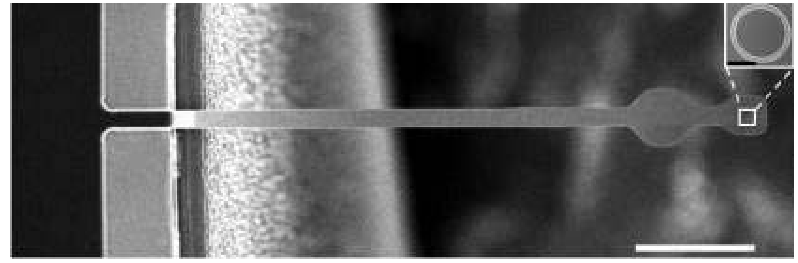
Cantilevers with Integrated Mesoscopic Samples

Sandip Tiwari, Cornell University, ECCS - 0335765

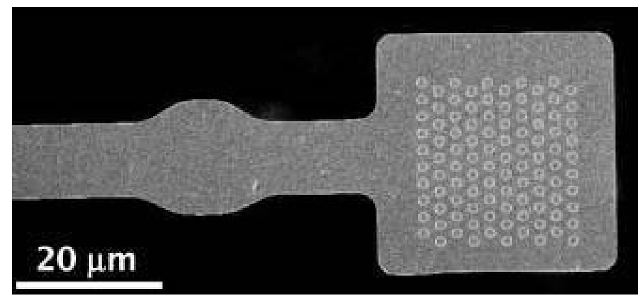
A normal (resistive) metal ring threaded by a magnetic flux can support a dissipationless current. Such a persistent current follows from a quantum mechanical treatment of the metal's conduction electrons bound by the periodic potential of the ring.

This project studies persistent currents in normal metal rings using a cantilever as a torsional magnetometer.

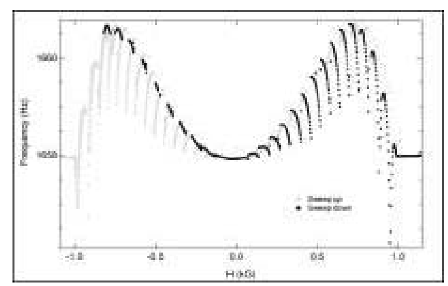
To make these measurements, we have fabricated high sensitivity cantilevers with integrated metal rings. At T = 300 mK, the force sensitivity of the cantilevers is measured to be 1.6 aN/Hz. We have measured superconducting persistent currents in Al rings and are proceeding with our measurements of persistent currents in the normal state.



SEM micrograph of a fabricated silicon cantilever. The cantilever is 40 µm wide. Inset shows a detail of the single Al ring at the end of the cantilever.



SEM micrograph of a fabricated silicon cantilever with an array of rings.



Cantilever's resonant frequency showing periodic oscillations due to flux quantization in the Al ring at the cantilever's end.

Jack Harris, Yale University
Work performed at Cornell NanoScale Facility

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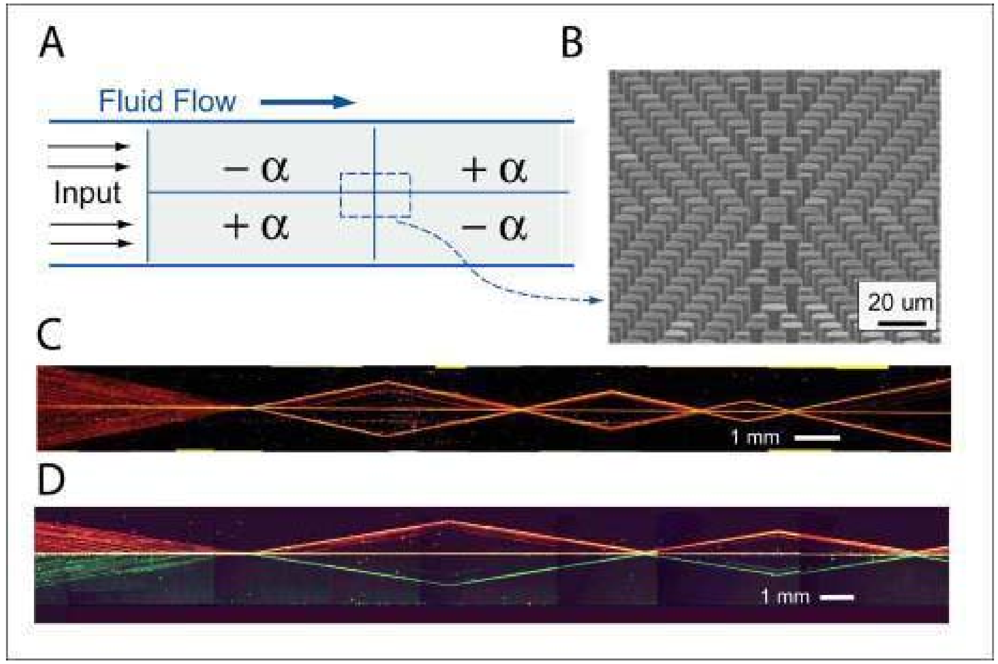
Hydrodynamic Metamaterials: Nanofabricated Arrays to Steer, Refract and Focus Streams of Biomaterials

Sandip Tiwari, Cornell University, ECCS - 0335765

It is possible to direct particles entrained in a fluid along trajectories much like rays of light in classical optics. An asymmetric-post array forms the core hydrodynamic element and is used as a building block to construct nanofluidic metamaterials and demonstrate refractive, focusing and dispersive pathways for flowing beads and cells. The core element is based on the concept of *deterministic lateral displacement* where particles choose different paths through the asymmetric array based on their size: particles larger than a critical size are displaced laterally at each row by a post and move along the asymmetric axis at an angle to the flow, while smaller, sub-critical particles move with the flow. These modular, nanofluidic metamaterials form a rich design toolkit for mixing, separating and analyzing cells and functional beads on-chip.



Complex nanofluidic metamaterial
A. Schematic of a complex metamaterial constructed by tiling several focusing, defocusing, and refractive elements.

B. SEM image showing the interface between four sub-elements.

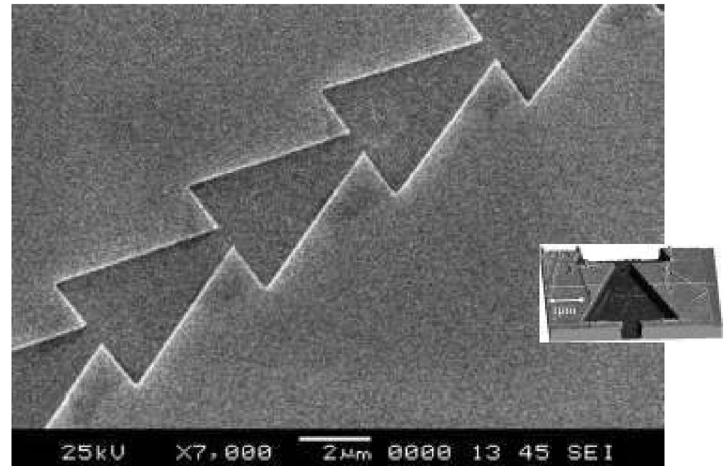
C&D Time exposure images showing particle motion through a series of different elements, motion is from left to right.(C) using just a single inlet and single outlet port. (D) with two separate inputs allowing two different-colored bead streams in the top and bottom halves of the device.

Robert Austin, Princeton University
Work performed at Cornell NanoScale Facility

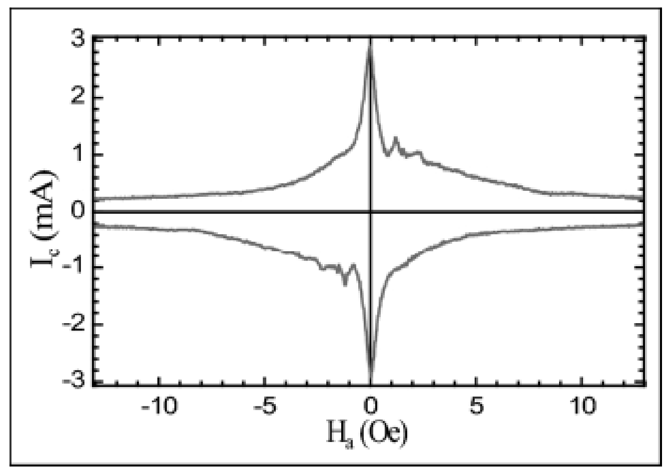
Probing Vortex Dynamics in Superconductors with Nanoscale Weak-Pinning Channels

Sandip Tiwari, Cornell University, ECCS - 0335765

Vortices are quantized bundles of magnetic flux that thread many different superconductors over a particular range of applied magnetic field. For technological applications of superconductors in large magnetic fields, controlling the dynamics of magnetic flux vortices that penetrate the superconductors is important, as the motion of many vortices can cause unwanted dissipation. By etching asymmetric patterns for the channel walls, we are able to produce a vortex ratchet, which results in the directed motion of vortices when driven with an oscillatory force with zero mean. Such ratchets may provide controllable model systems for investigating the dynamics of certain molecular motors. At low temperatures, and in the absence of pinning and dissipation, a vortex can be described quantum mechanically and may exhibit phase coherence, allowing for the possibility of a vortex interfering with itself or tunneling between two different positions. Studies of such behavior helps guide fundamental understanding and could provide a new route for quantum computing.



Scanning electron microscope (SEM) image of ratchet channel. Inset: Atomic force microscope (AFM) image of ratchet channel.



Measurement of critical current as a function of magnetic field for set of vortex ratchet channels showing asymmetry with respect to current and field directions.

Britton Plourde, Syracuse University
Work performed at Cornell NanoScale Facility

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SRC Highlights

Disentangling the Charge Transport Mechanisms in Organic Semiconductors
Hartmut Höchst, Synchrotron Radiation Center, DMR 0537588

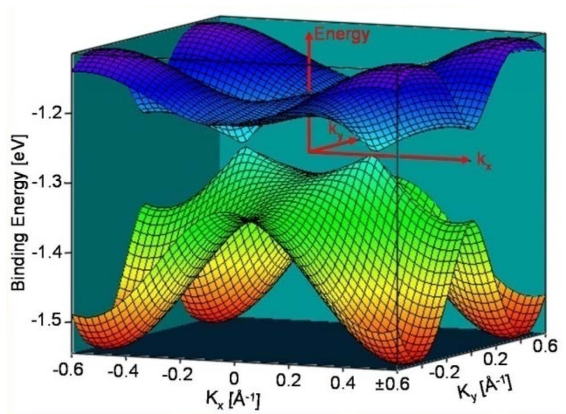
NEXAFS Spectroscopy of Tailored Molecules for Solar Cell Applications
F. J. Himpsel, Physics Dept. UW-Madison
Synchrotron Radiation Center operated under Grant No. DMR-0537588

Observations of a kink in the dispersion of f-electrons
Tomasz Durakiewicz, Los Alamos National Laboratory
The Synchrotron Radiation Center operated under Grant No. DMR-0537588

Disentangling the Charge Transport Mechanisms in Organic Semiconductors

Hartmut Höchst, Synchrotron Radiation Center, DMR 0537588

Intellectual Merit: This work sheds light on a decades-old problem of how charges are transported through a crystal consisting of organic molecules. Dr. Höchst and his collaborators utilized the tunabilty of the synchrotron radiation in their experiments on Pentacene, a prototypical organic semiconductor, to understand how charges are transported through this material. Furthermore, their experiments on the interaction between charges and lattice vibrations in crystalline Pentacene films demonstrated that vibrations can, astoundingly, both aid and hinder charge transport.



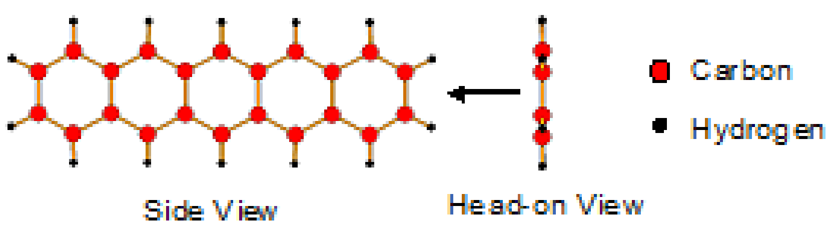
Band structure of the highest occupied molecular orbital region of Pentacene as determined from angle resolved photoemission spectroscopy with synchrotron radiation.

R. C. Hatch, D. L. Huber, and H. Höchst, "Electron-phonon Coupling in Crystalline Pentacene Films," Phys. Rev. Lett. **104,** 047601-1–047601-4 (2010)

Disentangling the charge transport mechanisms in organic semiconductors

Hartmut Höchst, Synchrotron Radiation Center

Broader Impacts: Understanding charge transport through organic semiconductors is key in explaining why these materials are promising candidates for novel electronic applications such as flexible computer displays, spray- or paint-on solar cells, and "printed" electronics, with mass production coming off a rotary printing press rather than by the elaborate and tedious production steps currently involved in the fabrication of electronic circuits. Considering the much simpler manufacturing processes and their comparatively low environmental impact, solar cells based on organic molecules can be a key in solving the world's energy crisis.



Pentacene is a molecule comprised of carbon and hydrogen atoms. Researchers make Pentacene crystals on top of metals and other materials. These organic crystals behave just like conventional semiconductors (i.e. silicon).

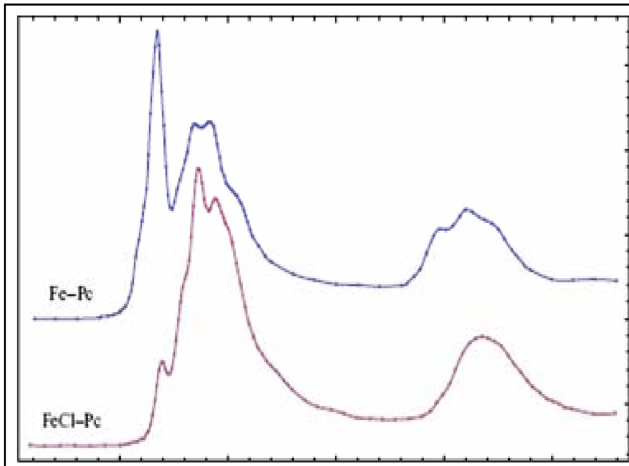
NEXAFS Spectroscopy of Tailored Molecules for Solar Cell Applications

F. J. Himpsel, Physics Dept. UW-Madison

Synchrotron Radiation Center operated under Grant No. DMR-0537588

Intellectual Merit: The key obstacle to using sunlight as a significant alternative energy source is the cost of solar cells. The cost of both materials and production can be reduced by replacing crystalline silicon with inexpensive organic dyes. Plants use such dyes for photosynthesis. While it is possible to create dye-sensitized solar cells, their efficiency needs to be improved. In order to overcome these limitations Himpsel's group started a systematic investigation of dye molecules using synchrotron light. It involves an international collaboration with synthetic chemists and theorists in Spain. The ultimate goal is to provide feedback on how to systematically optimize the molecules used in dye-sensitized solar cells.

P. L. Cook, X. Liu, W. Yang, and F. J. Himpsel, NEXAFS Spectroscopy of Biomimetic Dye Molecules for Solar Cells, J. Chem. Phys. ***131****, 194701 (2009).*



Iron is widely used by nature for charge transfer and is an inexpensive element for use in solar cells. NEXAFS spectros-copy distinguishes the two oxidation states involved in the charge tranfer, +2 (blue) and +3 (red).

Home of Aladdin

NEXAFS Spectroscopy of Tailored Molecules for Solar Cell Applications

F. J. Himpsel, Physics Dept. UW-Madison

Broader Impacts: Currently, the best efficiency in dye-sensitized solar cells is reached with dyes based on expensive metals, such as ruthenium. This project means to systematically identify efficient, yet inexpensive dyes and designs for solar cells, for example by going from ruthenium to iron or manganese, which is used by nature in photosynthesis. A successful feedback from spectroscopy to synthetic chemistry and solar cell design would lead to inexpensive solar cells that could be mass-produced. Our nation would have a viable alternative and environmentally friendly energy resource.

The collaboration with Spain makes graduate students and postdocs familiar with international interactions and brings in the significant know-how about solar energy.

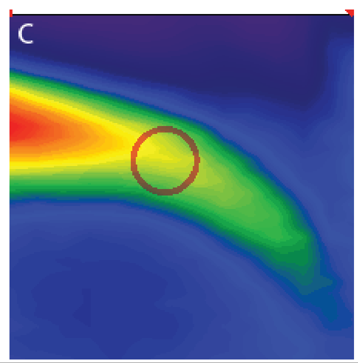
This work was supported by the NSF under Award Nos. DMR-0520527 (MRSEC) and DMR-0537588 (SRC).
A proposal to the NSF (CHE-1026245) has been recommended for funding by the program director. Its title:
"International Collaboration in Chemistry: Molecules at Nanostructured Surfaces for Solar Cell Applications"

Observations of a kink in the dispersion of f-electrons

Tomasz Durakiewicz, Los Alamos National Laboratory
The Synchrotron Radiation Center operated under Grant No. DMR-0537588

Intellectual Merit: In every electronic device a noticeable amount of the electricity flowing through it is wasted. As the electricity flows through the device it encounters resistance which heats up the device and prevents it from performing optimally. This issue can be solved by a physics phenomenon known as superconductivity. Superconductivity happens when matter becomes so cold that all electrical resistance disappears. With no resistance there is no heat and the electricity can flow much more efficiently. Using synchrotron radiation produced at the Synchrotron Radiation Center a team from the Los Alamos National Laboratory team studied the electron configurations of f-electrons (outer shell of the atom) in a handful of different elements such as uranium. These observations resulted in witnessing peculiar behaviors and patterns in these atom's structures which have potential connections to creating higher temperature superconductors.

Tomasz Durakiewicz, John Joyce, Kevin Graham, Yinwan Li – Los Alamos Alamos National Laboratory



High resolution angle resolved photoemission spectra taken at SRC showing the location of the kink in the dispersion of f-electrons.

Observations of a kink in the dispersion of f-electrons

Tomasz Durakiewicz, Los Alamos National Laboratory

Broader Impacts: One of today's main hurdles in maintaining a superconducting state is that it must be at extremely low temperatures such as -321°F which is costly. The benefits of superconducting materials are apparent when looking at the efficiency of power transmission through the electric grid. Currently the combination of inefficiencies in power production combined with running the electricity through thousands of miles of wire results in less than a 30% efficiency due to the wasteful conversion into heat. Having a substance that can remain in a superconducting state at warmer temperatures is less costly and makes streamlining this technology more feasible.

Work supported by the US Department of Energy, Office of Science, Division of Materials Science and Engineering, and the LANL LDRD Program. The SRC is operated under NSF Grant No. DMR-0537588.

