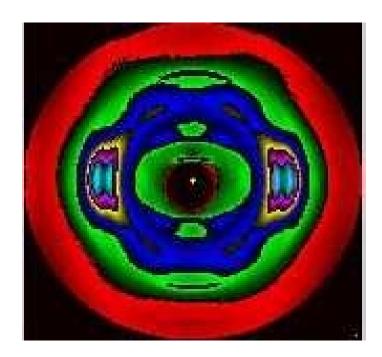
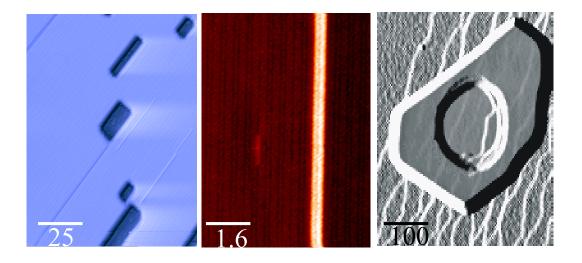
DIVISION of MATERIALS RESEARCH RESEARCH AND EDUCATION HIGHLIGHTS FY 2001



DIVISION of MATERIALS RESEARCH Research and Education Highlights, FY 2001

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Acknowledgment

This report derives almost entirely from the FY 2001 program reports prepared by the Program Directors of the Division of Materials Research. I deeply appreciate their dedication and professionalism. W. Lance Haworth, Executive Officer, DMR 18 August 2001

Division of Materials Research Highlights FY 2001

INTRODUCTION

The Division of Materials Research (DMR) is the unit of the Federal Government with primary responsibility for the overall health of materials research and education in the nation's colleges and universities. Materials research integrates a wide range of activities spanning both science and engineering. These extend from investigations of phenomena in condensed matter physics and solid state chemistry to research on functional materials including metals, ceramics, polymers, biomaterials, and electronic, photonic and magnetic materials. Materials research addresses the synthesis, processing, characterization, and properties of materials together with the prediction and control of materials behavior, encompassing the discovery and understanding of materials and condensed matter phenomena and the basis for their

translation into technological application. Its practitioners include physicists, chemists, materials scientists, and engineers, and it benefits from the participation of researchers from an even wider range of disciplines such as biochemistry, biology, earth sciences, mathematics, science. computer and medicine. The technological and societal significance of the field is immense: "Everything is made out of something". DMR supports education, fundamental research and facilities that are critically important to the future advancement of industries and technologies ranging from electronics and communications to information technology, transportation and



aerospace, energy, environmental protection, manufacturing, medicine and health care, packaging, and civil infrastructure.

The DMR budget (current plan) in FY 2001 is \$209.75 million. Most of these funds are allocated to nine core programs, namely Condensed Matter Physics, Solid State Chemistry, Polymers, Metals, Ceramics, Electronic Materials, Materials Theory, Materials Research Science and Engineering Centers, and National Facilities and Instrumentation. NSF's Budget Office requires that some of the DMR funds be held in accounts outside the core programs; these include, for example, funds for the NSF priority areas in Information Technology Research and Biocomplexity in the Environment.

Within this framework, DMR strongly encourages high-risk research with potential for high scientific or technological impact; support for women and minorities; projects integrating research and education; and projects with the broad multidisciplinary and interdisciplinary approach needed to address many of the complex and challenging problems in materials research.

NSF's Strategic Goals involve support for People, Ideas, and Tools. The DMR current plan for FY 2001 includes \$16.13M for <u>People</u> (primarily through Research Experiences for Undergraduates and the CAREER program), \$154.88M for research and education awards to individual investigators, groups and centers under <u>Ideas</u> (such awards also include stipends for graduate students and support for faculty salaries), and \$37.16M for <u>Tools</u> (including user facilities and instrumentation awards).

Special Emphasis Areas in FY 2001

In addition to core research and education activities built around individual investigator programs and support for centers, instrumentation and national user facilities, DMR provided support for a wide variety of crosscutting activities in FY 2001. Some of these include:

- NSF priority areas in Nanoscale Science and Engineering (\$58.82M from DMR in FY 2001), Information Technology Research (\$7.28M), and Biocomplexity in the Environment (\$1.07M). DMR is a key player in the 'nano' area and has a significant role in ITR, and DMR staff were heavily involved in administering both these NSF-wide competitions in FY 2001.
- Interdisciplinary research and university-industry cooperation, through Focused Research Groups (FRGs), centers and GOALI awards for example.
- A broad spectrum of activities in education and human resource development, thematic workshops, and international activities in materials research and education.

Focused Research Groups (FRGs) are collaborative, interdisciplinary materials research projects. They are normally smaller than MRSECs and involve three or more investigators, and they represent a significant and growing



DMR grantees contributed several articles to the special 'Nanotech' issue of Scientific American in September 2001

investment for the Division. The FRG concept has been adopted by other MPS Divisions and also (under various names) in NSF-wide competitions such as nano and ITR. FRG proposals are co-reviewed among DMR programs and other NSF programs as needed. The Division now supports about 50 active FRG awards (including new awards under the Nanoscale Science and Engineering competition in FY 2000).

DMR efforts to support human resource development and foster diversity in the materials field also continue to grow. Among many examples, supplementary support to DMR grantee Douglas Osheroff (DMR-0107408) provided funds for travel and local expenses for 54 African-American students to attend the Annual National Conference of Black Physics Students held at Stanford University this year. DMR supported a total of 61 Site awards for Research Experiences for Undergraduates in FY 2001, and 120 precollege teachers participated in Research Experiences for Teachers at many of these REU Sites in FY 2001. Further details of REU and RET activities are given later in this report.