SRC Home of Aladdin

MRI Highlights

Multi-User X-ray Diffraction System for Advanced Materials Analysis
Robert J. Lad (University of Maine), DMR-0521043

Applications of an Undergraduate FE-SEM facility
David M. Tanenbaum (Pomona College), DMR-0618417

Zero-Background Scatterless Hybrid Slits for Synchrotron and In-house SAXS Applications
Cyrus R. Safinya, University of California-Santa Barbara, DMR 0619171

High-Resolution S/TEM at U. Wisconsin & U. Puerto Rico
Paul M. Voyles, University of Wisconsin-Madison, DMR 0619368

IRENI: Infrared Environmental Imaging
Carol J. Hirschmugl, University of Wisconsin-Milwaukee, DMR 0619759

X-ray MicroCT Imaging of Self-Healing Polymers
Paul V Braun, UIUC, DMR-0721324

MRI: Acquisition of a Fast-Pulse-Laser for a Local Electrode Atom Probe
G.B. Thompson, M. L. Weaver, T. Klein, W. Butler and D.E. Nikles
University of Alabama, Tuscaloosa, AL, DMR-0722631

Development of Efficient Thermal Neutron Position Sensitive Detectors
Anton S. Tremsin, University of California at Berkeley, DMR 0753599

Development of an Ultra-fast Optical Spectroscopy System for Multi-disciplinary Studies
Kenneth J. Rothschild, Trustees of Boston University, DMR 0821450

Development of a Portable Laser Heating System
Ho-kwang Mao, Carnegie Institution of Washington, DMR 0821584

Defect evolution in diblock copolymer films
Lee Park, Ward Lopes, Claire Ting (Williams College), DMR-0922400

MRI: Acquisition of Nanoindentation System at UPRM
Agnes M. Padovani (U. of Puerto Rico-Mayaguez), DMR-0922994

Rare Earths in Sol-Gel Glasses
Daniel M. Boye, Davidson College DMR-0959552

Acquisition of a Confocal Raman / AFM Hybrid System
Felicia S. Manciu, University of Texas–El Paso, DMR-0723115

Development of an Intense Positron Annihilation Spectrometry System for Nanophase Characterization
Ayman I. Hawari, North Carolina State University, DMR-0521270

Development of Synchrotron Infrared Microspectroscopy Imaging using a Multielement Detector (IRMSI-MED) for Diffraction-Limited Chemical Imaging
Carol J. Hirschmugl (University of Wisconsin-Milwaukee), DMR-0619759

IRENI at the SRC
Carol J. Hirschmugl (University of Wisconsin-Milwaukee), DMR-0619759

Major Research Instrumentation (MRI): Development of an In-Situ Neutron Scattering Facility for Research and Education in the Mechanical Behavior of Materials
P. K. Liaw, University of Tennessee, Knoxville, DMR-0421219

Local Electrode Atom Probe – Tomographic Characterization of III-V Semiconductor Structures
James S Speck, University of California Santa Barbara, DMR-0821168

Eliminating Parasitic Slit Scattering in Small Angle X-ray Diffractometers
C. R. Safinya, UC Santa Barbara, DMR-0619171

MRI: Acquisition of an Atomic Force Microscope for Undergraduate Research and Education
Dean A. Waldow, Pacific Lutheran University, DMR-0619826

Dual Beam FIB/FESEM at Missouri S&T
F. Scott Miller (Missouri S&T), DMR-0723128

Atom Probe Tomography of Advanced GaN-based LEDs
James Speck, University of California-Santa Barbara, DMR 0821168

MALDI Imaging and Traveling Wave Ion Mobility Mass Spectrometry in Materials Research
Chrys Wesdemiotis, The University of Akron, DMR-0821313

Multi-User X-ray Diffraction System for Advanced Materials Analysis

Robert J. Lad (University of Maine), DMR-Award 0521043

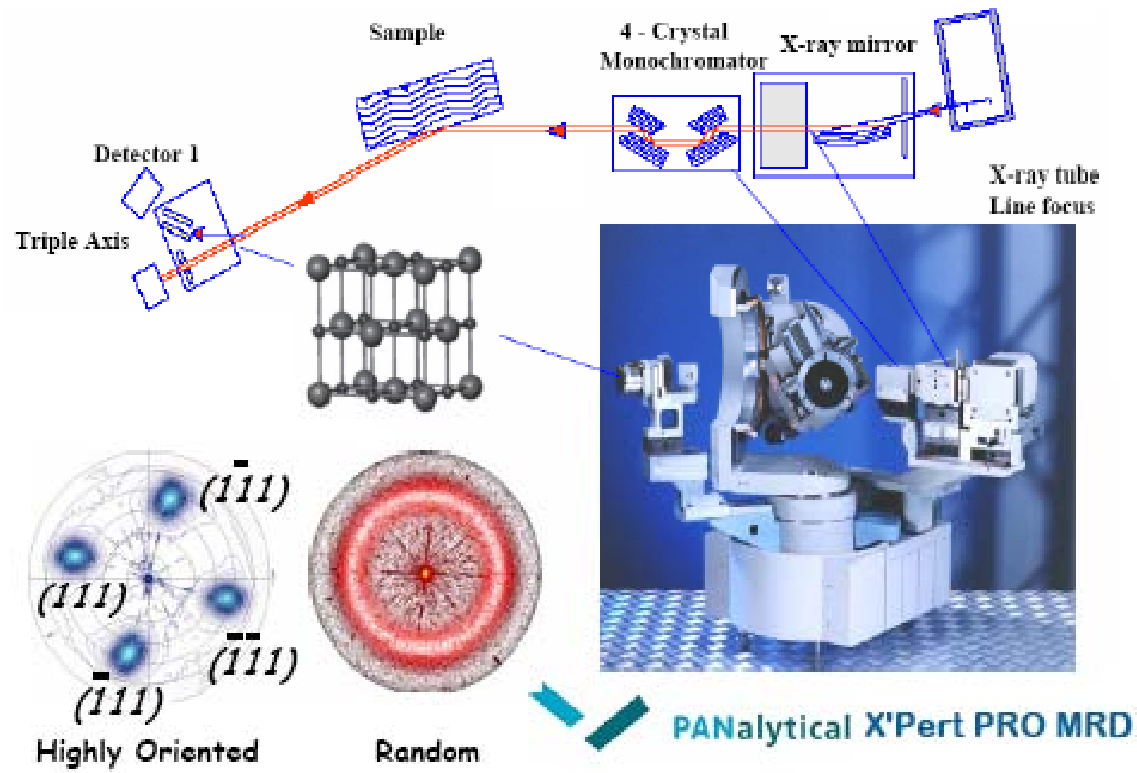
THE UNIVERSITY OF MAINE

Project Summary

A high resolution X-ray Diffraction (XRD) system is providing critical information about the structural properties of materials at the atomic, molecular, and nanometer scale. Specific measurement capabilities include phase analysis, reciprocal space mapping, pole figure analysis, reflectometry, rocking curve analysis, stress and texture analysis, and topography.

Types of Materials Analyzed by XRD at UMaine

- zeolites and powder catalysts
- piezoelectric single crystals
- AlN/InN and Ni/TiO_2 multilayer structures
- poly-silicon and silver oxide films
- Pt-Rh alloy electrode structures
- As-S-Se and metal oxide gas sensing films
- oxynitride wear resistant coatings
- wood/carbon fiber composites
- carbon nanotubes
- cellulose films and fibers
- nanoporous inorganic membranes



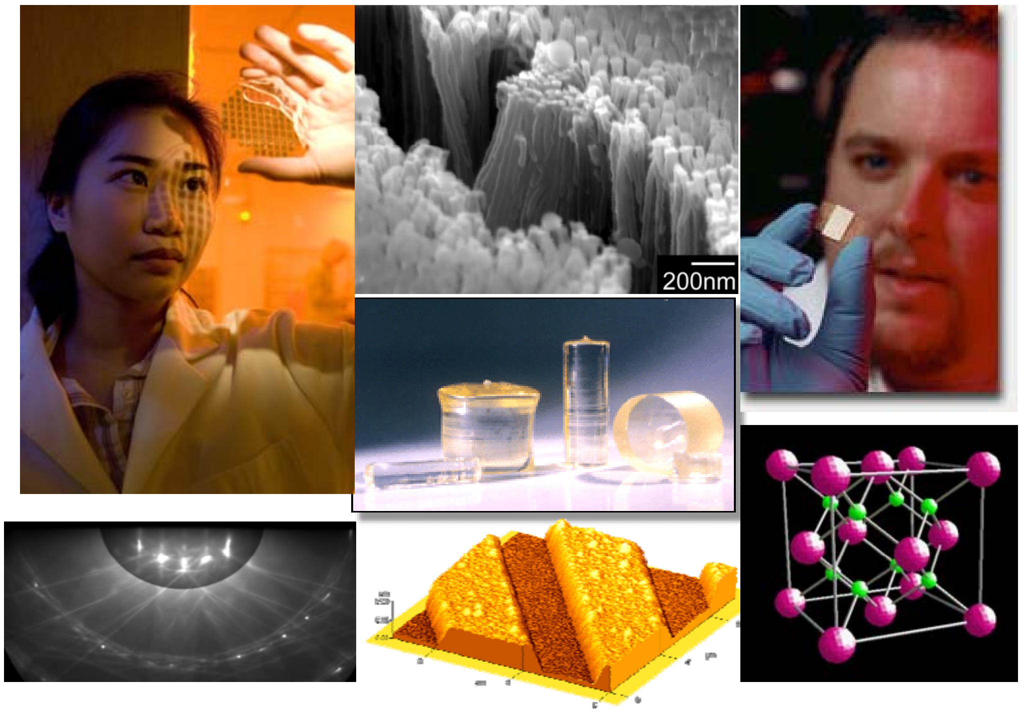
Example: X-ray diffraction analysis of Zr-Si-O-N thin films used as tough hard high temperature coatings, diffusion barriers in microelectronics, and optical coatings

Project Outcomes

Education and research tool for 6 postdocs, >30 graduate students, 17 IGERT students, 6 GK/12 students, >20 REU and RET participants, and >25 undergraduate students; >20 publications and use in collaborative projects with numerous industry partners.

Multi-User X-ray Diffraction System for Advanced Materials Analysis

Robert J. Lad (University of Maine), DMR-Award 0521043



IMPACT on the State of Maine

- ✓ Maine Economic Development via Industry Collaborations and Technology Transfer
- ✓ Educational Training of Maine's Next Generation Workforce

XRD Use for Educational Programs

Expanding Your Horizons
Maine Principals Association Science Fair
Research Experience for Undergraduates (NSF)
Research Experience for Teachers (NSF)
IGERT Sensor Engineering Informatics (NSF)
IGERT Functional Genomics (NSF)
GK-12 Sensors! (NSF)
Bates College Chemistry
Consider Engineering
Nanoscience Day

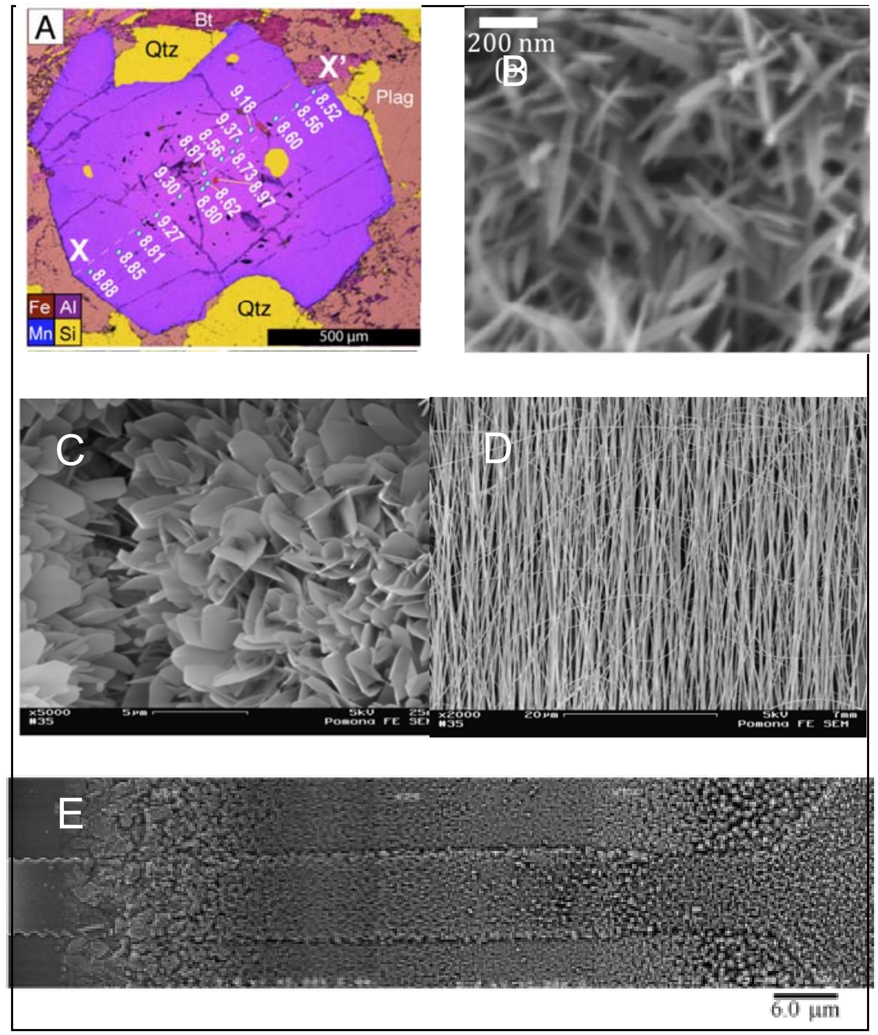
XRD Use by Maine Industrial Partners

Ascendant Energy (Rockland, ME)
Applied Thermal Sciences (Sanford, ME)
AVX Tantalum (Biddeford, ME)
BiODE, Inc. (Westbrook, ME)
Environetix Technologies (Orono, ME)
Fairchild Semiconductor (S. Portland, ME)
FHC Inc. (Bowdoin, ME)
Flexplay Inc. (Saco, ME)
The Jackson Laboratory (Bar Harbor, ME)
Maine Medical Research Institute (Scarborough, ME)
Mainely Sensors (Orono, ME)
Marca Coating (Saco, ME)
Nanoscale Components Inc (Camden, ME)
NanoSpire Inc. (Buxton, ME)
National Semiconductor (So. Portland, ME)
Orono Spectral Solutions Inc. (Old Town, ME)
Stillwater Scientific Instruments (Orono, ME)
Zeomatrix (Orono, ME)

Applications of an Undergraduate FE-SEM facility

David M. Tanenbaum (Pomona College), DMR- 0618417

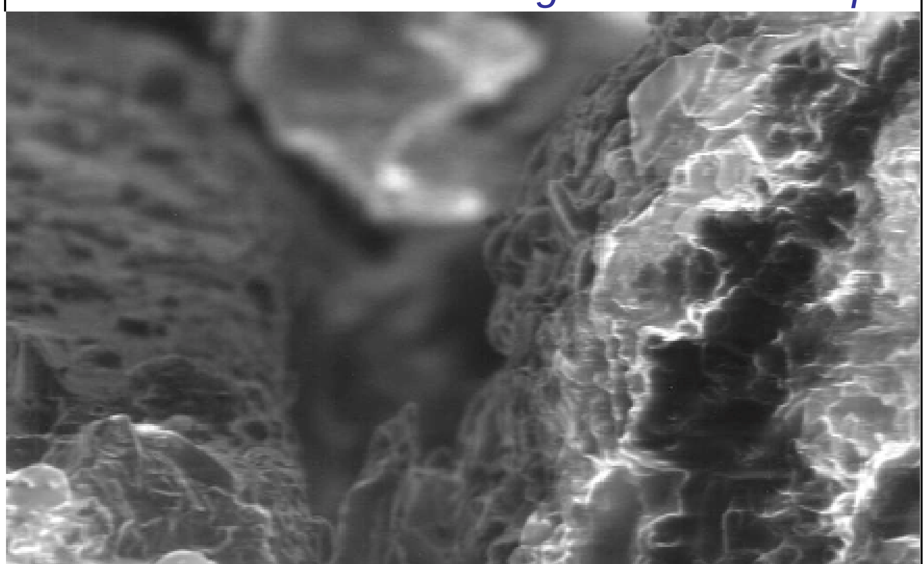
Our FE-SEM facility was accessed ~300 times during the 2009-2010 academic year, almost entirely for research by undergraduates working for principal investigators from four different institutions and covering Art, Biology, Chemistry, Engineering, Geology, and Physics. A sampling of some images acquired with the system are shown. A) Garnets analyzed with their oxygen isotope ratio indicated on top of X-ray intensity maps reveal geologic history. B) Manganese oxide nanostructures grown for battery electrodes. C) Calcium carbonate crystals are structural members in lizard eggshells. D) Aligned electrospun collagen fibers for tissue engineered cornea materials. E) TiO_2 nanostructures as a function of CVD temperature on a micro-hotplate array.



Outreach with an Undergraduate FE-SEM facility

David M. Tanenbaum (Pomona College), DMR- 0618417

Physics teachers from Los Angeles area high schools visit Pomona College for a workshop.



Plant material imaged as part of Light Explorations, an Art class at Pomona College.

Our FE-SEM facility was used in 7 different courses taught by faculty in departments from Chemistry, Physics, Geology, and Art in the past year. Over ten engineering clinic and science senior thesis students from 4 colleges used the SEM in research related to their senior exercises. We trained 38 new student users in the 2009-2010 academic year, working with 14 different principal investigators from 4 different institutions and covering Art, Biology, Chemistry, Engineering, Geology, and Physics. Over 25% of the new students trained are women, and they represent a diverse set of ethnic groups. In addition, we do demonstrations for groups from age 6 through adults, including high school science teachers.

Zero-Background Scatterless Hybrid Slits for Synchrotron and In-house SAXS Applications

Cyrus R. Safinya, University of California-Santa Barbara, DMR 0619171

The newly developed scatterless single crystal/metal hybrid slits greatly improves performance in synchrotron and in-house SAXS instruments. The hybrid slit produces no detrimental slit scattering commonly associated with conventional metal slits, leading to a much simplified SAXS design and greater performance in terms of flux and resolution. In both synchrotron and in-house experiments, the use of the scatterless slits has led to ~3X improvement in usable photon flux at sample position without compromising resolution.
The scatterless slit is been adopted by several synchrotron SAXS beamlines and is likely to become a standard feature in SAXS design. The dramatic performance enhancement resulting from the scatterless slits technology, and its low cost (at a fraction of the total instrument cost) has generated broad and rapid interest in the SAXS community and is been incorporated at several synchrotron beamlines around the world (e.g. ESRF, ALS, SSRL). The general scatterless design concept can be used to significantly boost the performance of a large number of existing SAXS instruments.

Reference: Y. Li , R. Beck, T. Huang, M.C. Choi, M. Divinagraci, “Scatterless Hybrid Metal-Single Crystal Slit for Small Angle X-ray Scattering and High-resolution X-ray Diffraction”, *J. Appl. Cryst.* **42**, 1134-1139 (2008)

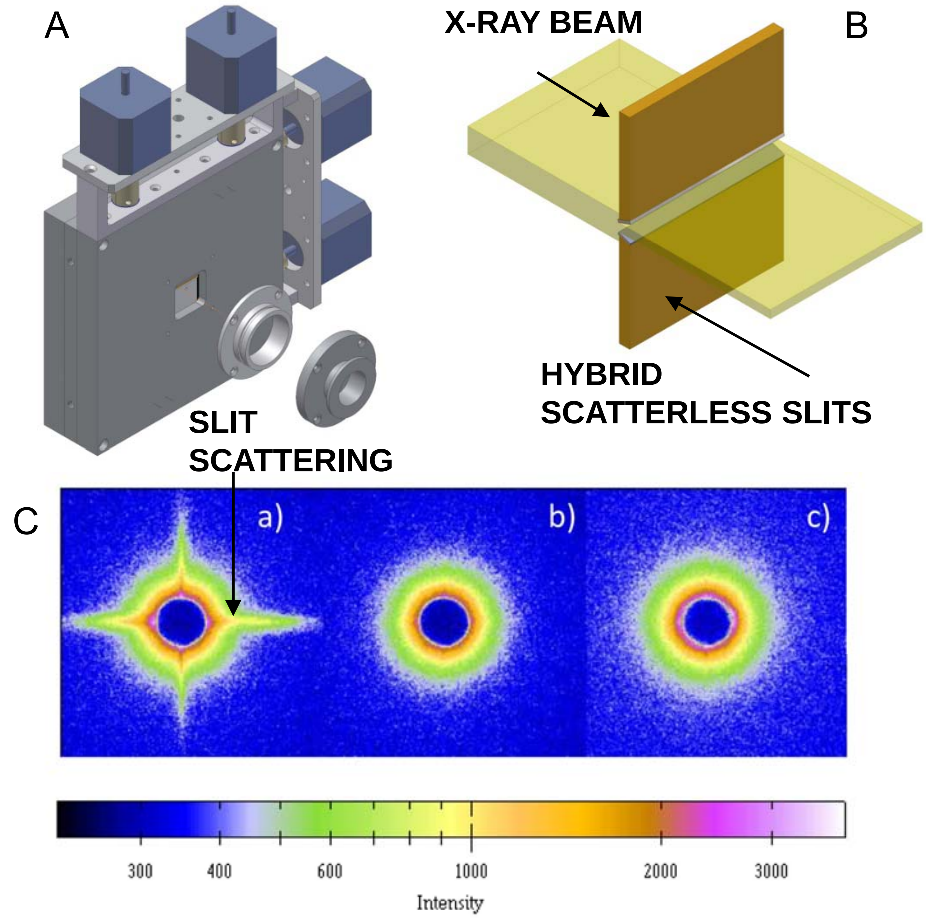


Fig. (A, B) Vacuum compatible scatterless slits developed at UCSB for synchrotron and in-house SAXS. (C) 2D SAXS background taken at ESRF beamline D2RM showing complete elimination of slit scattering (streaks in image a) when the scatterless slits were used (b). A simplified SAXS design results in 3X more flux without compromising resolution (c).

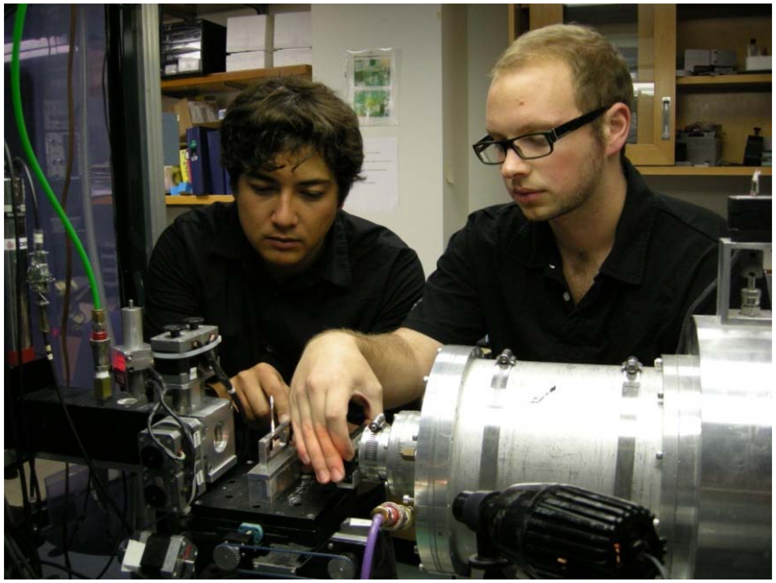
MRI: Development of an Ultra-High Resolution Small Angle X-Ray Scattering Instrument for Characterizing Supramolecular Assemblies

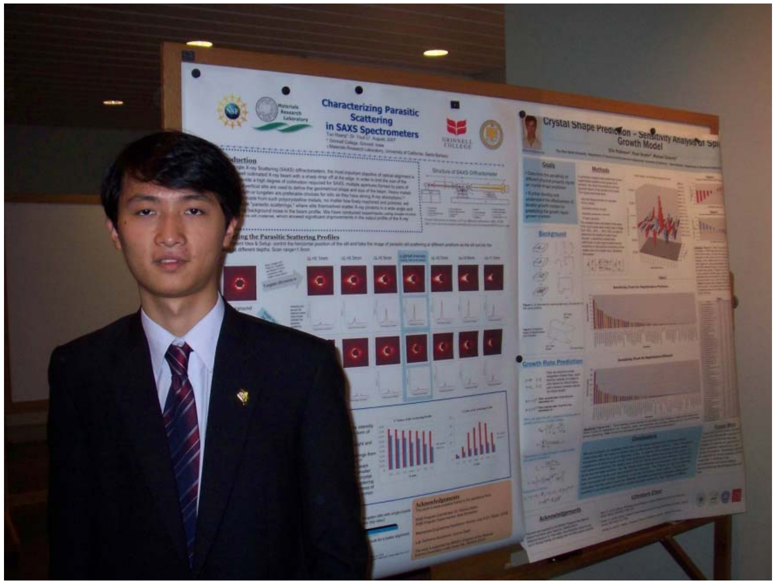
Cyrus R. Safinya, University of California-Santa Barbara, DMR 0619171

Broader Impact: The newly developed scatterless slits for SAXS is gaining wide interest in the SAXS community and we are collaborating with scientists at several synchrotron SAXS facilities in the world (incl. ESRF, ALS & SSRL) to implement this new technology, which can lead to significant enhancement in SAXS capability for broad areas of research.

Education: The participants including undergraduate and graduate students and postdoctoral researchers are educated in x-ray instrumentation science and SAXS methods for nanoscale characterization of supramolecular assemblies. PICTURED (TOP RIGHT): UCSB undergraduate research assistants Gabriel Harmon and Kyle Peterson, who are participants in the project, working on the in-house SAXS instrument.

Outreach: The PI's participate in multiple outreach programs at UCSB for undergraduate and high school teacher research internships. We actively recruit and encourage undergraduate students to work on this project to gain valuable first hand research experience. PICTURED (BOTTOM RIGHT): RISE intern Thomas (Tuo) Huang (Grinnell College, Iowa) who was mentored by co-PI Li, presents his work in a poster. Inspired by his research experience, Thomas is currently pursuing graduate study at Northwestern University.



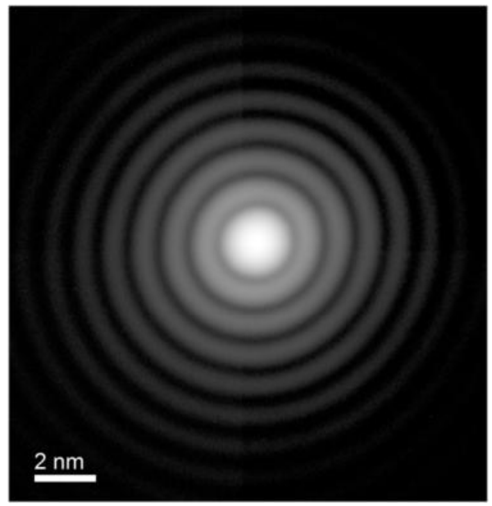


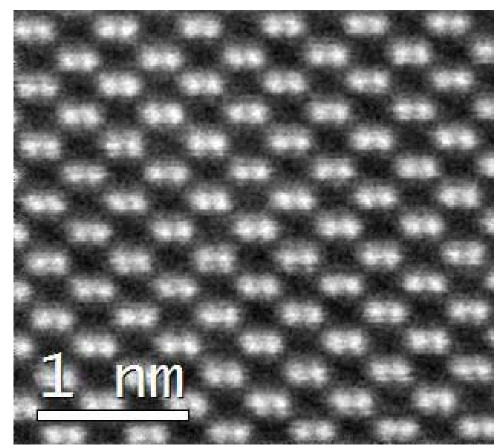
High-Resolution S/TEM at U. Wisconsin & U. Puerto Rico

Paul M. Voyles, University of Wisconsin-Madison, DMR 0619368

The University of Wisconsin Materials Science Center has installed a high-performance FEI Titan scanning transmission electron microscope (STEM) with spherical aberration corrector. It can acquire images with <0.1 nm spatial resolution and has full analytical capability.

The project investigators will use the Titan to study doping of semiconductors, the structure and dynamics of glasses, multitarget nanoparticle labeling of bio-macromolecules in cells, therapies based on inductive heating of magnetic nanoparticles, the reactivity of geological nanophases and nanopores, and natural-material catalysts for environ-mental remediation. The Titan will impact research from ~20 other research groups in the physical and biological sciences and engineering.

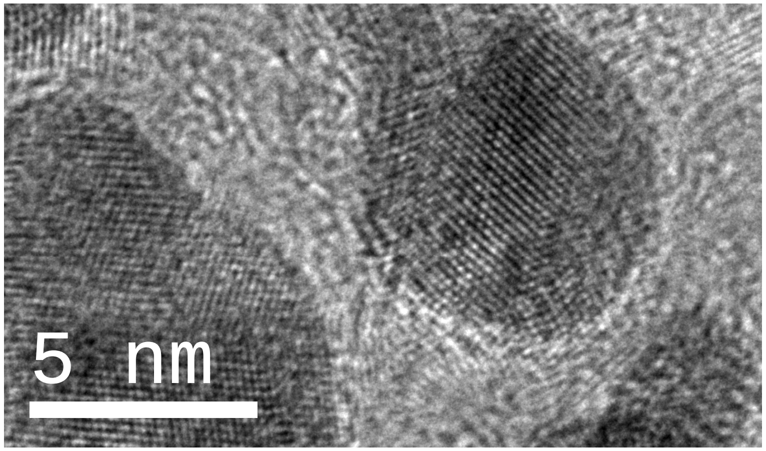




Top right: the UW Titan STEM / TEM; top left: a coherent nanoprobe for diffraction; bottom right: a <0.1 nm resolution STEM image of silicon, showing bright silicon atomic columns.

High-Resolution S/TEM at U. Wisconsin & U. Puerto Rico

Paul M. Voyles, University of Wisconsin-Madison, DMR 0619368



Top: UPRM students Yarilyn Cedeno and Edwin de la Cruz work on the Titan via the Internet. Bottom: a HRTEM image acquired from UPRM.

The Titan is shared by UW Madison and the University Puerto Rico, Mayaguez (UPRM), a Hispanic-serving institution. A dedicated remote operation station which can control all aspects of the Titan except sample exchange has been installed at UPRM. In August 2009, Voyles spent a week at UPRM training 9 faculty, staff, and students to operate the Titan.

The Titan will support research at UPRM on magnetic nanoparticles, catalysis, metal composites, and phase stability of meteorites. It is the first TEM at UPRM and the second high-resolution TEM on the island of Puerto Rico.

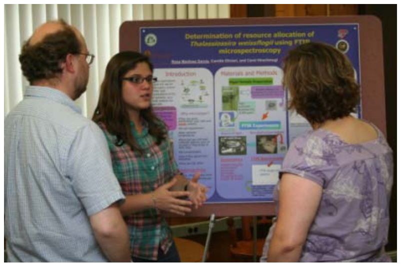
IRENI: Infrared Environmental Imaging

Carol J. Hirschmugl, University of Wisconsin-Milwaukee, DMR 0619759

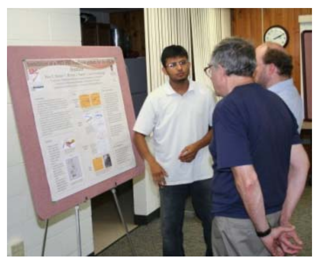
A sensitive infrared microscope that will greatly expand the ability to monitor the chemistry of small biological structures will afford new opportunities to track biochemical adaptations in living cells. UWM and the Synchrotron Radiation Center are spearheading this effort. The microscope will be available for users across a wide array of disciplines (e.g. physics, nanoscience, biology, chemistry, veterinary science, biomedical engineering, environmental science and geology), providing a new interdisciplinary tool to the broader scientific community.

IRENI: RET participants and REU students

Carol J. Hirschmugl, University of Wisconsin-Milwaukee, DMR 0619759



Poster presentations to SRC scientists, talks to fellow students and working at the IRENI facility were all part of the experience for the REU and RET participants.



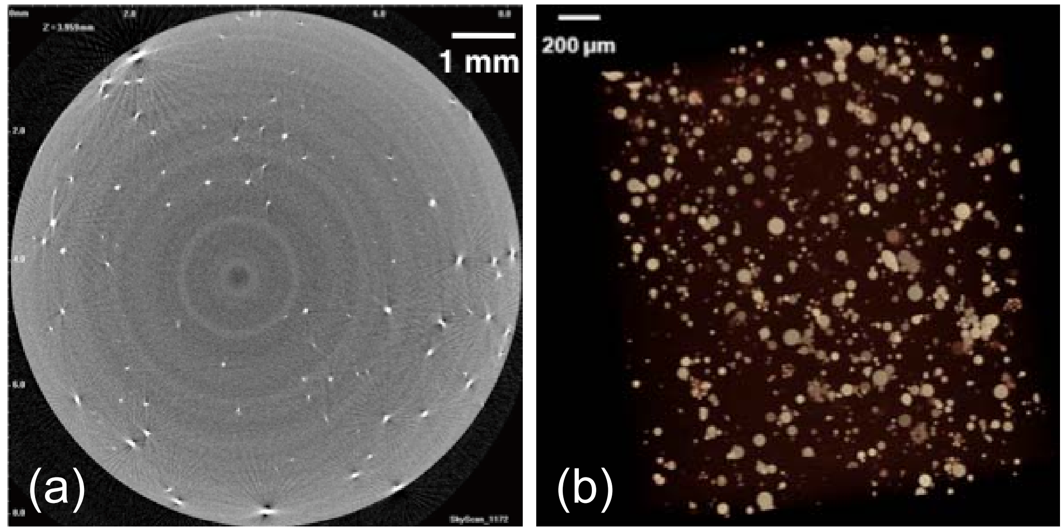
REU student and RET participants (Rosa Martinez, Puerto Rico University; Nirav Shilav U-Maryland-BC, and Theresa Phillips, Bigfoot Highschool, Walworth WI) used IRENI for their research projects during the summer of 2009. Tours for middle school students were also part of the outreach efforts.

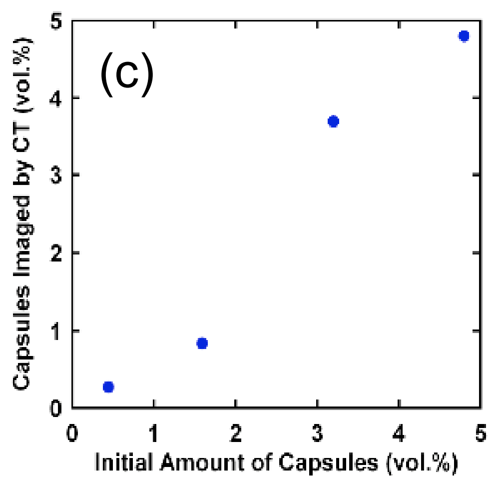
The REU students worked on biochemistry and physics experiments, while the RET teacher worked on a geochemistry project. The participants were given many opportunities to speak about their work with experts to learn how to have scientific discussions.

X-ray MicroCT Imaging of Self-Healing Polymers

Paul V. Braun (Univ. of Illinois at U-C), DMR-Award # 07-21324

Under support of the NSF, we have finished installation of a multiscale X-ray tomography imaging system. This system provides 3D non-destructive imaging capabilities from the nanometer to millimeter scale, as well as contrast on a wide variety of materials. We have used the Bio-MicroCT in this system to image micron-scale microcapsules in self-healing polymer blocks. Bio-MicroCT images are extremely useful in quantify the capsule survival rate when incorporated into the polymer, since the x-ray CT method is nondestructive. The volume ratio of capsules measured by CT was compared to the weight ratio of capsules blended into epoxy polymer, and a near linear correlation was observed for the first time.





(a) Cross-sectional tomography image of Iodobenzene-filled microcapsules in polymer.

(b) 3D reconstruction of all microcapsules in the polymer block.

(c) Measured total capsule volume vs. capsule volume in fabrication of sample.

Research of Profs. J.S. Moore, N. R. Sottos, and S. R. White

Multiscale X-ray Tomographic Imaging System

Paul V. Braun (Univ. of Illinois at U-C), DMR-Award # 07-21324

ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

BECKMAN INSTITUTE
AT THE UNIVERSITY OF ILLINOIS

imaging technology group

- Located in the Imaging Technology Group, which provides open access and training to the University of Illinois community.

- Accessible to scientists and engineers across campus and beyond, including scientists from industry and national laboratories.

- Full time staff enabling access even to untrained users.

- Samples can be imaged under various environments (humidity, tension/pressure, aquaria), which is especially beneficial for biological samples.

- Fully operational for over a year with >50 users from many different scientific disciplines.

MRI: Acquisition of a Fast-Pulse-Laser for a Local Electrode Atom Probe
NSF-DMR-0722631

G.B. Thompson, M. L. Weaver, T. Klein, W. Butler and D.E. Nikles
University of Alabama, Tuscaloosa, AL

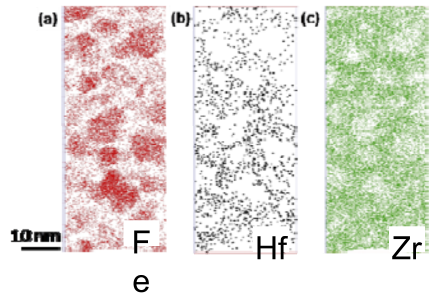
Intellectual Merit:

Atom probe microscopy provides 3-dimensional reconstructions of individual atoms' spatial location and identity. **The acquisition of the pulse laser allows thermal heating to assist the field evaporation process of the atom probe to characterize,poor electrical conductors and brittle intermetallics.**

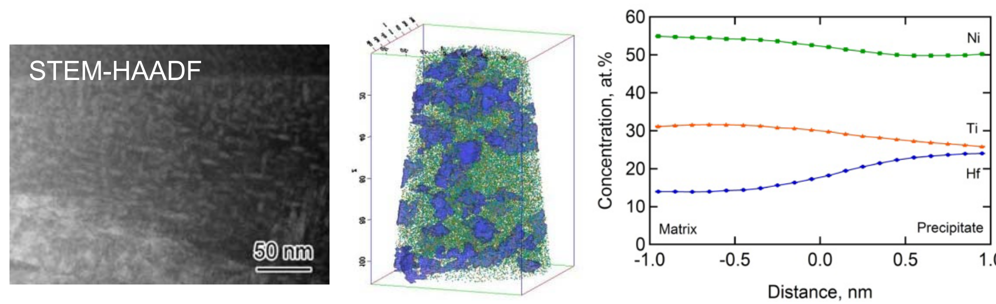
The upgrade in instrumentation has impacted several research programs, including

1) Precipitation studies in High Temperature Shape Memory Alloys
2) Atomistic oxidation studies in thermal barrier coatings
3) Semiconductor devices
4) Magnetic ribbons for energy applications
5) Magnetic materials for next-generation storage media hard drives
6) Precipitation in irradiated stainless steels

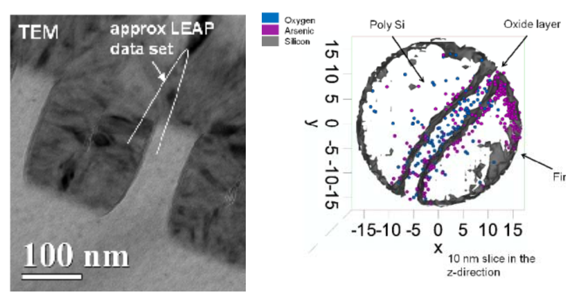
The laser LEAP serves UA community as well as external users from U. of FL, U. of MI, MIT and others.



Chemical Partitioning in $(Co_{1-x}Fe_x)_{88}Zr_7B_4Cu_1$ Soft Magnetic Nanocrystalline Alloys. Collabration between UA-Naval Research Laboratory



Nanoscale precipitate composition of $Ni_{50.7}Ti_{26.93}Hf_{22.3}$, these precipitates have dramatically increased the shape memory transformation temperature and structural stability. Collaboration between UA-NASA



Ar dopant distribution in a FinFET semiconductor device.

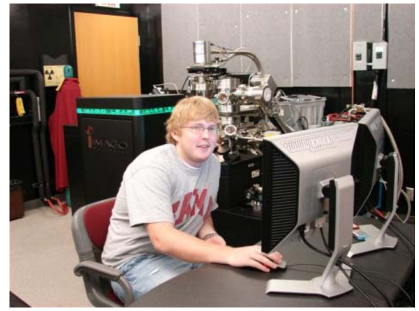
MRI: Acquisition of a Fast-Pulse-Laser for a Local Electrode Atom Probe
NSF-DMR-0722631

G.B. Thompson, M. L. Weaver, T. Klein, W. Butler and D.E. Nikles
University of Alabama, Tuscaloosa, AL

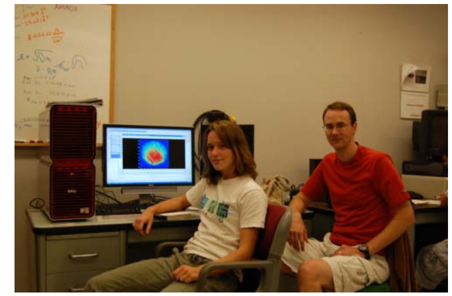
Broader Impact

The Local Electrode Atom Probe (LEAP) and its laser upgrade has been used in numerous out-reach and workforce development activities.