Over the past six years DMR has co-sponsored a series of workshops in different regions of the world with the goals of identifying specific areas and future directions for cooperation between US and foreign investigators in materials research and education, and to begin the development of a Materials World Net for international communication in the field of materials. Several of the workshops are now bearing fruit. An NSF Dear Colleague Letter issued FY 2000 and updated in FY 2001 describes opportunities for cooperative activities in materials research between US and European researchers to be supported by NSF and the European Community. DMR plays a leading role in this partnership which involves three NSF Directorates together with the EC Growth Programme. Five NSF awards were made this year and more than 30 additional proposals are under review in the current phase of the competition. Comparable



arrangements for international cooperation are now being actively explored by NSF and its counterpart agencies in Canada, Mexico, and South America, and also by NSF and national funding agencies in Europe to complement the NSF-EC interaction. A workshop held in South Africa last year to address opportunities for US-African cooperation in materials research and education has already stimulated the development of regional materials networks in Africa.

Crosscutting and Coordination Activities

DMR was involved in all NSF priority areas (formerly termed "initiatives") in FY 2001. The Division plays a major administrative and funding role in Nanoscale Science and Engineering (Nano), and provides significant support in funding and staff time to in the Information Technology Research (ITR) priority area. These activities in Nano and ITR are addressed in more detail below. DMR funds have a small but significant impact on Biocomplexity in the Environment (BE). The 21st Century Workforce priority area is focused primarily in NSF's Directorate for Education and Human Resources; DMR supports this priority area through MPS contributions to minority programs.

Inter-agency Activities

Nanoscale Science and Engineering and the National Nanotechnology Initiative (see also <u>High Risk</u> <u>Investment Areas</u>, below):

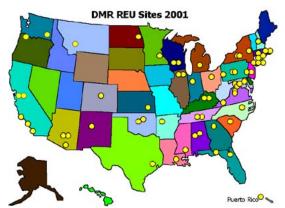
The NSF Nanoscale Science and Engineering Priority Area involves all NSF directorates and forms part of the multi-agency National Nanotechnology Initiative announced in FY 2000. MPS and Engineering are the two lead NSF directorates and DMR plays a key role in the overall MPS and NSF effort in this rapidly emerging area of science and technology. DMR-supported efforts in nanoscale science and engineering include every program in the Division and range from individual-investigator awards and focused research groups to multidisciplinary centers. Tom Weber (DD/DMR) is a member of the Interagency Working Group; Lance Haworth (EO/DMR) co-chairs the NSF Working Group. DMR Program Directors played a major role in the FY 2001 NSF Nano competition; Ulrich Strom (PD, MRSECs) served as NSF-wide coordinator for the Centers competition, and LaVerne Hess (PD, Electronic Materials) and Andy Lovinger (PD, Polymers) coordinated DMR's participation in the Interdisciplinary Research Team and Exploratory Research competitions. DMR accounted for a significant fraction of the total NSF investment in nanoscale science and engineering in FY 2001 (\$58M out of approximately \$150M). DMR invested \$11.08M in new awards under the NSF Nanoscale Science and Engineering competition in FY 2001, including support for 7 Exploratory Research awards, 25 Interdisciplinary Research Teams, and 5 Centers. Another 82 awards in nanoscale science and engineering amounting to over \$26M were made independently by DMR core programs.

Intra-agency Activities

DMR is a major participant in an increasingly wide range of intra-agency activities. DMR staff contribute

a significant fraction of their time and effort to planning and implementing these activities. The NSF-wide 'nano' and 'ITR' competitions in particular expanded rapidly from FY 2000 to FY 2001with correspondingly large demands on DMR staff time and effort. Some examples of intra-agency activities in FY 2001 include:

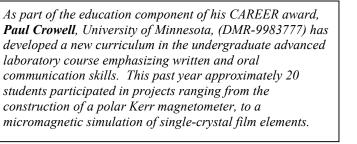
- REU Sites (11 competitive awards for \$2.07M). Overall, DMR supported about 760 REU students at REU Sites, MRSECs and National Facilities in FY 2001 and several hundred more REU students through individual-investigator awards).
- Research at Undergraduate Institutions (7 competitive awards for \$1.84M, down from 18 awards for \$2.35M in FY 2000)

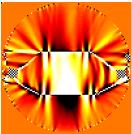


- About 120 pre-college teachers participated in Research Experiences for Teachers (RET) activities at REU Sites, Centers and Facilities supported by DMR in FY 2001. These RET awards were funded primarily by the MPS Office of Multidisciplinary Activities.
- DMR played a significant role in the NSF-wide Information Technology Research Priority Area in FY 2001. Bruce Taggart and Daryl Hess (PDs, Materials Theory) coordinated DMR's participation in the ITR competition and contributed much time and effort to the overall NSF review process. DMR

supported (in whole or in part) to 5 five-year "medium" ITR awards and 5 three-year "small" ITR awards through the NSF-wide competition for a total of \$7.28M in FY 2001 funds.

- DMR played a supporting role in the NSF Priority Area on Biocomplexity in the Environment in FY 2001. David Nelson (PD, Solid-State Chemistry) coordinated the BE activity for DMR. The Division provided \$1.05M for support of new awards through the NSF BE competition in FY 2001.
- CAREER awards (42 competitive awards in FY 2000 for \$10.8M, up from 33 awards for \$9.6M in FY 2000)





High Risk Investment Areas

Some examples of 'high risk' investments in DMR are given below. *In addition every DMR program supports a broad spectrum of awards involving various degrees of risk.* Program directors are encouraged to support high-risk awards, where appropriate, through matching support from the Division Reserve account.

Nanoscale Science and Engineering

In FY 2001 the NSF Nanoscale Science and Engineering Priority Area focused on six high-risk/high-reward research areas. DMR plays a key role in this initiative (see <u>Interagency Activities</u>, above). The six focus areas are:

• *Biosystems at the Nanoscale.* Research in this area supports the development of a fundamental understanding of nanobiostructures and processes, nanobiotechnology, and techniques for a broad range of applications in biomaterials, biosystems-based electronics, agriculture, energy, and health.