1) UA's Nanoscience and Engineering High School Research Summer Internships
   - Kristy Tippey (Central High) and Hiram Purser (Hillcrest High) performed characterization of wire drawn stainless steel to determine materials sensitivity to corrosion
2) HBCU visiting summer faculty program (an extension to DMR-9976488, DMR-0349851, and DMR-0907673; introducing HBCU faculty to Materials Sci. and Eng.)
   - Dr. Sundar Nagy (WVSU) and his student, Jennifer Thompson, did atom probe reconstruction of Fe(Cu)Pt magnetic materials
3) Work force development
   - Graduation of graduate students including Karen Torres (Hispanic Am.) to NIST-Gaithersburg, Michael Bester to ORNL, Diondra Means (African Am.) to Texas Instruments.



Chad Hornbuckle, a former REU, using the LEAP. His work lead to an internship at Naval Research Lab where he prepared samples to be analyze in the LEAP. Chad is now pursuing a Ph.D. at UA.



Professor Thompson working on atom probe reconstruction with Kristy Tippey, a former high school intern now a engineering undergrad at UA

Workforce development of graduate students: Diondra Means, Bianzhu Fu, and Karen Torres

UA will host the 2012 International Field Emission Society conference, the premier atom probe meeting, demonstrating UA's emergence as an atom probe research leader.

IFES 2012
JULY 22-27, 2012
53rd International Field Emission Symposium

Development of Efficient Thermal Neutron Position Sensitive Detectors

Anton S. Tremsin, University of California at Berkeley, DMR 0753599

Research Goal: to develop neutron counting detection technology with high spatial (~55 μm) and temporal (~1 μs) resolution and high detection efficiency (~40% for thermal and cold neutrons).

Principle of neutron detection:

- ^{10}B or Gd-doped microchannel plates convert incoming neutrons into highly energetic particles escaping into adjacent pore;
- Secondary electrons are produced upon collision with the pore walls;
-Electron avalanche results in a signal of 10^3-10^6 electrons for each detected neutron, which can be easily detected by a Medipix2 or Timepix readout with no readout noise.

Neutron radiography

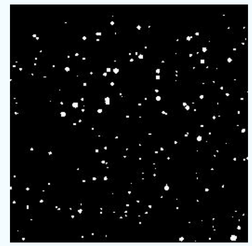


Fig. 2. Single frame image of neutron events accumulated over 30 μs .

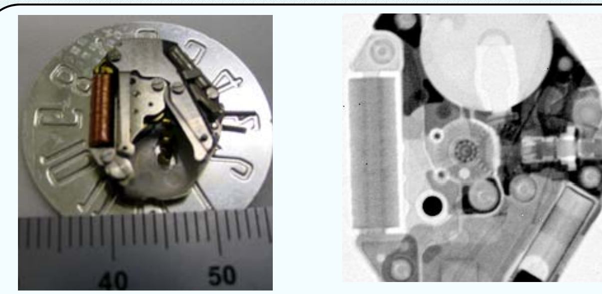


Fig. 3. Photograph (left) and neutron radiographic image (right) of a wrist watch taken at the cold neutron beamline. Data acquisition time 180 sec. High efficiency and high spatial resolution allow detailed radiography in comparatively short acquisition times

Key research challenges:

• Efficient neutron conversion into an electron avalanche for detection with high efficiency;
• Conservation of reaction products in the local area to avoid image blur;
• Engineering design of MCP-Medipix2 combination with minimized distance and high acceleration voltage between them to preserve high spatial resolution of event localization;
• Fast, reliable, noiseless readout electronics and data acquisition software;
• Data analysis and processing tools

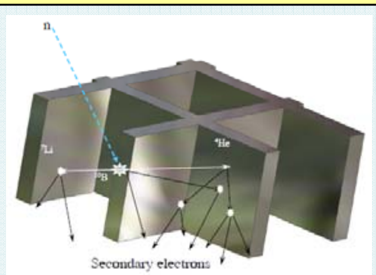


Fig. 1. Neutrons interact with 10B atoms inside the MCP glass. Reaction products create an electron avalanche in a single pore, which is ~8 μm, preserving spatial information of the event within 10 μm.

Application to be improved/enabled by this technology:

• Phase, texture, material composition and strain measurement with high spatial resolution in transmission Bragg edge diffraction mode;
• Stroboscopic studies of dynamic processes with unique contrast of neutron imaging, e.g. water propagation, air-liquid mixture flow, fuel injection in car engines, etc;
• Studies of dynamic magnetic fields within thick samples utilizing neutron spin interaction with magnetic fields.

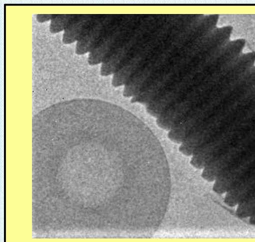


Fig. 4. Neutron transmission image of bent steel screw. 100 sec acquisition.

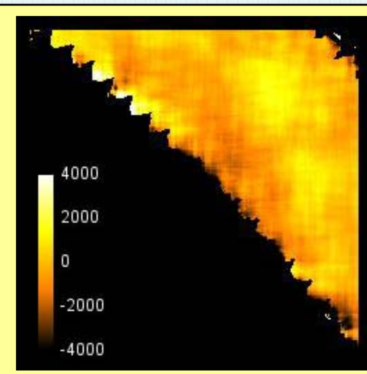


Fig. 5: Strain map image of the steel screw shown in Fig. 4. The strain is calculated from 110 Bragg edge positions λ_0 mapped across the sample. The color bar indicates strain values in μstrain.

Development of Efficient Thermal Neutron Position Sensitive Detectors

Anton S. Tremsin, University of California at Berkeley, DMR 0753599

Broader impacts

Development of high resolution neutron counting detectors based on microchannel plate technology can be very useful for scientists outside of materials research community. Such diverse areas as plant root growth and dynamics of water uptake, water transport within wood samples, dynamics of fuel injection and oil distribution in car engines can benefit from the unique contrast mechanism of neutron radiography. Neutrons have relatively large interaction cross sections with lighter atoms as they interact with nucleus instead of electron as in case of X-rays. There are also several isotopes which have very large cross section of neutron absorption (e.g. ^{10}B, ^{157}Gd, ^{6}Li, Cd) which can be used to enhance the contrast in the images. At the same time neutrons can penetrate thick metal samples.

Another attractive application for the developed neutron detection technology is the non-destructive studies of material composition of precious museum objects. We have conducted a proof-of-principle experiment to verify our sensitivity to a small change in bronze composition, which may allow accurate mapping of internal components in terms of timing, as bronze composition was changed at a certain time in certain places. Fig. 6 shows the three samples we have measured: pure copper, and two bronzes: Cu-80% Sn-10%, Pb-10% and Cu-88% Sn-8%, Pb-4%. With time of flight technique we can separate these bronze compositions by the position of Bragg edge, Fig. 7.

Fig. 6. Photograph of three different materials imaged in transmission diffraction time-of-flight mode on a pulsed neutron beamline. **Top:** bronze with Cu-80% Sn-10%, **middle:** is pure copper, **bottom:** Pb-10% and Cu-88% Sn-8%, Pb-4%.

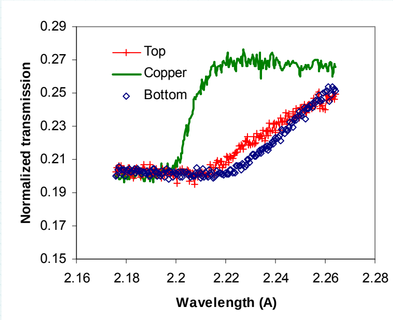


Fig. 7. Bragg edge measured in transmission mode of three different samples shown in Fig. 6. The difference in Bragg edge between top and bottom bronzes can be used for spatial mapping of bronze composition within archeological samples.

Student participation in our development of the detection technology provides them with a unique opportunity of muti-disciplinary training. The development, assembly and testing of neutron counting detectors on neutron beamlines involves many aspects of state-of-the-art instrumentation manufacturing and utilization. It starts with the mechanical design of individual components and the full detector assembly, design and implementation of data processing electronics, writing data acquisition software and development of algorithms for the analysis of the experimental data.

Rahul Barwani, the undergraduate student at UC Berkeley was involved in detector development and has learned useful skills during that work.

Development of an Ultra-fast Optical Spectroscopy System for Multi-disciplinary Studies

Kenneth J. Rothschild, Trustees of Boston University, DMR 0821450

This is the first year of a 3-year project in the Photonics Center at Boston University to develop a broad spectral range, ultra-low noise, ultrafast optical spectroscopy instrument for multidisciplinary research. The instrument will incorporate many innovations that will open up a new window for understanding a variety of fundamental processes in biology, chemistry, and materials science.

Accomplishments to date include:

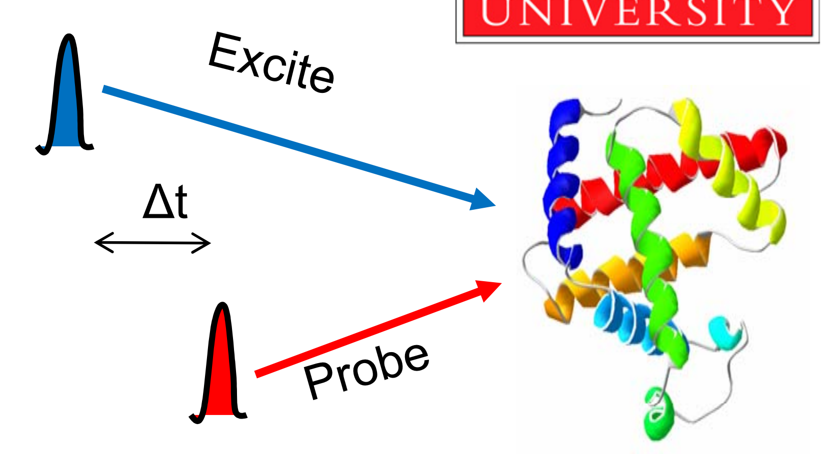
•*Ti:sapphire oscillator and regenerative amplifier system operational.*

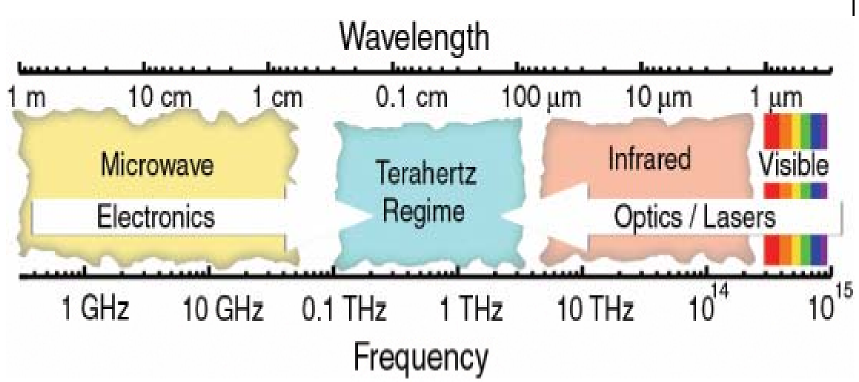
•*UV-Vis-NIR Optical Parametric amplifier system operational with wavelength tuning range extending out to the 2 micron range.*

•*Mid-IR Optical Parametric amplifier system i operational, typically generating > 15 mJ at 2220 cm^{-1} with ~ 100 fs pulse-width.*

•*Novel THz spectrometer under development.*

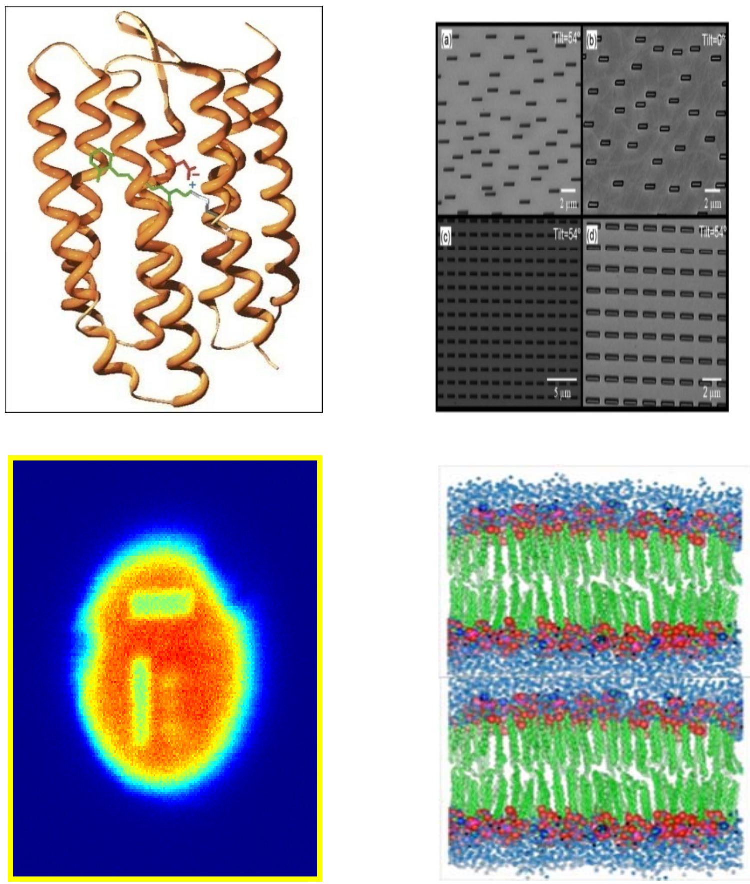
•*New collaborations facilitated in biomolecular studies, nanoplasmonics, metamaterials and complex chemical systems.*





Development of an Ultra-fast Optical Spectroscopy System for Multi-disciplinary Studies

Kenneth J. Rothschild, Trustees of Boston University, DMR 0821450



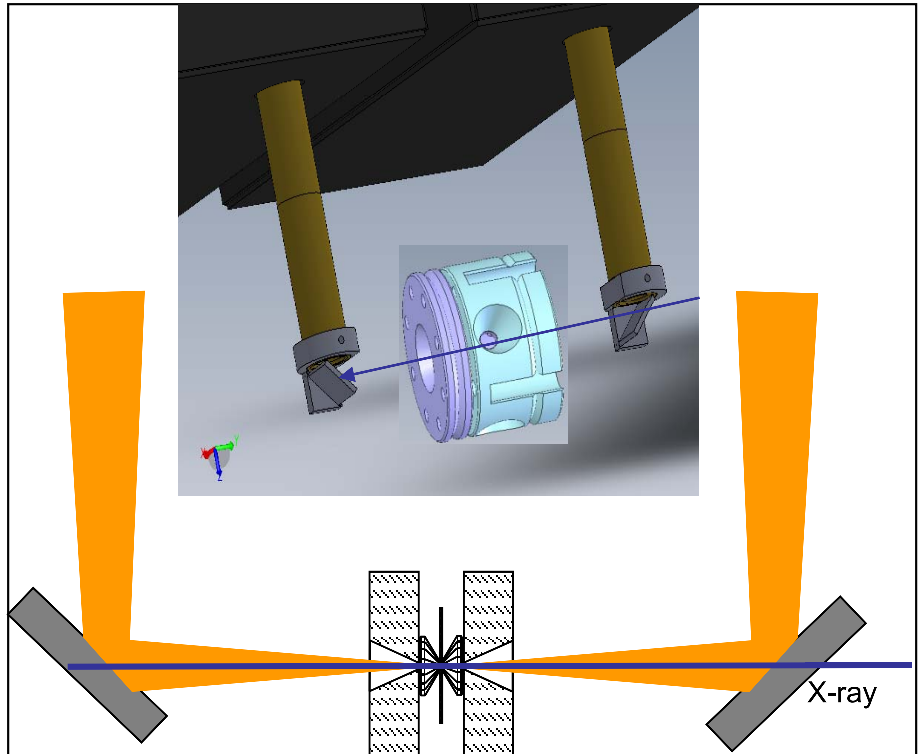
The promise of ultrafast optical spectroscopy in condensed matter physics, chemistry, biology, materials science, and engineering stems from its ability to temporally resolve phenomena at the fundamental sub-picosecond timescales of nuclear and electronic motion. This NSF-MRI instrument development project is facilitating basic studies in a variety of disciplines. Examples include (see Figures clockwise from top left): Signal and energy transduction in rhodopsins, Nanoplasmonic structures (with H. Altug, BU), Molecular basis of anesthetic in biological membranes, and 3D Lithographic fabrication (Peter So, MIT). As part of our outreach effort we are conducting tours and involving REU students in the instrument development. For more information on research at the Femtospec Laboratory and NSF-MRI Facility go to http://physics.bu.edu/femtospec/

Development of a Portable Laser Heating System

Ho-kwang Mao, Carnegie Institution of Washington, DMR 0821584

A portable laser heating microscope has been developed for a broad range of materials studies at extreme pressure-temperature conditions. The essential features include:

- Portability
- Co-axial alignment
- Modular design
- Extended temperature coverage down to 500 K and up to over 10,000 K.
- Flexible for a variety of applications in high pressure research for different environments, including in synchrotron and neutron applications and optical spectroscopies.



The developed laser heating system behaves like a microscope head, flexible enough to be integrated with other measurements, such as at synchrotron beamlines and with optical systems.

Development of a Portable Laser Heating System

Ho-kwang Mao, Carnegie Institution of Washington, DMR 0821584

The developed system is being integrated at many beamlines at the Advanced Photon Source. The flexibility of the system allows for studies of materials under high pressure-high temperature conditions at various specialized beamlines.

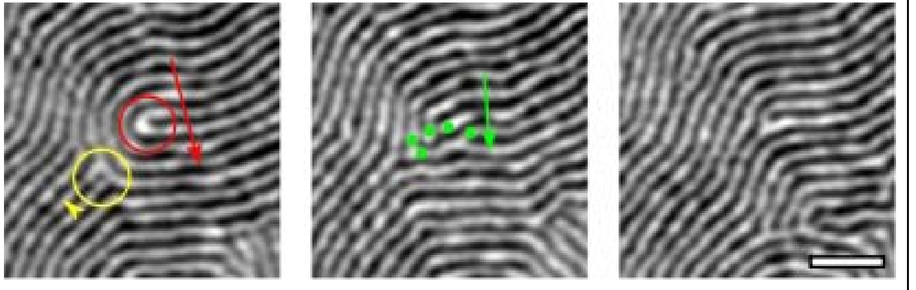
Previously, laser heating systems were integrated with synchrotron x-rays at a few dedicated high pressure beamlines, and limited to x-ray diffraction only. With the portable system, it allows for studies of materials behavior at high pressure and high temperature with many newly developed x-ray techniques, such as imaging, spectroscopy, and inelastic scattering, at specialized beamlines. For example, at least seven beamlines at the Advanced Photon Source showed their interests in using the portable system.

Defect evolution in diblock copolymer films

Lee Park, Ward Lopes, Claire Ting (Williams College),

DMR- MRI 0922400

This multi-user instrument MRI grant was used to fund the purchase of two Agilent AFM at Williams College. These AFMs are being used in both research and teaching in multiple departments. A highlight from Ward Lopes' research is provided here (physics.)



Annihilation of dipole configuration of disclinations. Images are separated by 20 minute intervals. The scale bar is 300 nm long. The first image indicates a +1/2 disclination (red circle) and a -1/2 disclination (yellow circle). The Burgers vector for the configuration of the two disclinations (the sum of the red and yellow arrows) is the green vector with magnitude 6 repeat spacings in the second image.

The Lopes lab is studying weakly segregated diblock copolymer systems with striped (smectic) symmetry, tracking defects as a function of time and temperature. to better understand pattern formation and evolution. They have found that disclinations in weakly segregated, cylindrical phase, PS-b-PMMA diblock copolymers primarily annihilate in dipole configurations (one disclination with positive winding number and one disclination with negative winding number). These preliminary results are the first experimental evidence that the dynamics of ordering in different systems with the same smectic symmetry can be different. In future work, they will quantify the relative frequency of dipole, tripole and quadrupole annihilations in this diblock copolymer system. The observation of a dipole annihilation with a Burgers vector of magnitude 6 repeat spacings is shown above. Individual dislocations created by the annihilation are indicated in the second image. By time of the scan of the third image, most of the dislocations from the dipole annihilation have annihilated with other dislocations from outside of the image boundaries.

Acquisition of AFM systems

Lee Park, Ward Lopes, Claire Ting (Williams College),
DMR- MRI 0922400

All of the research at Williams College is carried out by undergraduate research assistants. To date there have been ~ 15 students from different labs (chemistry, physics, biology, computer science) trained in the use of the AFM for a broad range of applications, In addition, the AFM will be used extensively in a Materials Chemistry course in the Fall of 2010. A new set of laboratory experiments for an upper level chemistry course (Chemistry of Materials, Chem 336) focusing on tools and strategies for nanofabrication has been developed and will be offered in the fall of 2010.

We have also begun planning for a professional development course (to be offered for the first time during the summer of 2011) for community college, high school, and middle school teachers that will focus on modern microscopy methods. The course will be designed as a 3- or 5-day workshop, with hands-on time on a variety of imaging instruments available at the college, including AFM, SEM, TEM, fluorescence microscopy, confocal microscopy, polarizing microscopy.

Finally, we have worked with another group of undergraduates during the summer of 2010, under the auspices of the Williams Instructional Technology (WIT) program; these students have been designing and implementing an on-line instrument sign-up system that will facilitate the many users and parts associated with the AFMs on campus (and will also be extended to other shared equipment on campus.) This system will be operational by the end of summer 2010.

MRI: Acquisition of Nanoindentation System at UPRM

Agnes M. Padovani (U. of Puerto Rico-Mayaguez), DMR-Award # 0922994

❖ A **G200 Nano Indenter** from Agilent Technologies, Inc. was acquired for this major Hispanic institution. Its installation & training were completed on August 13, 2010.

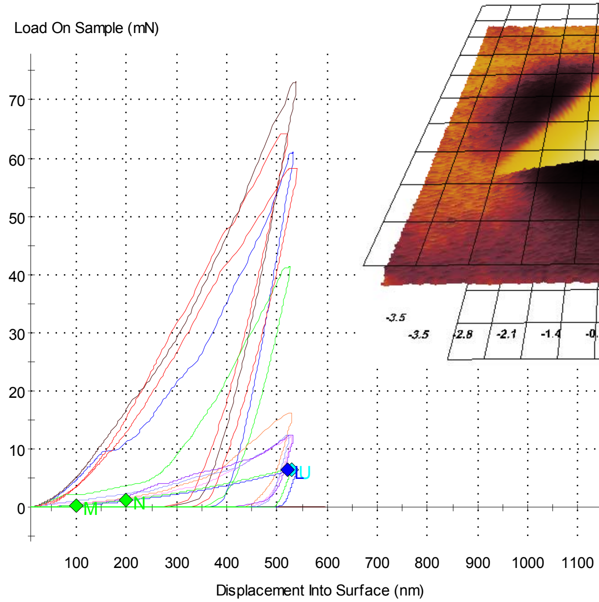
❖ ***Intellectual Merit:***

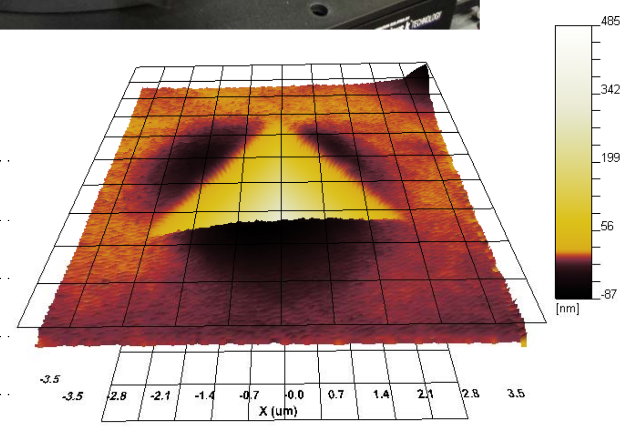
The scientific merit was centered on the outcomes of three research projects:

❖ ***Block Copolymer SIBS Thin Films for Applications in μ-Sensors and μ-Fuel Cells***: The study of fundamental nanomechanical properties such as elastic modulus, hardness, and film adhesion helps to understand the integration capability of these polymer nanocomposites.

❖ ***Characterization of Al/AlB_2 Functional Composites***: Mechanical properties are critical for understanding the particle matrix interaction that leads to the bulk mechanical behavior of these novel composite materials.

❖ ***Characterization of PEO Layer in Surface Modified Titanium Alloys***: The characterization of mechanical properties at the submicron scale is being used to evaluate the osseointegration capability of these surfaces.





MRI: Acquisition of Nanoindentation System at UPRM

Agnes M. Padovani (U. of PR-Mayaguez), DMR-Award # 0922994

❖ ***Broader Impacts:***

❖ The system is the *first available in a Hispanic serving higher education institution in Puerto Rico*. Training of students in this state-of-the-art instrument is impacting a new cadre of underrepresented minority and enhancing the education pipeline by providing a venue for education and training in advanced characterization techniques.

❖Five users received full training in the G200 Nanoindentation system during the week of August 9-13, 2010. These included the PI (Padovani), a full-time technician, and 3 graduate students (2 MS students from Mechanical Engineering and 1 PhD student from Chemical Engineering).

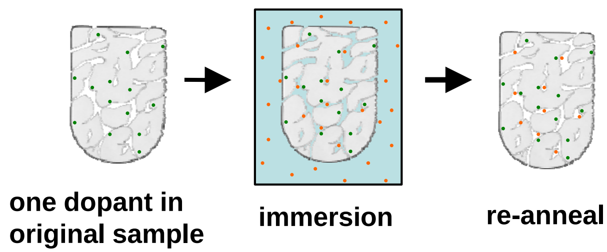
❖ Two additional training sessions were organized to demonstrate the basic instrument capabilities and these were attended by: 14 graduate students (MS and PhD), 3 undergraduate students, and 4 faculty members from 5 different engineering departments at UPRM (ESM, Mechanical, Chemical, Civil, and Electrical & Computer Engineering).

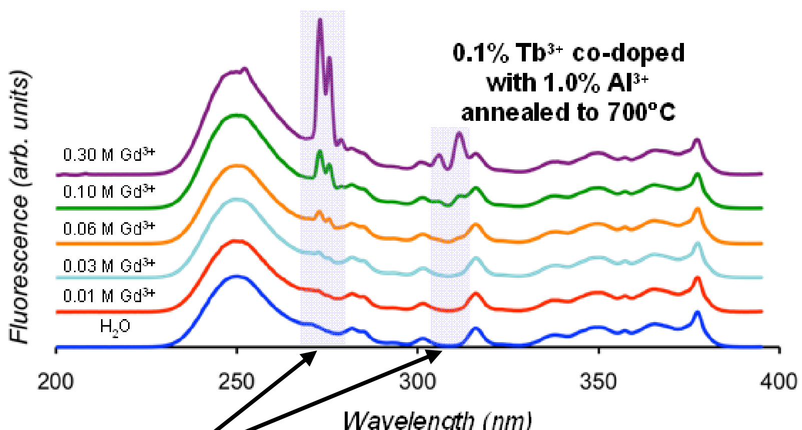
Rare Earths in Sol-Gel Glasses

Daniel M. Boye, Davidson College **DMR-Award 0959552**

Post Annealing Immersion

- New technique for studying pore network
- Fluorescent ions introduced into porous network via solutions, varying dopants and concentrations
- Energy transfer between different dopants monitored to determine proximity

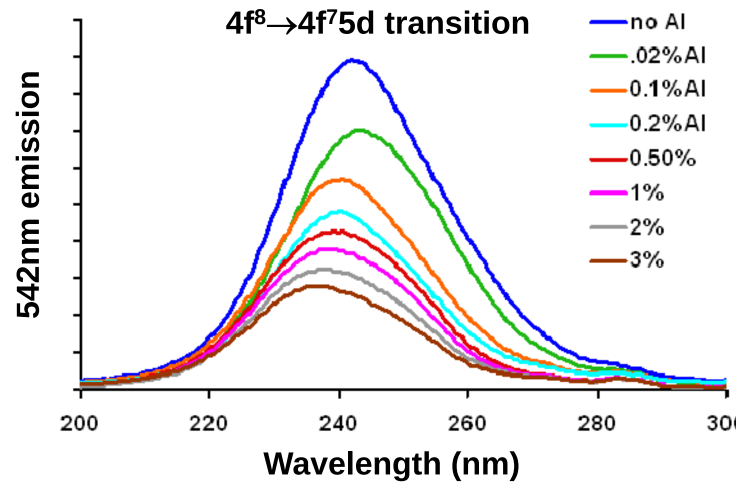




Tb^{3+} emission result of energy transfer from excited Gd^{3+} ions

Aluminum Co-doping

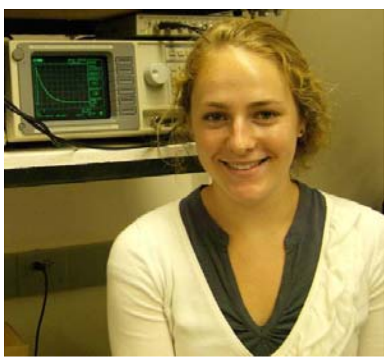
- Al co-doping can significantly increase emission yield independent of Rare Earth ion used
- Continuing work in our group to study mechanism
- Monitor emission of Tb^{3+} green emission when excited through its $4f^8 \rightarrow 4f^7 5d$ transition which is more sensitive to host coupling compared to $4f^8 \rightarrow 4f^8$ transitions
- Decreasing emission with increasing Al concentration indicates weaker coupling to host



Rare Earths in Sol-Gel Glasses

Daniel M. Boye, Davidson College   DMR-Award 0959552

Kate Arpino
2nd Place Poster Award at DPC'10 !!!



Co-PIs

Hamilton College: Ann Silversmith, Physics
Whitman College: Kurt Hoffman, Physics

Undergraduate Research Participants

Hamilton College: Sarah Fobes, Zane Glauber, Kate Arpino, Andrew Beyler
Davidson College: Lindsey Martin, Patrick Panuski (high school student)
Whitman College: Dylan Wenzlau, Genderzon Montejo, Freddy Sanchez, Tyler Harvey

Professional Communication

- 1 article published
- 1 article accepted for publication
- 2 articles submitted for review
- 3 senior theses
- 4 conference posters
- 5 oral presentations
- 6 attended 17th International Conference on Dynamical Processes in Excited States of Solids (DPC'10), ANL, Chicago

Curriculum Development

Lindsey Martin works on new phosphor lifetime laboratory exercise

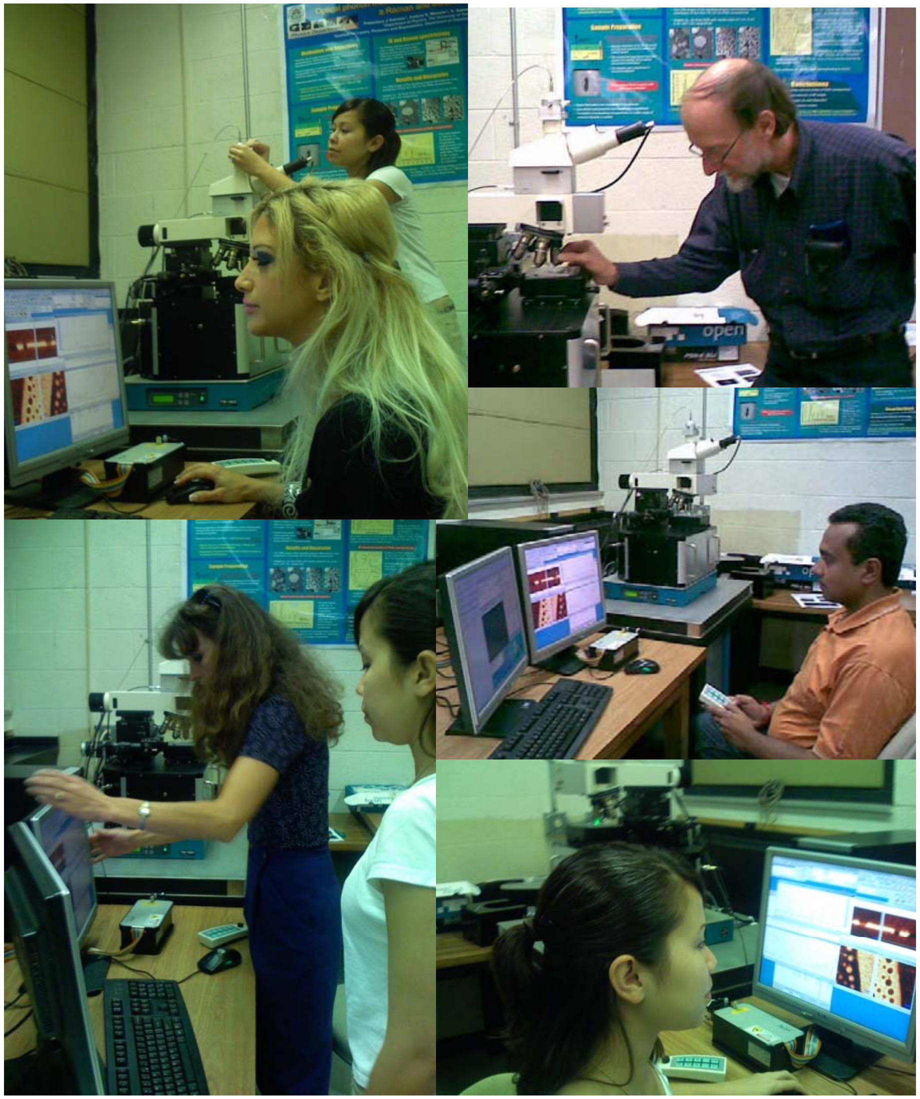
New sample synthesis

Genderzon Montejo examines aerogels from a new synthesis technique for our research efforts

ACQUISITION OF A CONFOCAL RAMAN/AFM HYBRID SYSTEM

FELICIA S. MANCIU, UNIVERSITY OF TEXAS AT EL PASO,
DMR 0723115

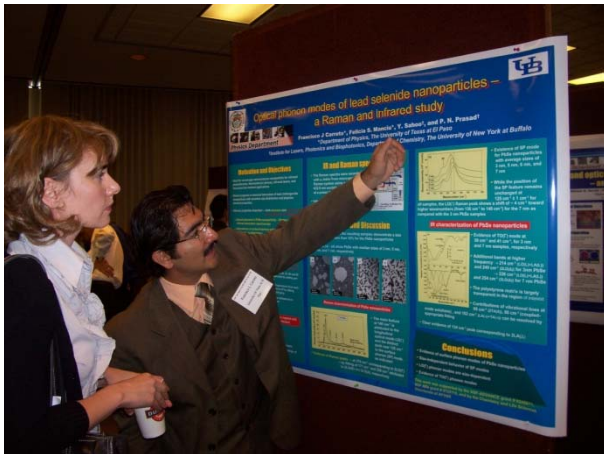
- **The research performed with this instrumentation enhanced our understanding of important fundamental and applied nanoscale phenomena**



- **F. S. Manciu**, J. R. Govani, W. Durrer, L. Reza, and L. A. Pinales: "*Inhibition of urinary calculi – a spectroscopic study*", submitted.
- **F. S. Manciu**, A. Ramirez, W. Durrer, J. R. Govani, R. R. Chianelli: "*Spectroscopic analysis of a dye-mineral composite – a Raman and FT-IR study*" **J. Raman Spectroscopy**, vol. **39**, Issue 9, 1257-1261 (2008).
- **F. S. Manciu,** Y. Sahoo, F. Carreto, and P. N. Prasad: "*Size-dependent Raman and infrared studies of PbSe nanoparticles*", **J. Raman Spectroscopy**, vol. **39**, Issue 9, 1135-1140 (2008).

ACQUISITION OF A CONFOCAL RAMAN/AFM HYBRID SYSTEM

FELICIA S. MANCIU, UNIVERSITY OF TEXAS AT EL PASO,
DMR 0723115



- **Education:** Research results presented at conferences demonstrating the instrument capabilities.

- **Outreach:** Local high school teachers who were participating in a two-week NSF NCLT (National Center for Learning and Teaching in Nanoscale Science & Engineering) Teacher Professional Development Workshop held at UTEP learned about size and scale by observing samples using the confocal Raman and AFM. Program Director, Dr. Eric Hagedorn reported that teachers greatly valued interacting in small groups with Dr. Manciu in her laboratory.

- The system was also used to characterize samples of PVDF for curricular materials being developed by Drs. Michael Eastman and Eric Hagedorn for a U.S. Army Office of Research Materials World Module grant. Undergraduate science majors taking UNIV 1301 will learn to interpret the data as part of their course.

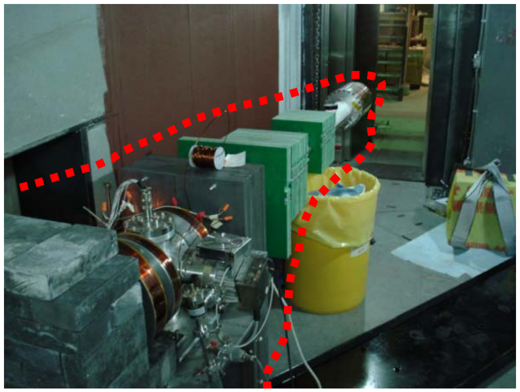
Development of an Intense Positron Annihilation Spectrometry System for Nanophase Characterization

NSF Award # 0521270

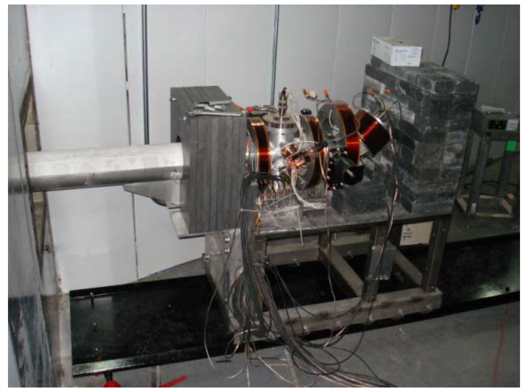
North Carolina State University
The University of Michigan
Oak Ridge National Laboratory

PULSTAR Positron Beam

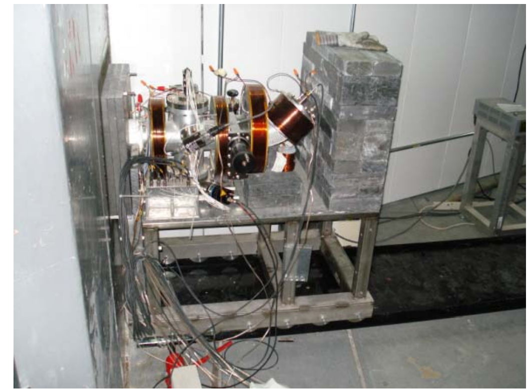
Nano-phase Investigation Using Anti-matter



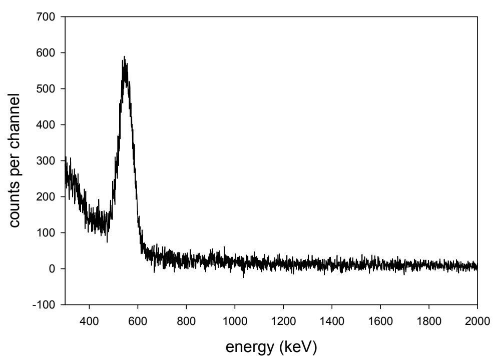
The positron beam-line (within the red border) prior to insertion in to the PULSTAR reactor's beamport #6. The beam-line is ~15 feet long.