- Nanoscale Structures, Novel Phenomena, and Quantum Control. Research in this area explores the
- novel phenomena and structures that appear on the nanoscale. *Device and System Architecture*.
- Research aims to understand interactions among nanoscale devices, the design of nanoscale systems, and their integration into architectures for various operational environments.

To bring the nanoworld to everyone, the University of Wisconsin MRSEC (Thomas F. Kuech, DMR-0079983) has developed a series of short web-based 'picture books' accompanied by hands-on demonstrations that illustrate nanoscale materials and devices. (<u>http://www.mrsec.wisc.edu/edetc/nano/index.html</u>). This work is the basis for a lead article in the Smithsonian's Muse magazine Spring 2001 issue dedicated to nanotechnology. (<u>www.musemag.com</u>).

- *Nanoscale Processes in the Environment*. Research in this area focuses on probing nanostructures and processes of relevance in the environment from the Earth's core to the upper atmosphere and beyond.
- *Multi-scale, Multi-phenomena Modeling and Simulation at the Nanoscale.* Research on physical, mathematical, chemical and biological modeling and simulation techniques in the nanoscale range includes quantum mechanics and chemistry, molecular simulation, grain and continuum-based models, stochastic methods, and nanomechanics.
- Societal Impact of Scientific and Technological Advances on the Nanoscale. Research on economic, ethical, legal, and other societal aspects will be explored in order to anticipate potential impacts. This

includes studies of life cycle economic assessments for nanoscale processes and systems and the potential impact of nanotechnology on everyday life as it moves to a commercialization stage.

The largest number of NSF proposals was received in the *Nanoscale Structures, Novel Phenomena and Quantum Control* focus area in the FY 2001 competition, and DMR's role was correspondingly focused quite strongly – though not exclusively - on this aspect of the competition.

The National High Magnetic Field Laboratory

In FY 1991 DMR began support for the National High Magnetic Field Laboratory, operated by a consortium involving Florida State University, the University of Florida and Los Alamos National Laboratory. The project was perceived at the time as one with high risk and high potential for payoff in fundamental research. In the ensuing ten years, the NHMFL has developed from a design blueprint to reach fruition as the world's premier laboratory for the exploration of matter under high-field conditions, attracting the very best scientists and engineers as participants and users. In January 2001 NSF support for the NHMFL was renewed for a further 5-year period on the basis of a comprehensive review conducted during the previous year; the funding levels planned for FY 2003 and beyond are subject to the outcome of further review in FY 2002.

At the NHMFL's Center for Integrating Research and Learning two signature programs, Research Experiences for Undergraduates and Research Experiences for Teachers, provide mentorships through which students participate in authentic laboratory experiences. 43 teachers have been challenged to extend their understanding of how science is done in the real world and to create classroom materials for over 2,200 K-12



The Spallation Neutron Source (SNS)

The SNS is now under construction at Oak Ridge National Laboratory. NSF and DoE staff are exploring NSF's future role in providing a full suite of instruments for the high-power target station currently under construction. NSF's participation will help the US regain worldwide pre-eminence in research and education in neutron science with applications to materials science, condensed matter science, chemistry, earth science, biology and engineering.

Exploratory Research

DMR supported thirteen individual awards for exploratory research in FY 2001. Four of these were made without external review under the "Small Grants for Exploratory Research" program, and nine through the following panel review in NSF-wide competitions (nanoscale Science and Engineering, and Biocomplexity in the Environment). These awards are typically made for up to \$100,000 for one year and specifically enable investigators to pursue high-risk, exploratory projects. In addition, the MRSEC program explicitly encourages Centers to provide seed funding for high-risk projects and exploratory research; the MRSECs invested about \$4 million in such efforts in FY 2001 for the support of more than 50 individuals and small groups.

DMR HIGHLIGHTS

Highlights of DMR activities in FY 2001 are given in this section, organized by their focus on people, ideas and tools respectively.

1. **PEOPLE**

Research Experiences for Undergraduates and Teachers

DMR supported the research efforts of well over 1000 undergraduates in FY 2001, including 760 at REU Sites, MRSECs and National Facilities, and several hundred more through individual-investigator awards.

About 350 students participated in summer research experiences at 36 locations established through the annual NSF-wide REU Site competition. Two Sites are co-funded with the Division of Physics, one with Chemical and Transport Systems (Directorate for Engineering), and two with the Four are affiliated with Materials Research NSF-EPSCoR program. Science and Engineering Centers. In addition, 23 MRSECs supported by DMR in FY01 incorporated REU Sites as an integral part of the MRSEC efforts; about 380 students participated. DMR user facilities including the National High Magnetic Field Laboratory and the Synchrotron Radiation Center also supported REU Sites involving 30 students. (http://www.nsf.gov/mps/divisions/dmr/research/c reusites.htm) About 120 pre-college teachers participated in Research Experiences for



Teachers (RET) activities in 26 DMR REU Sites, including those within centers and facilities, during FY 2001. Support for these RET activities was provided by the MPS Office of Multidisciplinary Activities.

"This research experience provided me with the additional insight as to how I want to inspire my students towards a science career. The research projects gave me new ways in which to incorporate basic knowledge and techniques into my lesson plans. I was most impressed by the spirit of collaboration and the excitement of research that was exhibited by everyone I came into contact with. It was the sharing of ideas and information that made the biggest impression on me. This is the feeling I want to bring back to my students, that science is interesting, challenging and exciting." Dara Stone, Chestnut Accelerated Middle School, Springfield, MA (U Mass - Amherst MRSEC RET participant)

Minority-Serving Institutions Link with MRSECs.



DMR supports two Collaboratives to Integrate Research and Education, CIRE; one between the U. of Puerto Rico at Humacao (Fredy Zypman, DMR-9872689) and the MRSEC at the U. of Pennsylvania (Michael L. Klein, DMR-0079909), the other between Florida A&M University (Hamid Garmestani, DMR-9982872) and the MRSEC at Carnegie Mellon University (Gregory S. Rohrer, DMR-0079996). The Collaboratives are designed to improve minority education in materials-related areas by using both the human and practical resources of the MRSECs to establish joint research programs and sponsor summer exchange programs. A new masters' program in materials physics, the first graduate program at UPR-

Humacao, has been developed through the collaboration with Penn. The annual Penn-UPR CIRE meeting was held in Puerto Rico in October 2000. The meeting featured Alan MacDiarmid who gave an inspirational talk to over 400 undergraduate and high school students in Humacao. This was the first meeting Prof. MacDiarmid attended after he was recognized with the 2001 Nobel Prize in Chemistry earlier that month. (http://www.lrsm.upenn.edu/lrsm/outr.html#CIRE).

Minority Research Planning Grants enable new minority faculty to jump-start their research and obtain preliminary results they can build upon. Prof. Theodore Goodson just completed a very successful MRPG at Wayne State University (DMR-9908418) in which he studied the photodynamics of polymers. As a result, he published papers in Phys. Rev. B, J. Phys. Chem., and Chem. Phys. Lett., with additional papers in press in J. Appl. Phys. and Macromolecules. He trained one MS and two undergraduate students and had Detroit high-school students work in his lab. His subsequent full proposal has now been funded (DMR-0088044).

The Macrogalleria, a pioneering educational polymer web-site by Prof. Lon Mathias (U. Southern DMR-9950760) Mississippi, is continuing to garner broad recognition. NSF Director Rita Colwell described it in these terms in one of her speeches: "Many of you have seen the wonderful Web Site called 'Macrogalleria'. It is set up like a shopping mall. The site



bills itself as 'the Internet mall where you netsurfers can learn all kinds of nifty stuff about polymers and polymer science'. The student or the Internet surfer clicks on the shops and learns that polymers are everywhere. As he or she ascends to the different levels of the mall, more complex concepts are conveyed." The Macrogalleria was recently selected by <u>Scientific American</u> as one of its "50 Top Websites" and only one of five in chemistry. This follows many other distinctions, such as the Education Index Top Site and the Top 5% of Chemistry Sites. The worldwide popularity of the Macrogalleria is so high that it has already been translated into Afrikaans, French, and Spanish, and is being translated into Italian and Portuguese.

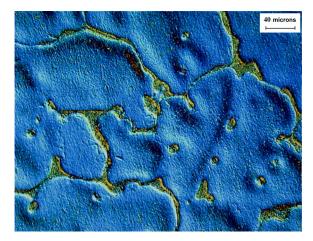
Fostering CAREERS. Prof. Kristi Anseth (U. Colorado) was named The Materials Research Society (MRS) Outstanding Young Investigator for 2001. Prof. Anseth is a CAREER grantee whose work on polymeric biomaterials for tissue engineering is co-funded by DMR and NSF's Bioengineering Division (BES-9734236). Remarkably, Prof. Anseth's student Amy Burkoth won ACS Student Award in Applied Polymer Science the 2001. Two years ago the MRS Outstanding Young Investigator was another DMR CAREER grantee, Prof. Anne Mayes of MIT (DMR-9817735). These



distinctions for young scientists in highly interdisciplinary fields exemplify DMR's success in fostering a diverse and internationally leading workforce of scientists and engineers.

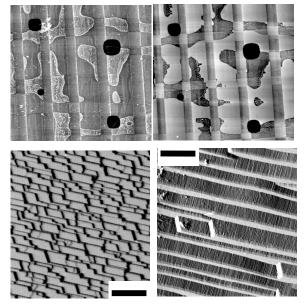
As part of his CAREER award, Andrew Rappe of Penn (DMR-9702514) has developed instructional JAVA applets and HTML tools to aid in teaching advanced general chemistry and to expose undergraduates to modern materials modeling techniques. He is collaborating with Prof. Charlotte Zales of Immaculata College. Resources are publicly available on the Web. Two functional applets are currently available: (1) Maxwell-Boltzmann distribution which simulates the motion of a gas of Argon atoms and is designed to reinforce ideas in probability distributions and randomness, and (2) Atomic quantum mechanics which shows the calculation of "atomic wavefunctions" using density functional theory. Applets under construction address surface science, kinetics of greenhouse gases, and molecular dynamics simulations of biomolecules.

Prizes for Imagery and Imagination.

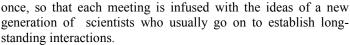


Paula Crawford, a Ph.D. student working with Prof. M. Glicksman at Rensselaer Polytechnic Institute (DMR-9633346) was awarded first prize in 'Artistic Microscopy,' and a second prize in 'Engineering Materials' from the American Metallographic Society at the ASM Materials Week in Cincinnati, Ohio. Her elegant micrograph reveals the distribution of a second (intermetallic) phase in a cast aluminum-copper alloy.

Jennifer Giocondi, a graduate student working with Greg Rohrer at Carnegie Mellon University (DMR-0072151), won two first place prizes for exhibits in the Ceramographic Competition of the American Ceramic Society during its 103rd Annual Meeting and Exposition in March 2001. The stunning images show photochemical decoration of domains in barium titanate (upper) and nanofaceting on the surface of strontium titanate (lower), and demonstrate the ability to deposit materials selectively on a sub-micron scale.