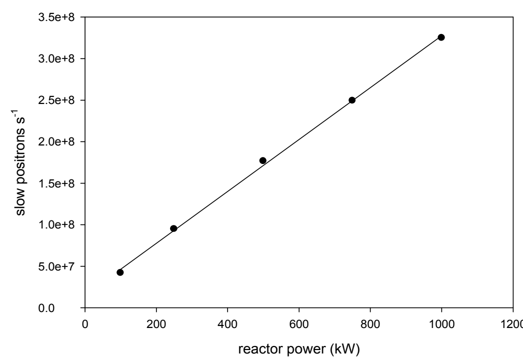


The positron beam-line partially inserted into to the PULSTAR reactor's beamport #6.



The positron beam-line fully inserted into to the PULSTAR reactor's beamport #6.





Recent results of positron generation by the PULSTAR reactor using the positron beam-line shown above. The results indicate a beam intensity exceeding 3 x 10^8 e+/s at full reactor power (1-MW). On-going modification to the beam-line are expected to raise this number substantially. The figure on the left shows the signal of e^- - e^+ annihilation (i.e., 511 keV gamma-rays) in the detector.

World Record 5 x 10^8 e+/s at FRM-II (20-MW) reactor in Munich, Germany.

Development of Synchrotron Infrared Microspectroscopy Imaging using a Multi-element Detector (IRMSI-MED) for Diffraction-Limited Chemical Imaging

Carol J. Hirschmugl (University of Wisconsin-Milwaukee),

DMR-Award 0619759

A novel facility - IRMSI-MED - has been designed and realized for measuring the chemical makeup of biological single cells *in vivo* and providing insight into how sub-cellular structures function in a living cell. Importantly, the rapid measurements that IRMSI-MED will afford will track the changes in their chemical makeup allowing scientists to understand the organism's response to changing environmental conditions. The development of this chemically sensitive infrared microscope with multiple, parallel detection channels will greatly expand the ability to examine such biological structures, and to track their changes over minutes.

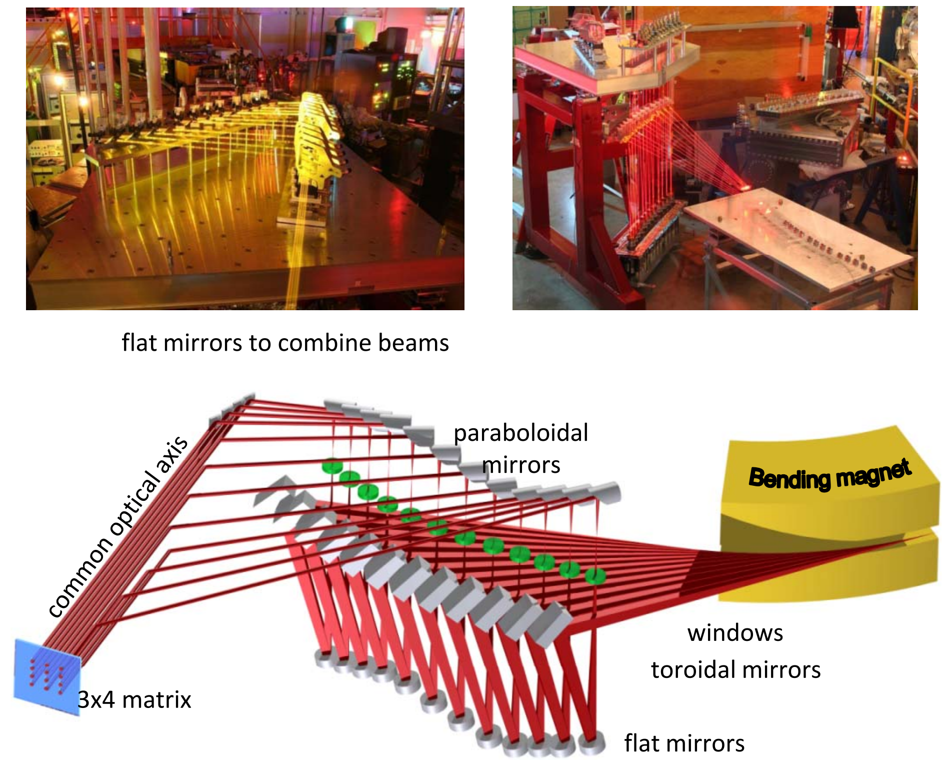


Figure: The bottom panel shows a schematic of the novel IRMSI-MED facility. The top panels show the realization of IRMSI-MED with an initial laser alignment (right) and *in situ* with synchrotron light (left).

Development of Synchrotron Infrared Microspectroscopy Imaging using a Multi-element Detector (IRMSI-MED) for Diffraction-Limited Chemical Imaging

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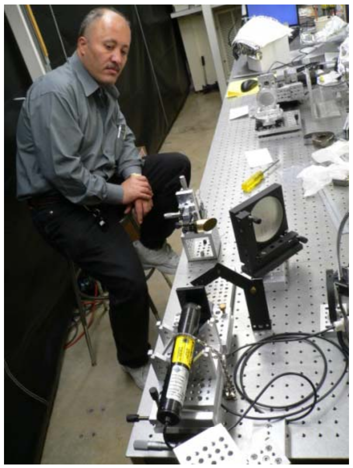


Dr. El Bayarri (SESAME, Jordan) working on alignment issues during assembly of IRMSI-MED.

“At Risk” High School Students visiting the SRC and running experiments at the IR Facility.

•During the realization of IRMSI-MED, Dr. El Bayarri (Jordan), who is directing the assembly of an IR facility at SESAME (Synchrotron in the Middle East to promote Peace and Science), participated in the assembly of the IRMSI-MED facility.

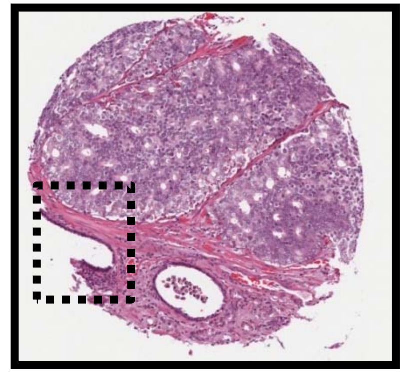
•High School Teachers from Milwaukee Public Schools participating in RET at UWM have arranged visits for their students to SRC where they will use IRMSI-MED for demonstration experiments.

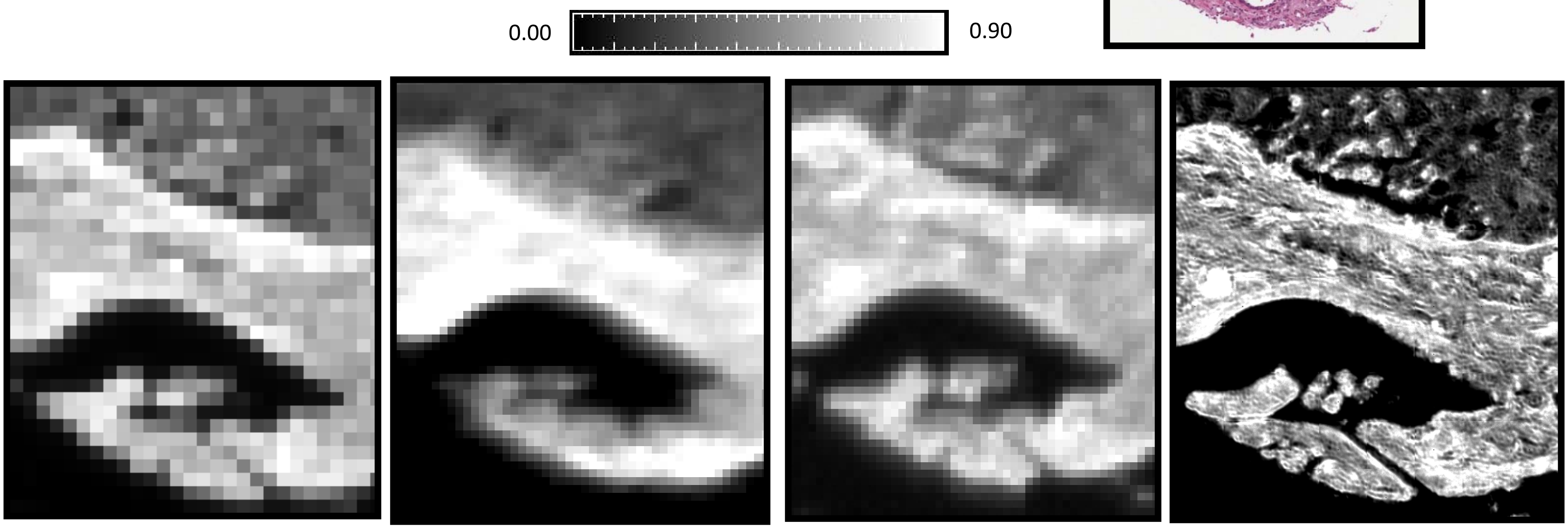
•IRMSI-MED microscope will be available for users across a wide array of disciplines (e.g. soft matter condensed physics, nanoscience, biology, chemistry, veterinary science, engineering, environmental science and geology), providing a new interdisciplinary tool to the broader scientific community.

IRENI at the SRC DMR-Award 0619759

M. Nasse, M. Walsh, R. Bhargava and C.J. Hirschmugl
University of Wisconsin-Milwaukee and University of Illinois Urbana Champaign

- Improve Spatial Resolution
- Improve Temporal Resolution (4 hrs -> 1 minute)
- Improve Signal/Noise





Spotlight FTIR
Point mapping mode
10µm

Spotlight FTIR
Linear Array
6.25µm

Varian (Biorad/DigiLab)
FTIR
Focal Plane Array
5.5µm

IRENI Beamline
Focal Plane Array
Up to 0.54µm

**Images of CH stretch regions*

Major Research Instrumentation (MRI): Development of an In-Situ Neutron Scattering Facility for Research and Education in the Mechanical Behavior of Materials (DMR-Award # 0421219)

P. K. Liaw, H.Choo, L. Li (Ph.D. Student)
Department of Materials Science and Engineering, the University of Tennessee, Knoxville, TN 37996, USA
International Collaborator: Prof. T. Ungar from Eötvös University, Hungary

To complement the development of an in-situ neuron scattering facility at Spallation Neutron Source (SNS), Oak Ridge National Laboratory, Tennessee, preliminary experiments using diffractions were conducted to study the mechanical behaviors of nanocrystalline (nc) materials.

Specimen:

Nc Ni-18wt.%Fe alloy (wt.%: weight percent) (Ni-18Fe)

Mechanical experiments:

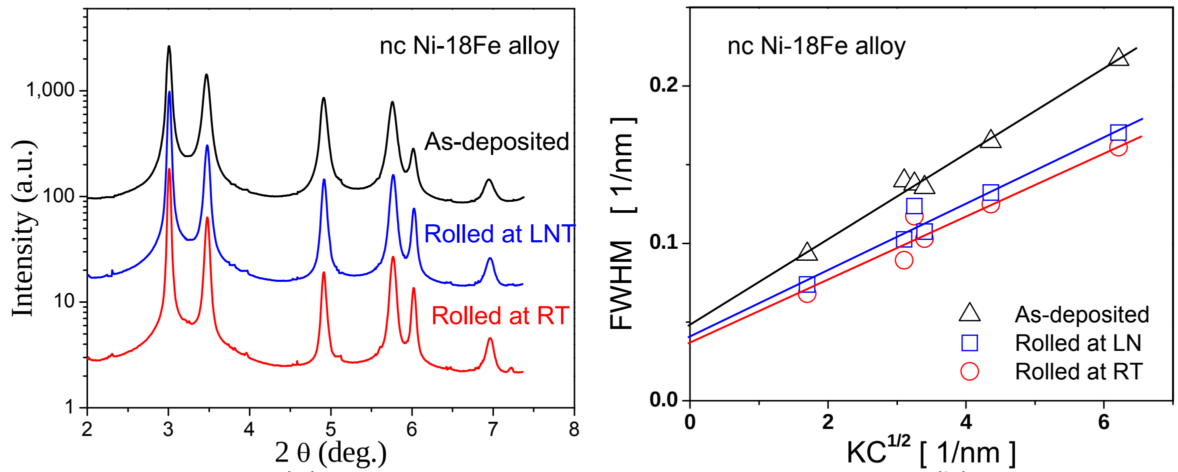
1. Rolling deformations performed at both room temperature (RT) and liquid-nitrogen temperature (LNT).
2. Diffraction experiments

Diffraction-analysis methods:

1. Qualitative method: modified William-Hall method[1]
2. Quantitative method: diffraction line-profile analysis (performed by convolutional-multiple-whole-profile (eCMWP) programs.

New findings:

Concomitant reductions in the densities of both dislocations and twins and an increase in the crystallite size, which has never been observed before.



(a) (b)

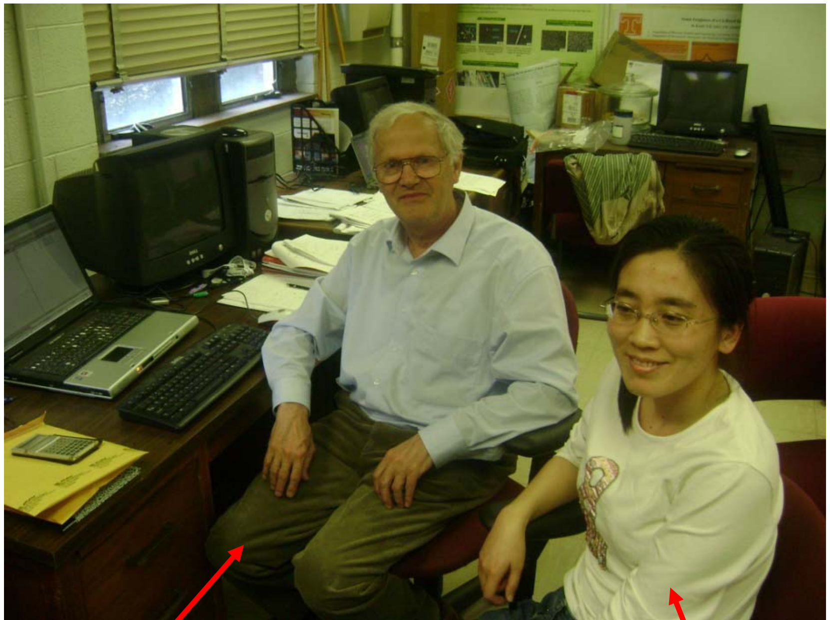
Figure 1(a) Comparison of diffraction patterns for the as-deposited, RT-rolled, and LNT-rolled nc Ni-18Fe alloys shows that peak-widths are shrinking after rolling deformation at both RT and LNT. (b) Modified William-Hall plots quantitatively show the increased grain size [reciprocal to the full-width at half-maximum (FWHM) intercept] and decreased dislocation density (proportional to the slope of line).

Sample	ρ [$10^{16}m^{-2}$]	$\langle x \rangle_{area}$ [nm]	β [%]
Initial	3.7 (±0.5)	14 (±1)	3.2 (±0.8)
RT -rolled	2.2 (±0.4)	31 (±3)	1.5 (±0.3)
LNT -rolled	1.8 (±0.3)	26 (±3)	2.2 (±0.3)

Table 1. The eCMWP fitting values for the average dislocation density (ρ), area-averaged mean crystallite size ($\langle x \rangle_{area}$), and twin-boundary frequency (β) of the as-deposited, RT-rolled, and LNT-rolled nc Ni-18Fe alloys, respectively. It clearly shows the dislocation density and twin-boundary frequency decreased concomitantly with grain growth.

Major Research Instrumentation (MRI): Development of an In-Situ Neutron Scattering Facility for Research and Education in the Mechanical Behavior of Materials (DMR-Award # 0421219)

P. K. Liaw, H. Choo, L. Li (Ph.D. Student)
Department of Materials Science and Engineering, the University of Tennessee, Knoxville, TN 37996, USA
International Collaborator: Prof. T. Ungar from Eötvös University, Hungary



Prof. Ungar

Li Li

A photo taken during Prof. Ungar's 6 weeks' visit at The University of Tennessee in Spring 2008

Outreach Activities

- Prepared a talk for The 2008 Mineral, Metals & Materials Society (TMS) at New Orleans.
- Participated in the 2008 TMS Outstanding Student Paper Contest.

International Collaborations

- Worked with Prof. Ungar from Eötvös University, Hungary, on analyzing diffraction patterns for about 6 weeks at The University of Tennessee in March and April 2008.
- Li Li will visit Prof. Ungar's Lab at Budapest, Hungary, and learn diffraction line-profile analyses to continue the collaboration.

Local Electrode Atom Probe – Tomographic Characterization of III-V Semiconductor Structures

James S Speck (University of California Santa Barbara) DMR-Award #0821168

LEAP[1] produces 3-D compositional images at the atomic scale with high analytical sensitivity[2,3]. Correlation of observed physical properties in these structures with the elemental distribution. Provides insights into growth dynamics .

1. LED[4] structure: InGaN quantum wells grown on m-plane GaN were characterized to investigate Indium distribution. Initial investigations using standard statistical methods[5] (*unpublished*) reveal absence of In clustering in quantum wells.
2. It was proposed that the carrier localization in the active region (InGaN) that leads to enhanced recombination (higher efficiency) was due to Indium segregation. However, no such apparent Indium segregation has been observed in our results.
3. Magnesium clusters are observed in the p-GaN region.