Diversity and International Cooperation at the Frontier of Nanoscale Science and Engineering. Prof. Mildred Dresselhaus's research group at MIT (DMR-0116042) is engaged in nanostructural studies of carbon, bismuth and other materials. In addition to its outstanding research achievements, the group provides a fascinating example of the human side of materials research. Supported by the NSF grant are: Marcie R. Black, Electrical Engineering and Computer Science (EECS) graduate student; Sandra D. M. Brown, Physics graduate student (received Ph.D. June, 2000); Yu Ming Lin, EECS graduate student; Antonio G. Souza Filho, visiting Physics graduate student from Brazil (Brazilian Fellowship at MIT); Ado Jorio de Vasconcelos, Postdoc (Brazilian Fellowship with a supplement from NSF); Noriko Yoshizawa, Postdoc (Japanese Fellowship). Marcie Black and Dr. Yoshizawa are women and Dr. Brown is an Afro-American woman. Yu Ming Lin is an MIT graduate student in EECS from Taiwan. Dr. Vasconcelos is supported in part through an NSF-sponsored exchange program with Prof. Marcos A. Pimenta of the Federal University of Minas Gerais in Brazil. Antonio Souza Filho is a visiting graduate student from the Federal University of Ceara. Sandra Brown was partly supported by a fellowship from Lucent Technologies.. NSF's Division of International Programs supports the group's interactions with Japan and Brazil. **International Interactions.** DMR continued to sponsor a broad spectrum of workshops in FY 2001. Many of these bring together scientists and engineers from different parts of the world (as described in the Introduction section of this report) and include a significant focus on questions of workforce and human development. One example is the binational <u>U.S-Germany</u> <u>Workshop on Polymers</u> organized last year by Profs. Colleen Pugh and Wes Burghardt (DMR-0080058). Speakers in this highly prestigious workshop are young researchers (usually at the Assistant Professor level) who can attend only





2. IDEAS

The <u>2000 Nobel Prize in Chemistry</u> was awarded to Alan Heeger (UCSB), Alan McDiarmid (U. Penn.), and Hideki Shirakawa (U. Tsukuba) "for the discovery and development of conductive polymers". This achievement was highlighted in last year's report but the context of DMR support for the two US members of this triumvirate deserves further emphasis. The DMR Materials Research

Laboratory there supported the initial interaction between Heeger and McDiarmid at Penn leading to their seminal work. Heeger and McDiarmid



continue to be key participants in the MRSECs at Santa Barbara and Penn respectively. Alan Heeger has been a grantee in the Condensed Matter Physics Program for many years. His CMP-funded research has focused on the photophysics of conducting polymers. The



Polymers Program has supported both Heeger and McDiarmid through individual grants since the 1970s when their work on conductive polymers began; Heeger remains a current POL grantee (DMR-9730126 and 0099843). Research into electroactive polymers has brought forth plastic transistors, light-emitting diodes, lasers and other photonic devices, as well as applications such as "electronic paper" – to the point

where the Washington Post wondered in a Dec. 2000 editorial whether Silicon Valley should perhaps be



B

renamed "Plastic Valley"! Both the Polymers Program and the MRSECs have actively supported a broad diversity of effort in this area; current Polymers grantees include Profs. Rigoberto Advincula (U. Alabama), Guillermo Bazan (UCSB), David Curtis (U. Michigan), Larry Dalton (U. Washington), Nicholas Pinto (U. Puerto Rico), Benjamin Schwartz (UCLA), Fred Wudl (UCLA), and Luping Yu (U. Chicago).

Controlling nature's randomness.

Diffusion plays a fundamental role in a remarkably large number of physical phenomena, including crystal growth, molecular processes in living cells, and the formation of galaxies. A particle undergoing diffusion executes a random walk through space. If it were possible to tame the randomness of the diffusive process, it would have enormous impact on virtually all of the physical sciences and in many crucial technologies. Brage Golding and Mark Dykman at Michigan State University (DMR9971537) use optical tweezers to control the diffusion of a submicron sphere (A) between two normally equally likely sites in an optical trap (C). By changing the modulation phase of light shining on the particle, they can make the particle stay mostly

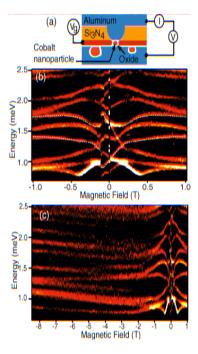


on the left side (B) or the right side (D) of the trap. In effect, they have created an optical orifice that behaves like a controllable pore for particle flow.

Quantum Computing.

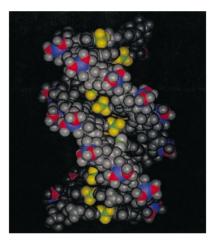
Siyuan Han and students, U. Kansas, DMR-9876874, have demonstrated that macroscopic quantum coherent oscillations between two states can be maintained over many cycles. The states are macroscopic superconducting currents in NbN SQUID devices. They execute about 10,000 oscillations before losing coherence. This is the first demonstration in the solid state of conditions that are a prerequisite to physical realization of <u>scalable, fault-</u>tolerant quantum computing.

Artificial Atoms. At the extreme nanoscale limit, artificial atoms and molecules are being fabricated. These have quantized electronic energy levels and it becomes possible to add and subtract electrons from among these levels. The fabricated structures include single electron transistors, quantum dots, etc. Dan Ralph, Cornell, DMR-0071631 is exploring the fundamental physics processes at work in this new regime, and how individual quantum states can be manipulated for sensor and memory applications. In magnetic cobalt nanoparticles (figures at right), the individual energy levels shift and jump as a magnetic field rotates the direction of the particle's magnetic moment, so that the energy of just one quantum state could be used to measure the orientation of the particle in magnetic memory applications.



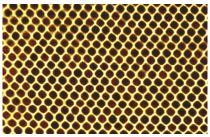
The materials science of genetic information. Activities linking solid-state chemistry with the study and exploitation of biological and environmental processes are beginning to emerge. For example,

double-stranded (ds) DNA has been shown to be a onedimensional semiconductor. Anisotropic conduction in the onedimensionally ordered solid double-stranded DNA films is attributed to the concerted movement of cations in the direction of the main axis of the of the ds-helices when an electric field is applied. Such movement raises the high-frequency longitudinal polarizability and thereby makes the resolved component of the high-frequency dielectric constant high. In a very significant development Adam Heller, University of Texas at Austin (DMR-98010700) has determined that the biological function of the insulator-to-semiconductor transition upon parallel alignment of the ds-DNA is protection against reversible chemical change by oxidation or reduction. Removing or adding an electron produces in an insulator a localized reactive radical. Adding a hole or electron to a band of a semiconductor, which extends over a large number of atoms, does not make any atom in the ensemble



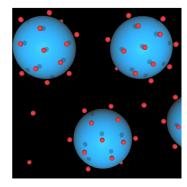
uniquely reactive. The organization of ds-DNA in aligned, polarizable arrays may prove to be a central evolutionary strategy for preserving genetic information. Alignment is expected in the life cycle of cells and organisms when their DNA is exposed and when it becomes vulnerable in a changed environment.

Nanoparticle arrays by colloidal assembly. Zhonglin Wang at Georgia Tech (DMR-9733160) has produced amazingly reproducible and relatively large (mm scale) films of monolayers of ferromagnetic cobalt nanocrystals using chemical / colloid-chemistry techniques. The method is simple relative to the competing CVD and PVD approaches that require highly specialized equipment. An example is shown in the figure at right. Here the distance between particles is 25 nm and the particles have uniform diameter of 11nm. A potential application is for high-



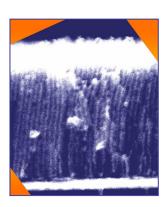
density magnetic storage, and Prof. Wang's results have attracted attention from IBM and Seagate.

Colloidal particles are receiving intense attention in biotechnology for attachment of proteins and other labels, cell-function assays, targeted drug delivery, gene therapies, and selective toxin removal. Controlling the interaction between particles will be one key to their successful application. Prof. Anne Mayes (MIT) (DMR-9817735) incorporated hydrophobic side-chains into latex particles in addition to the usual hydrophilic ones. At medium separations, the hydrophilic molecules extend into solution, contact those from other latex particles, and cause repulsion. However, at smaller separations the hydrophobic chains, initially collapsed away from the solvent, merge to create an attractive regime leading to adhesive bridges between particles.



Also working on colloids, Jennifer Lewis, U Illinois at Urbana-Champaign, DMR-0071645, has shown that negligibly charged colloidal microspheres (blue in the figure) aggregate in aqueous solution, but undergo a stabilizing transition upon addition of highly charged nanoparticles (red). This type of self-organization, or haloing, provides a new method for tailoring the behavior of complex fluids. The cover image at left is from Proceedings of the National Academy of Sciences (Braun et al., **98** (16), 8923 (July 31, 2001).

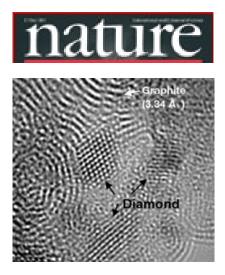
Mark Tuominen and Thomas Russell (U. Mass. Nanotemplates. Amherst) are supported by jointly by CTS and DMR through the Nanoscience Initiative on a project to generate novel block-copolymer nanostructural architectures (CTS-9871782). They recently succeeded in developing a new nanofabrication technique that allowed them to create magnetic nano-wire arrays from diblock copolymer templates. Through phase separation of these copolymers and field-effected orientation they obtain densely packed lattices of nanocylinders perpendicular to the substrate; these are then etched and filled with cobalt, thus generating arrays of nanowires 14 nm in diameter. The results were published in Science (290, 2126 (2000). Aspects of the work are also supported by the U Mass MRSEC (DMR-9809365). The research also included collaboration with IBM, which resulted in licensing of the nanowire arrays for magnetic storage to a new company named Paramount Capital.



Understanding Surface Coatings for Implants.

Prof. Jody Redepenning (U. Nebraska, DMR-9972587) works the development of new on hydroxyapatite/biopolymer composites. She is determining the influence of deposition conditions on chemical and physical characteristics of electrolytically produced calcium phosphate coatings. One provisional patent has been filed. Shown is a scanning electron micrograph image of an electrolytically prepared hydroxyapatite coating. The coating covers the surface of titanium beads such as those found on the exterior of hip and knee implants. The non-line-of-sight procedure used produces a relatively uniform coating on irregularly shaped objects.

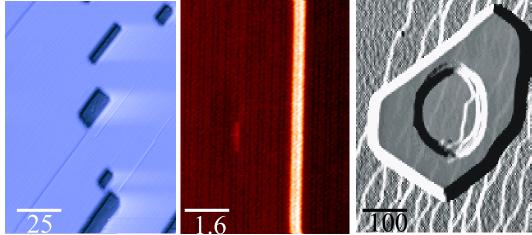




Nanoporous diamond. The conversion of silicon carbide to crystalline diamond-structured carbon at ambient pressure and temperatures at or below 1000°C, without plasma activation, was reported in Nature (v. 411, pp. 283-287, 2001).

This technique involves placing silicon carbide into glass tubes, heating it, and exposing it to a mixture of chlorine and hydrogen gases. A form of pure carbon almost identical to both natural and conventional synthetic diamond, but built of nanocrystals (just a dozen of atoms in cross-section), is produced. The transmission electron micrograph shows regions of both graphite and diamond. Like natural or other synthetic diamond, each carbon atom is tightly bonded to four neighbors, but the arrangement of these groups can be slightly different. *This method allows for synthesis of very hard, stiff, nanoporous, and ultra-light diamond and/or diamond-graphite nanocomposites* (Yuri Gogotsi, Drexel University., DMR-9874955 CAREER, and Michael McNallan, U Illinois - Chicago, CMS-9813400).