Fig. 1. Description of Atom Probe Operation

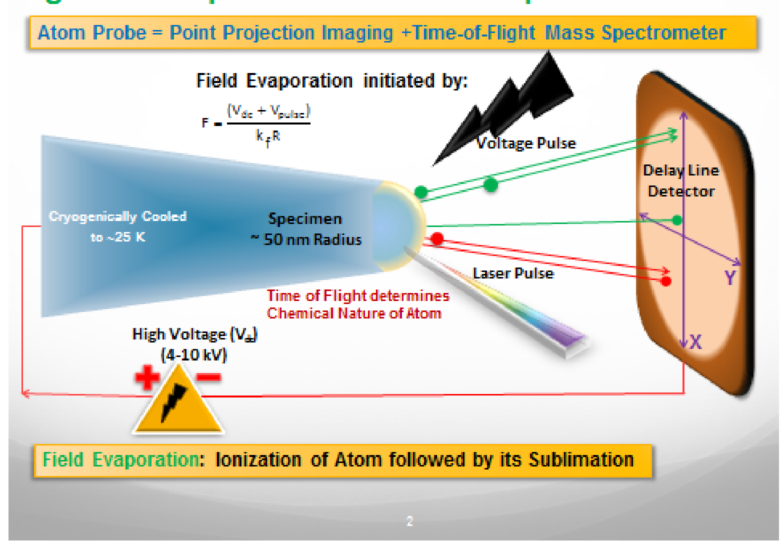
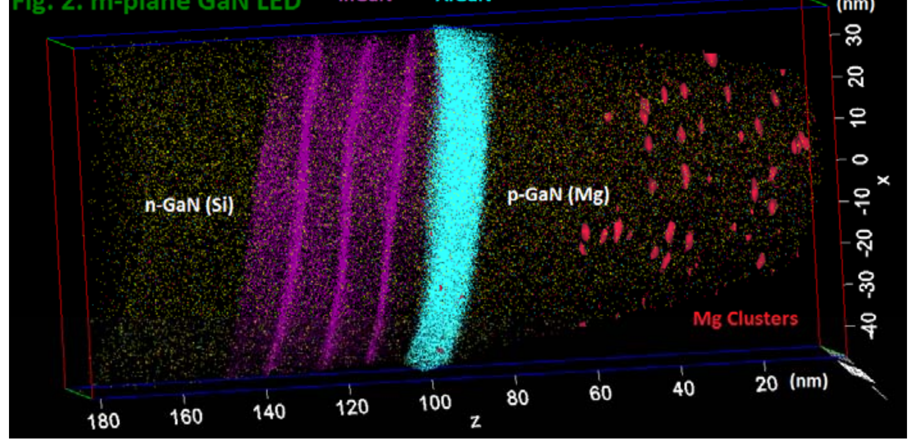


Fig. 2. m-plane GaN LED



Broader Impact of LEAP Facility at UC – Santa Barbara

James S Speck (University of California Santa Barbara), DMR-Award #0821168

Fig. 3. LEAP/TEM Analysis of AlInN

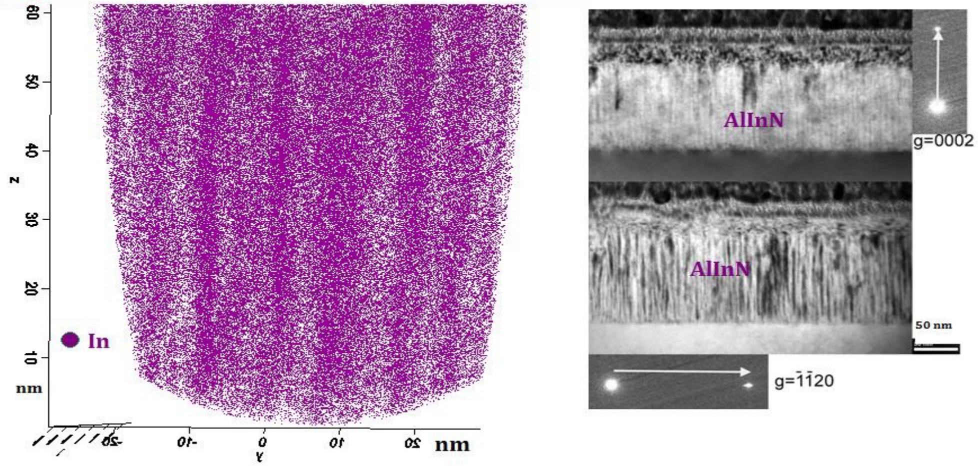
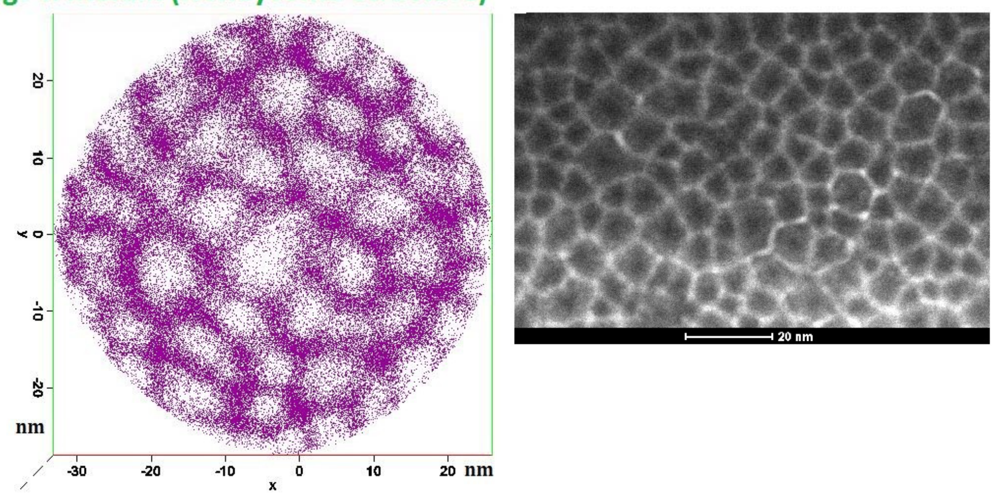


Fig. 4. Indium (Honeycomb Structure)



1. Fundamental understanding of III-V nitrides: Relate electronic properties of devices with structure / local composition

2. Synergistic approach to materials characterization through combination of LEAP and other allied analytical technique (TEM/SIMS). Figure 3 and 4 reveal a cross-correlative LEAP-TEM characterization performed on InAlN layers grown on m-plane GaN to quantify the extent of Indium phase separation and verify 3-D morphology of the “honeycomb” structure.

3. Disseminate Atom Probe Tomography fundamentals and give an overview of its potential applications through an elective course comprising of approx. 15 Lectures and 7 Practicals

4. Developing a sound in-house LEAP technical expertise encompassing many materials systems in order to make cross-discipline/industrial collaboration attractive.

Eliminating Parasitic Slit Scattering in Small Angle X-ray Diffractometers

PI: C. R. Safinya, Co-PI's: A. Butler, S. Feistein, Y. Li, J. Zasadzinski , UC Santa Barbara, DMR-0619171

Our instrumentation development effort has led to a new hybrid design of x-ray aperture slits, which has been demonstrated to almost completely eliminate the detrimental parasitic slit scatterings in small angle x-ray scattering (SAXS) instruments. Parasitic slit scattering is one of the most difficult-to-overcome resolution-limiting factors in current SAXS instrument design. The simple, yet effective hybrid slit design combines a highly polished single crystalline (Si) slit edge bonded to a Tungsten base (inset in C). By using a polished (1 0 0) Si slit edge that generates no SAXS signal, most of the parasitic slit scattering due to the polycrystallinity of the slit material can be eliminated, as shown in the experimental data (A, B, C) collected and analyzed by our 2007 summer RISE (Research In Science and Engineering) intern Thomas Huang (Grinnell College, Iowa) mentored by Co-PI Y. Li (UCSB MRL Summer RISE Intern Report, 2007)

This broadly applicable design concept represents a very cost-effective way to significantly upgrade the performance of a large number of existing and future SAXS instruments, which are essential tools used widely for nanoscale characterization in broad areas of research.

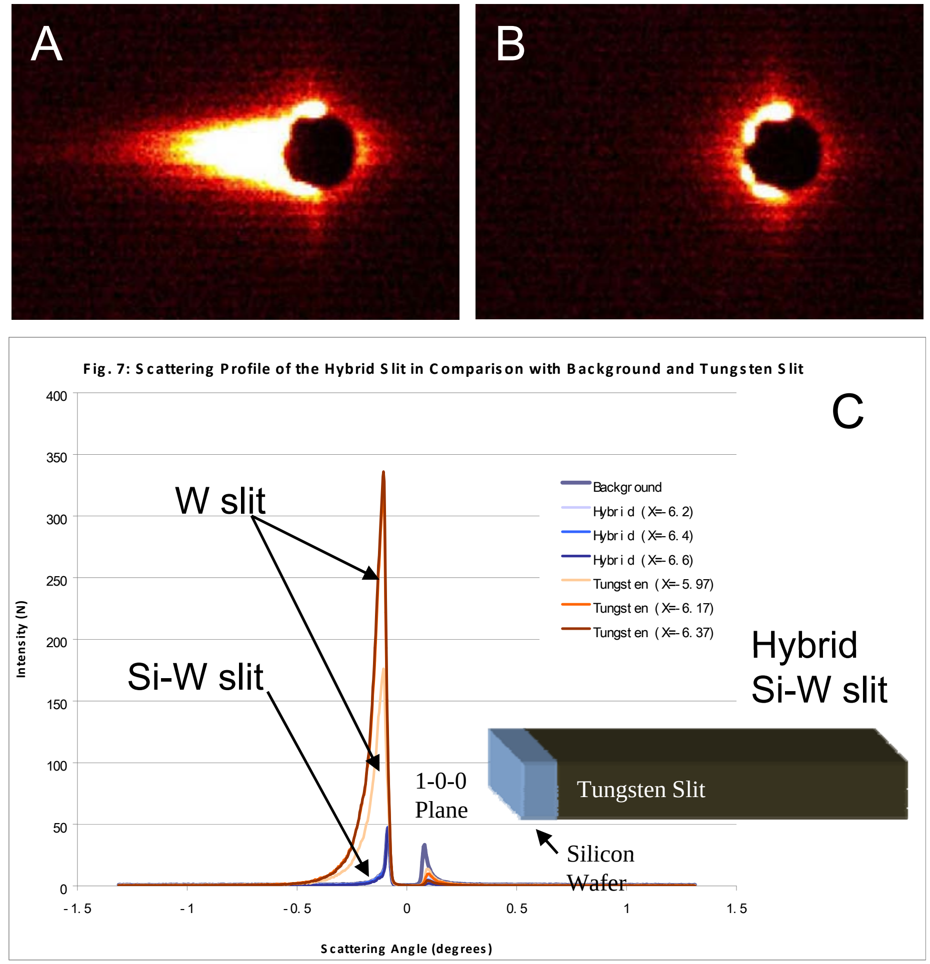


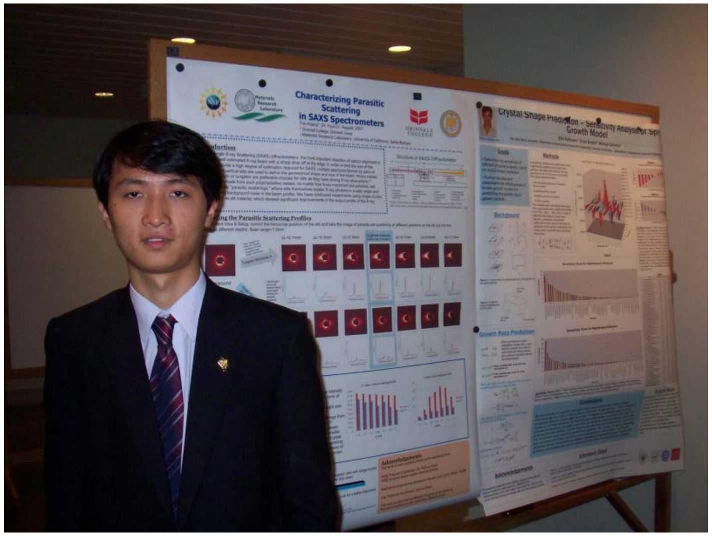
Figure (A, B) Slit scattering images from a traditional Tungsten slit (A) and a Si-W hybrid slit (B). The intensity profiles (C) across the beam stop (centered at X=0) show the dramatic reduction of parasitic scattering to the background level with the hybrid Si-W slit (inset)

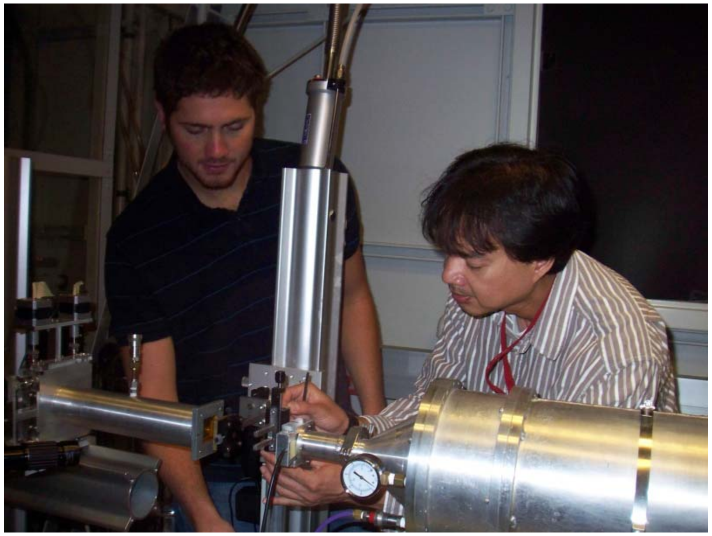
MRI: Development of an Ultra-High Resolution Small Angle X-Ray Scattering Instrument for Characterizing Supramolecular Assemblies

PI: C. R. Safinya, Co-PI's: A. Butler, S. Feistein, Y. Li, J. Zasadzinski , UC Santa Barbara, DMR-0619171

Education: **Multidisciplinary teams comprised of undergraduate and graduate students, and postdocs, with backgrounds in materials, physics and engineering,** are educated in x-ray instrumentation science and SAXS methods for nanoscale characterization of supramolecular assemblies. These skills are essential to successful careers in a broad range of areas including nanoscience and nanotechnology, polymer physics and chemistry, chemical and biomedical engineering.

Outreach: The PI's actively participate in multiple outreach programs at UCSB for undergraduate and high school teacher research internships. **Thomas (Tuo) Huang** (Top photo, presenting at UCSB summer research interns conference), a **MRL RISE Intern (2007)** from Grinnell College, Iowa, worked directly with mentor and Co-PI Dr. Youli Li to develop the scatter-free hybrid x-ray slit (see research highlights). Thomas worked closely with UCSB mechanical engineering undergraduate students **Nicholas Judy** (bottom photo, left), **Eric Walsh**, and staff research associate **Morito Divinagracia** (bottom photo, right), who are actively working on the MRI project together with other graduate students and postdoctoral researchers.

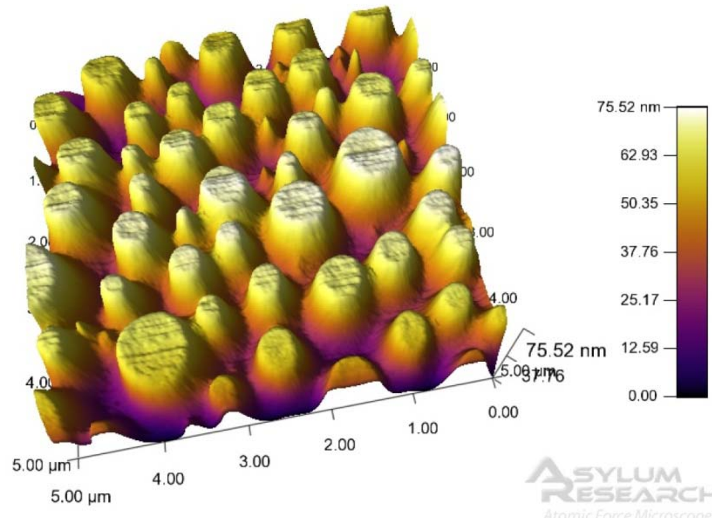




MRI: Acquisition of an Atomic Force Microscope for Undergraduate Research and Education

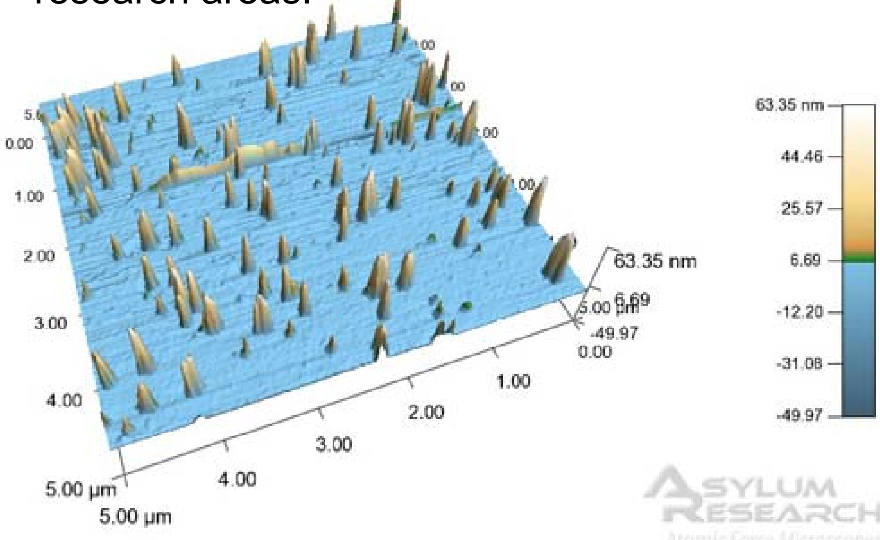
Dean A. Waldow, Myriam Cotten, and Paul H. Davis
Pacific Lutheran University, DMR-0619826

In the first year of this NSF-MRI grant, the majority of effort was spent comparing vendors, purchasing, and installing the atomic force microscope (AFM). The AFM was installed shortly before the end of our spring semester. In the remaining few months of the first year, progress was made in education, in outreach, and in each of three following three research areas.



AFM image of a Graft copolymer compatibilized thin film polymer blend demonstrating control of surface topography

1) The affect of different compatibilizers on high molecular weight nanometer scale thin film polymer blends was studied [Waldow]. **2)** The size and shape distribution of gold nanoparticles as a function of synthesis method and reaction conditions were studied [Davis]. **3)** Initial work on bilipid membranes on mica was begun in relation to antimicrobial peptide interaction with the bilipid membranes [Cotton].



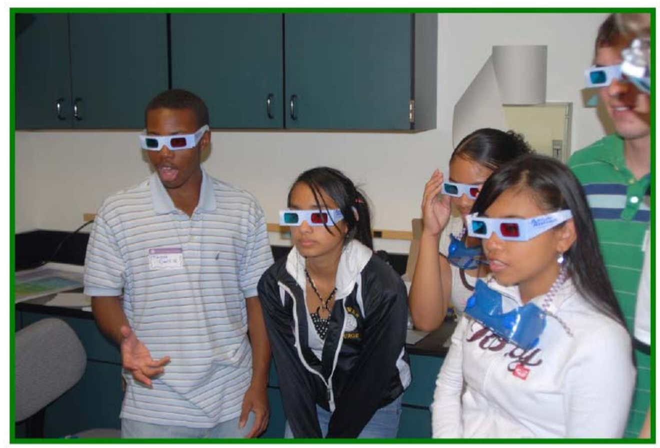
AFM image of gold nanoparticles

MRI: Acquisition of an Atomic Force Microscope for Undergraduate Research and Education

Dean A. Waldow, Myriam Cotten, and Paul H. Davis
Pacific Lutheran University, DMR-0619826 (Page 2)

Outreach: Undergraduate (UG) research students, the principal investigator (PI), and a co-PI hosted a hands-on material science / chemistry workshop for high school students from underrepresented groups in conjunction with the Washington State Mathematics, Engineering, and Science Achievement (MESA) program. Nanoscience and the AFM were key parts of the workshop with students participating in a demonstration of AFM.
(http://www.washingtonmesa.com/)

Education: UG students used the AFM in two classes: Instrumental Analysis and Biochemistry. Many UG summer research students were introduced to AFM during the summer research program. Students studied copolymer compatibilized polymer blend related research (2), gold nanoparticle research (2), and bi-lipid layers on mica surfaces for antimicrobial peptides (2).