Quantum Engineering of Nanostructures; C-K Shih et al./U. Tx, Austin; DMR-0071893 (Focused **Research Group).** In nanostructures where the length scale is near or smaller than the de Broglie wavelength of the electron, quantum confinement plays an important role in determining electronic structure. The ability to control the size and geometry of nanostructures therefore provides a means to



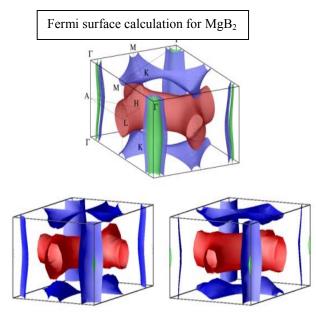
Ag/GaAs film

Ag nanowire

Pb/Si

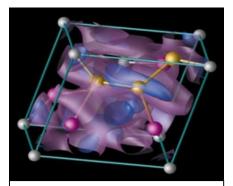
engineer and manipulate physical properties. This represents the conventional meaning of "quantum engineering." Recently, Shih et al. discovered that quantum mechanically confined electronic states have a strong influence on the formation and stability of nanostructures, thus giving rise to a new meaning for the words "quantum engineering." This FRG project explores both aspects of "quantum engineering" of nanostructures with different dimensionalities, illustrated by the three examples in the figure (dimensions are in nanometers). At the left an atomically flat silver film has been grown on a gallium arsenide substrate. The stability of the film is governed by electronic states arising from electrons confined in a 2dimensional quantum well whose properties are determined by the film thickness [Phys. Rev. Lett. 85, 5158 (2000), Science 292, 1131 (2001)]. The group is also exploring quantum engineering of nanostructures of other dimensionalities. A stable silver nanowire that evolved from the flat silver film is shown in the middle figure. Remarkably, the diameter of such wires is quantized, perhaps as a direct consequence of the quasiperiodic superstructure of the silver film which follows a Fibonacci sequence [Phys. Rev. Lett. 83, 3222 (1999)]. The third panel shows an engineered circular 'nanowell' in a metallic lead nanoterrace, this time on a silicon substrate. In this example atomic rearrangement following an STM pulse has been controlled to produce features with a predetermined diameter (120 nm) and precise depth (8 atom layers) even though the structure involves millions of atoms.

New materials sparked a flurry of activity in the materials theory community this year. In January,



superconductivity was discovered in the commonly available material MgB₂. The "high" transition temperature of 40K energized a great deal of theoretical and experimental work, reflected at a special session at the 2001 March Meeting of the American Physical Society in Seattle. Electronic structure calculations were presented by various DMR awardees including Marvin Cohen of U.C. Berkeley (#9520554), Amy Liu of Georgetown (#9973225), and Warren Pickett of U.C. Davis (#0114818). In collaboration with researchers at NRL, Liu used density functional theory to calculate the electronic structure and Fermi surface of MgB₂ (see Figure) and electron-phonon coupling strengths, a measure of the strength of the contribution of a particular phonon mode to the "glue" that binds the electrons into

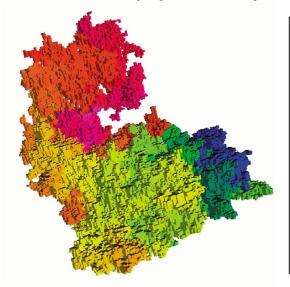
pairs in the conventional theory of superconductivity. The model is supported by currently available tunneling and thermodynamic data, and may help explain the high transition temperature and the puzzling way it depends upon the isotopic mass of the constituent elements. The adventure of exploring superconductivity in MgB_2 and related materials and their possible technological applications has only just begun!



Calculated electronic density of a candidate direct band-gap material CSn₂Si₂. The results suggest that a good interface with silicon based electronic circuits can be made.

The ability to predict from fundamental theory the properties of materials not found in nature or not yet synthesized continues to be developed. Motivated in part by the desire to construct a new material to improve the interface between electronic and photonic devices, Vincent Crespi of Penn. State (#9876232), Steven Louie and Marvin Cohen of UC-Berkeley (#0087088) worked in collaboration with materials scientists to design optoelectronic materials which could actually be fabricated. Electronic structure calculations using density functional theory together with a many-body perturbation theory method were used to determine candidate alloys involving only group IV elements which have desirable features: a lattice constant that matches well with that of silicon, a direct bandgap in the range of 0.7 to 1.0 eV that is optimal for optical transitions, and welldefined synthesis strategies that potentially enable production of bulk quantities of material. Two candidate materials were predicted, one of which is shown at left.

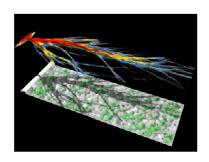
Magnetism, Crumpled Paper, and Avalanches. For a wide variety of systems, the response to an external stress is the production of discrete events with sizes that vary. For example, the Earth responds to stress between tectonic plates, paper emits intermittent sharp noises as it is crumpled, magnetic materials magnetize in jumps in response to an applied field. Tools used to describe second order phase transitions in equilibrium systems have been extended to describe these events in driven non-equilibrium systems. [This topic also comprises part of the 2001 Boulder Summer School]. Many investigators have been involved; these include **Daniel Fisher** of Harvard (#9976621) a pioneer in the field who studied charge density wave systems, **Alan Middleton** of Syracuse (#9702242, #0109614) who uses innovative numerical methods to advance the field, **Jean Carlson** of UCSB (#9813752) on earthquake faults, and **Jim Sethna** of Cornell (KDI #9873214, #9805422) who has been studying crackling noise [see http://simscience.org/crackling] and with **Karin Dahmen** of UIUC (#0072783) has been studying avalanches using a simple model of magnetic systems. These systems exhibit universal behavior on long length and time scales and yield to powerful renormalization group methods developed for phase transitions in equilibrium systems.



Fractal spatial structure of an avalanche. Fractal structures, as well as power laws, are characteristic of systems at their critical point. This moderate-sized avalanche involved the flipping of domains in the simulation. The colours represent time: the first domains to flip are coloured blue, the last pink. So far, there have been few experiments showing the spatial structure of avalanches. When results become available, a wealth of predictions of the scaling theories can be tested. Other systems display a qualitatively different kind of spatial structure, where the avalanche is made up of many small disconnected pieces, which trigger one another through the waves emitted as they flip. Adapted from J. Sethna et al. Nature 410, 242 (2001).