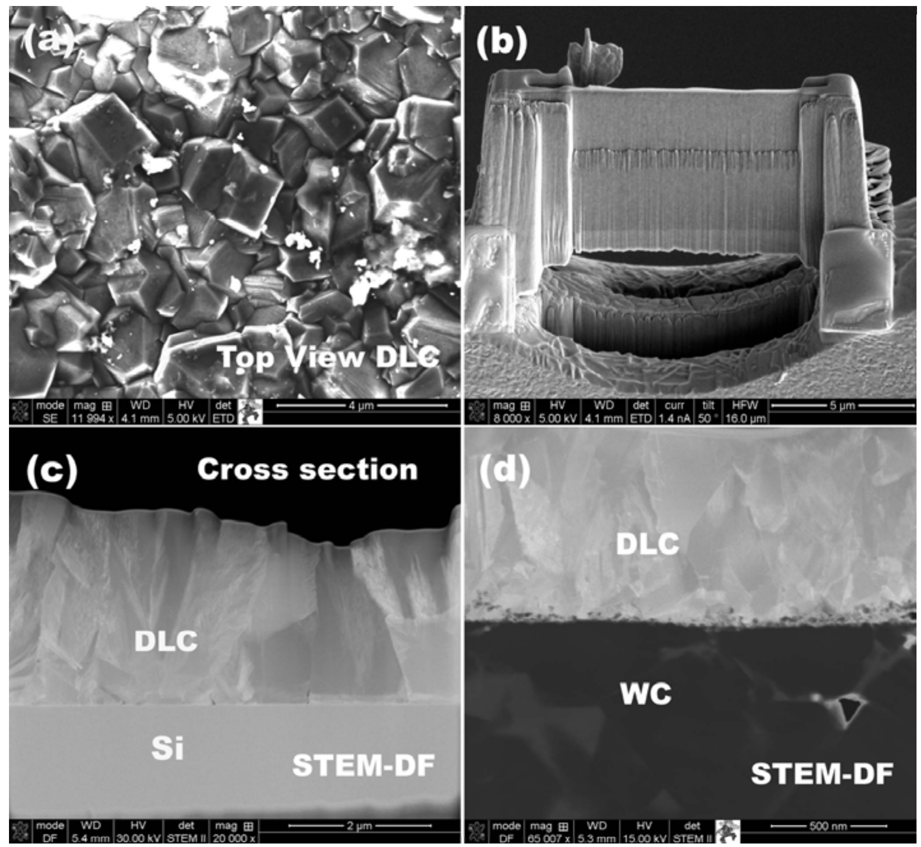


Dual Beam FIB/FESEM at Missouri S&T

F. Scott Miller (Missouri S&T), DMR-0723128

Diamond-like Carbon on Tungsten Carbide

Imaged at the left is a project in which diamond films are laser-deposited onto tungsten carbide substrates. Previously, this type of sample was extremely difficult, if not impossible to cross-section, yet you can see in the bottom row of images that both the diamond coatings and the tungsten carbide substrate are milled very smoothly with the focused ion beam. The Helios Nanolab 600 FIB is a very versatile instrument, and some of its imaging modes and capabilities are shown by this project. Fig. (a) is a top view secondary electron image, Fig. (b) shows the ion milling capabilities in making site-specific electron transparent lamella, and Figs. (c) and (d) show the excellent imagies produced by the 12 quadrant STEM detector.



Dual Beam FIB/FESEM at Missouri S&T

F. Scott Miller (Missouri S&T), DMR-0723128

The Helios Nanolab 600 has been used by a large number of undergraduate and graduate student researchers, as well as post-doctoral users from over 23 different research groups across ten different departments at Missouri S&T as well as several industrial groups. It has been integrated into the laboratory sections of three classes (Cell Biology, Scanning Electron Microscopy, and Transmission Electron Microscopy) and has been utilized in a variety of outreach activities. In the images at the left, high school students in a recent Materials Camp sponsored by ASM and hosted by the Department of Materials Science and Engineering disassemble smartphones to discover the large variety of materials necessary to produce the components of the phones. The students were able to analyze the components in the newly-renovated electron microscope suite, which will also house the recently acquired Tecnai G2 F20 STEM, partially funded by DMR-0922851

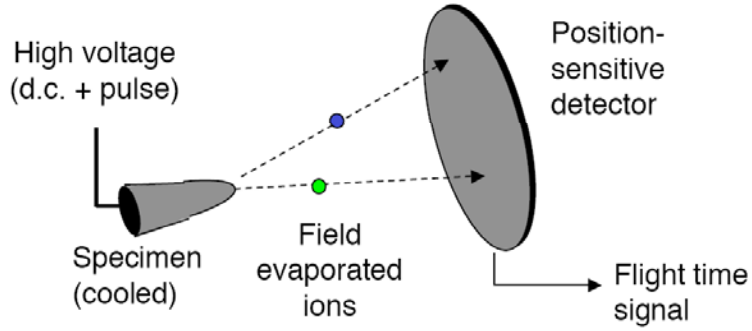
Atom Probe Tomography of Advanced GaN-based LEDs

James Speck, University of California-Santa Barbara, DMR 0821168

Atom Probe Tomography

3-D atomic scale chemical maps

- •Sharp tip (pcrepared by FIB or etching)
- •DC E-field + laser pulse (or E-pulse)
- •Atom position via position on detector
- •Atom nature via flight time



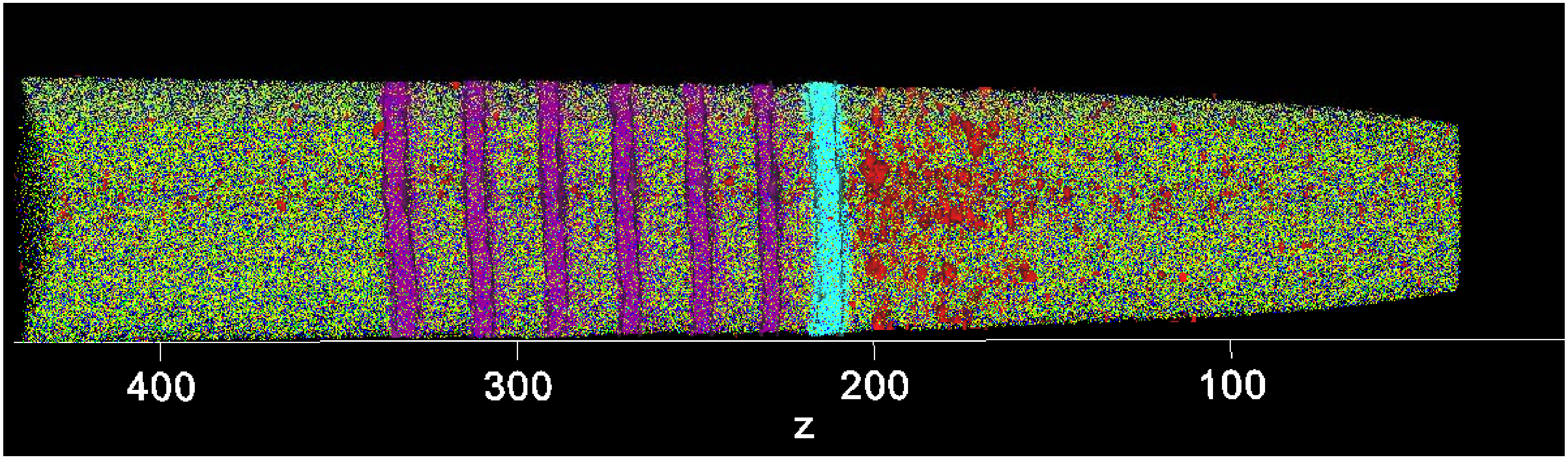
Atom probe reconstruction: GaN LED

Recorded at UCSB on Imago HR 3000 LEAP atom probe
m-plane, non-polar LED - 60 million atom data set
(left to right)
GaN:Si/6X In_xGa_{1-x} N/GaN QW/Al_yGa_{1-y}N/GaN:Mg

Key results

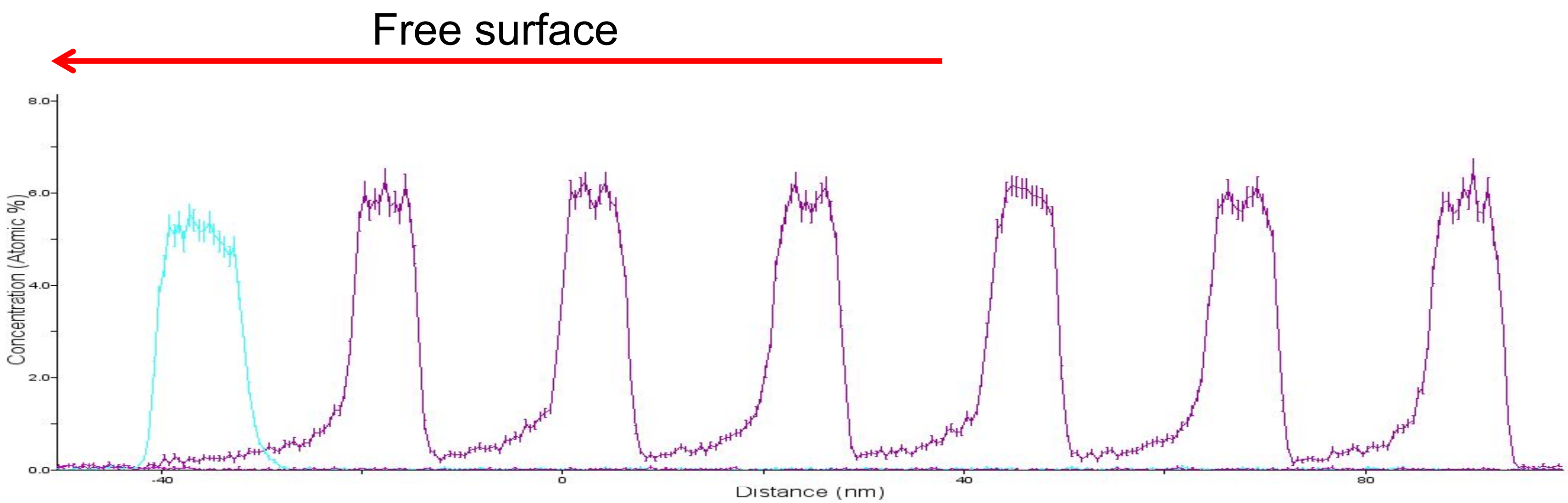
- •Homogeneous In_xGa_{1-x} N quantum wells
- •Mg clustering in GaN:Mg layer

Color code:
Ga+N: green; **In: purple**; **Al: aqua**; **Mg: red**



Atom Probe Tomography of Advanced GaN-based LEDs

James Speck, University of California-Santa Barbara, DMR 0821168



In: purple; **Al: aqua**
Note that the sample direction is reversed (free surface toward left in this image)

Detailed analysis of multiple quantum well (MQW) region

- Chemically homogeous $In_xGa_{1-x}N$ in the quantum wells
- Abrupt lower and upper interface with additional evidence of floating In layer that leads to additional indium incorporation in barrier layers

Broader Impact

Example of nanoscale chemical analysis with atomic scale, 3D resolution
Unparalleled resolution and dynamic range (from ~10^{17} cm^{-3} to bulk composition)

Training Activities

James Speck, University of California-Santa Barbara, DMR 0821168

Ravi Shivaraman
M.S. in Materials Science (ASU)
1+ year staff member at Imago Scientific
Temporary staff member – UCSB Microscopy and Microanalysis Facility (Summer 2009)
Ph.D. student – UCSB Materials Department (current)

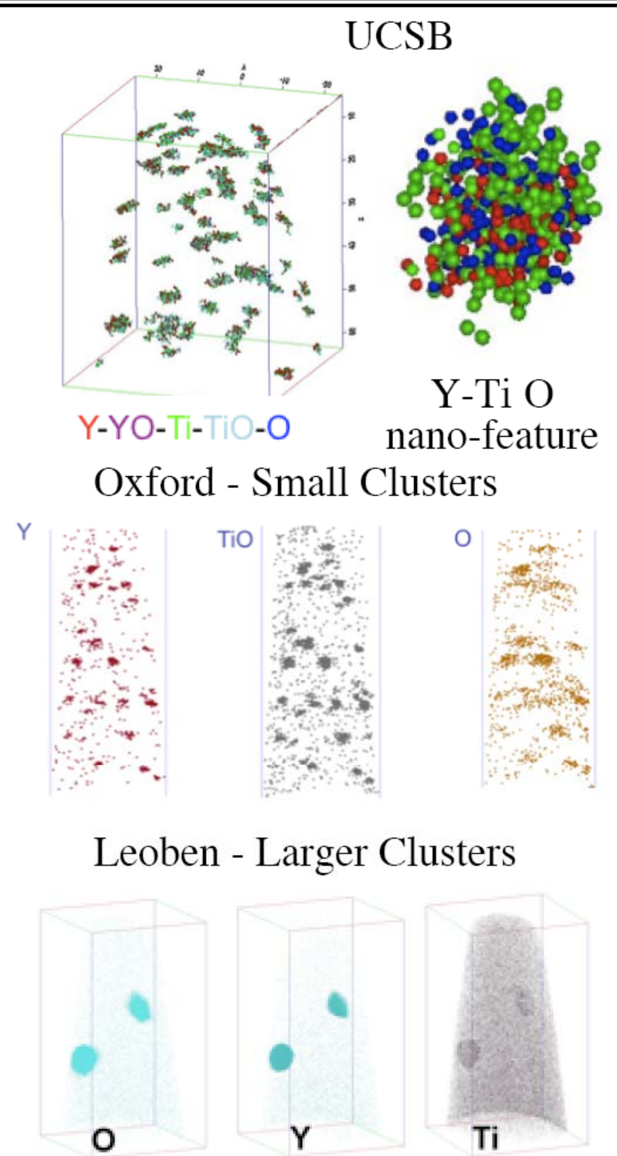
Nicholas Cunningham
MS in Mechanical Engineering (UCSB)
Ph.D student

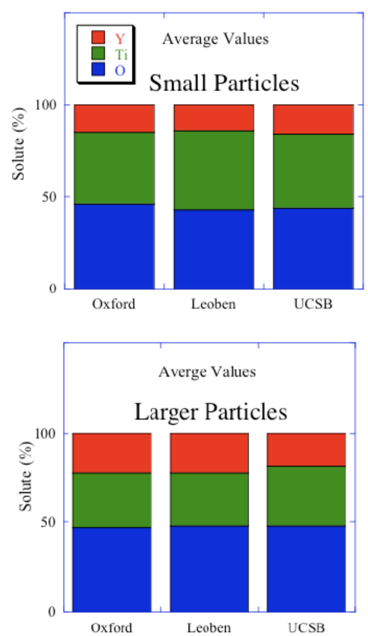
Summer 2009 LEAP (atom probe) Training Sessions

- **5 Participants**
- **6 Training Sessions**
- **8 Potential/Current Users**

International Activities

James Speck, University of California-Santa Barbara, DMR 0821168





UCSB-Oxford-Leoben Collaboration

Round-robin characterization of a reference advanced high temperature and radiation damage tolerant nano-dispersion-strengthened alloy with far from equilibrium nm scale Y-Ti-O precipitate clusters

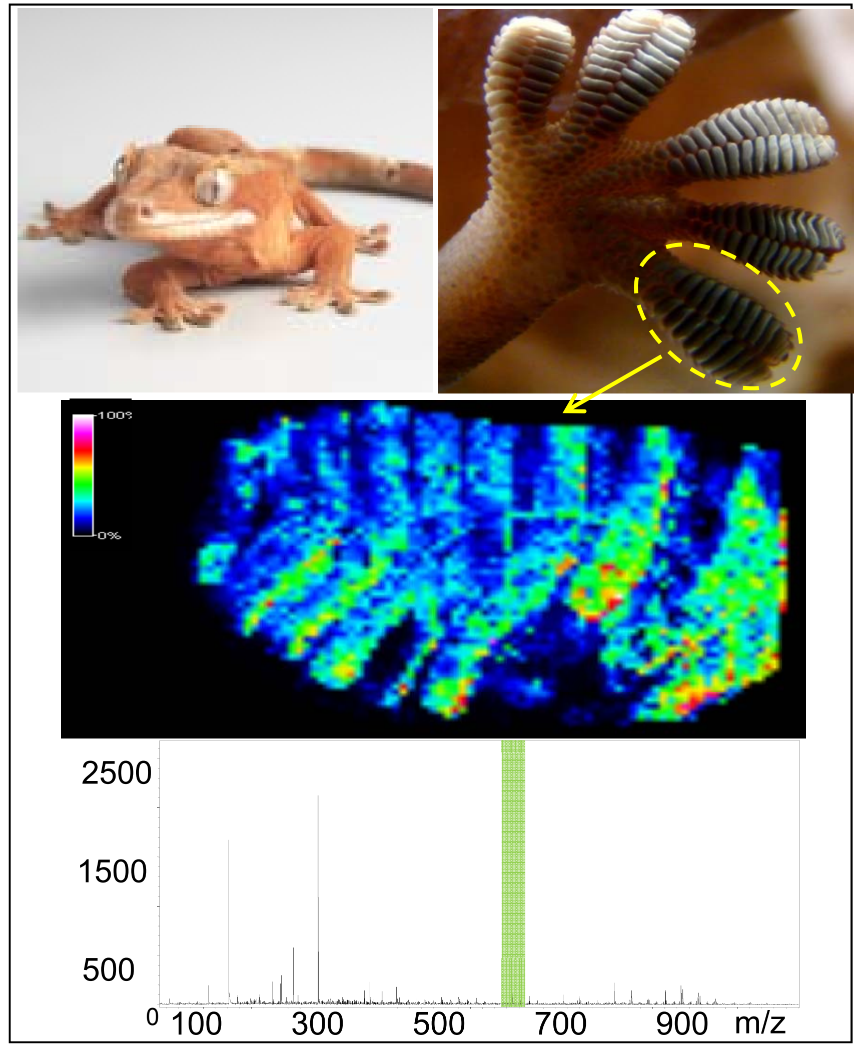
Excellent agreement between data from three laboratories

MALDI Imaging and Traveling Wave Ion Mobility Mass Spectrometry in Materials Research

Chrys Wesdemiotis, The University of Akron, DMR-0821313

Gecko Inspired Adhesives

Scientists have long admired the gecko's ability to walk up smooth surfaces, but have never fully understood how this works. The only explanation provided thus far has been that the gecko's amazing sticky power results from the complex hierarchal structure of the microscopic hair present on the gecko's toes. Recent collaborative research at the University of Akron between the groups of Peter Niewiarowski (Biology), Ali Dhinojwala (Polymer Science), and Chrys Wesdemiotis (Chemistry & Polymer Science) discovered many small molecules on the millions of hair strands (setae) within the gecko's toe using high-sensitivity MALDI imaging. Each molecule on the hair surface can be displayed in a distribution map with this most straightforward method. The information from these images is currently combined with high-resolution ESI tandem mass spectrometry and traveling wave ion mobility mass spectrometry to identify the exact structures of the small molecules. The knowledge gained from gecko's sticky toes will ultimately lead to novel synthetic adhesives that are both dry and self-cleaning.



MALDI imaging of the footprint from a gecko's single toe. The image displays the distribution of the molecule with *m/z* 649.

MALDI Imaging and Traveling Wave Ion Mobility Mass Spectrometry in Materials Research

Chrys Wesdemiotis, The University of Akron, DMR-0821313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CHEMICAL & ENGINEERING NEWS
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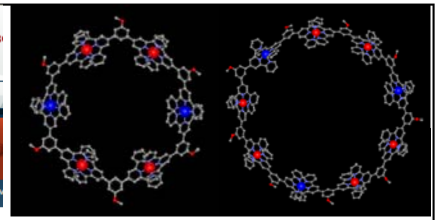
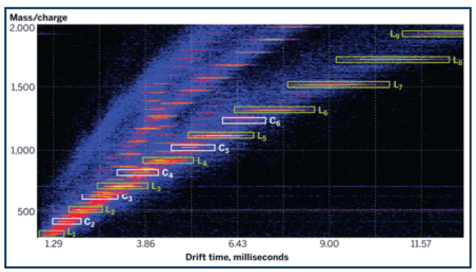
COVER STORY
Home » March 29, 2010 Issue » Cover Story » Positive Signals » Doubling Up On M
MARCH 29, 2010 | VOLUME 88, NUMBER 13 | PP. 35 - 37
Doubling Up On Mass Analysis
Coupling ion mobility spectrometry with mass spec provides sensitivity to analy
Mitch Jacoby





The first Traveling Wave Ion Mobility Mass Spectrometry (TWIM MS) studies of self-assembled supramolecules and supramolecular polymers have been reported and attracted considerable attention because such substances, which are designed for many different applications (e.g., sensors, drug release agents, photovoltaic materials), are difficult to characterize by other methods. The ACS magazine C&EN highlighted these results in a cover story entitled “Doubling Up On Mass Analysis.”

Undergraduate, graduate, and postgraduate students routinely utilize the instruments acquired with the MRI grant. McNair scholars and ACS-SEED high school students (both selected from groups that are underrepresented in science) have conducted research during the summer. The instruments have facilitated research across several departments at the University of Akron; they have also provided valuable analytical assistance to other academic institutions (Kent State University, Cleveland State University, College of Wooster, Kenyon College, Hiram College, Louisiana State University), hospitals (Akron General, SUMMA Health Care), and industrial corporations (Goodyear, Lubrizol, OMNOVA, DuPont, GoJo). Several industrial problems could be solved by analyses made possible with the new instruments.