Electron Flow in a High Mobility Two-Dimensional Electron Gas. Electron motion through high

mobility two dimensional electron gases is often thought to be nearly ideal. As shown in the figure, researchers at the Harvard MRSEC (Robert Westervelt, DMR-9809363) have discovered that electron flow from a quantum point contact forms narrow channels at distances well below the mean free path. The upper part of the figure shows the computed electron wave flow over the potential shown in the lower part (high potential is white, low is green). These calculations agree well with images of electron flow from a quantum point contact in a GaAs/AlGaAs heterostructure obtained by scanned probe microscopy at low temperatures. Although the statistically averaged parameters - mobility, mean free path - are the



same as in traditional pictures, the actual flow through a given nanoscale device shows additional structure. These developments improve our understanding of electron flow, with important effects on nanoscale electronic device design. (http://www.mrsec.harvard.edu).

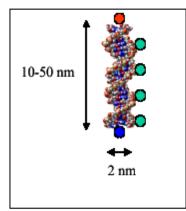


The Physics of Granular Materials. A case study published in the June 2001 issue of Physics World analyzes the impact of basic physics research on the wider fields of science and technology. In their case study based on citation mining, the authors highlight the enormous impact of the review article "The Physics of Granular Materials", published by researchers at the U. of Chicago MRSEC (Steven Sibener, DMR-9808595, and Leo Kadanoff, DMR-9400379 and DMR-8819860) in Science magazine in 1992. This single article garnered more than 300 citations since publication and helped launch the field of granular dynamics within condensed matter physics. What is particularly noteworthy is that about 20% of the citations of this article are from papers outside basic physics and involve applications as diverse as traffic flow, avalanche prediction, blood cell agglomeration, and fusion

plasmas. (http://MRSEC.uchicago.edu/MRSEC/).

Nano-Lightpipes. Everybody knows that it is impossible to propagate light through structures smaller than the wavelength of light. Researchers at the Caltech MRSEC (Julia Kornfield, DMR-0080065) have belied

this conventional wisdom, showing that light can propagate along waveguides whose lateral dimensions are only a few nanometers, or a few percent of the wavelength of light. The key is to exploit the tendency for electromagnetic excitations to "hop" between electric dipoles (such as fluorescent dye molecules or metal nanoparticles). The Caltech researchers demonstrated light propagation through two types of sub-wavelength-scale waveguides. The first is a DNA waveguide in which a fluorescence excitation hops from an optical donor molecule bound to one end of the DNA backbone to an acceptor molecule at the other end through dye molecules tethered at intervals in between (Figure). These fluorescence resonant energy transfer waveguides have so far shown that light can take several hops between molecules bound to DNA, and this can be extended to many hops along a longer waveguide. The second nanoscale waveguide structure is called a "plasmon wire", which is a chain of metal

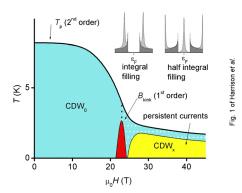


nanoparticles along which light hops from one particle to another. Light can even propagate around sharp corners and through nanoscale networks —all of which is impossible in conventional optical waveguides.

3. TOOLS

Providing broadly accessible, state-of-the-art information bases and shared research and education tools

Observation of Frohlich superconductivity in high magnetic fields. N. Harrison, C.H. Mielke, J.

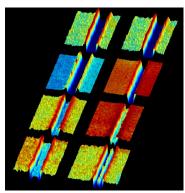


n high magnetic fields. N. Harrison, C.H. Mielke, J. Singleton, J. Brooks, M. Tokumoto, J. Phys.: Condens. Matter 13, L389 (2001). In 1954 Frohlich described a type of superconductivity caused by the motion of charge density waves. Charge density waves arise when electrons bunch up into wave-like oscillations and are one of the few macroscopic quantum phenomena observed to date. Some organic materials are known to have charge density waves which establish themselves only at very low temperatures (about one degree above absolute zero) and high magnetic fields, a half-million times stronger than the Earth's magnetic field. Such fields are available at the **National High Magnetic Field Laboratory** (DMR-0084173). Recent experiments by

NHMFL scientists, in collaboration with an Oxford University professor, have found compelling evidence of 'persistent currents' in this charge density wave. Persistent currents are electrical currents that travel without friction, just as in a superconductor. Frohlich-style superconductivity has never before been convincingly proven, but conditions in these materials in extremely high magnetic fields strongly suggest that this may be the long-awaited discovery.

Scientists Create 'Molecular Rulers' Enabling Precise Construction of Nanoscale Structures: P.S. Weiss and his colleagues at Penn State have discovered an effective and precise way to make ultra miniature metal wires in very close proximity to each other. The results, published in the 9 February 2001 edition of Science, describe the use of organic molecules as "molecular rulers" that permit the fabrication of

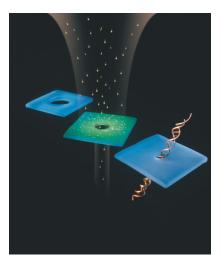
extremely thin wires from 15 to 70 nanometers wide and a few micrometers long that are spaced 10 to 40 nanometers apart. Their work is important because nanoscale construction methods have been limited to structures with larger, less controlled spacing than is expected to be useful in the continuing efforts to miniaturize electronic and optoelectronic devices used for circuits, high-density data storage, and sensors. In addition, their work is expected to serve as a test bed in the rapidly developing field of molecular electronics. The National Science Foundation's Major Research Instrumentation Program, the Army Research Office, DARPA, and the Office of Naval Research supported this research. It was conducted at Penn State's node of the National Nanofabrication Users' Network (CTS-9732194) which is co-funded by DMR.



Field emission scanning electron microscopy images depicting stages of a nanostructure reduction process.

Manipulating Matter at the Nanoscale. Several DMR research themes, such as spintronics, optics, nanoscience, etc. relate directly to emerging or mainstream technologies. However, and somewhat more typically, many awards are pioneering entirely new tools and techniques. An example is the work of Golovchenko, Harvard, DMR-0073590. Golovchenko is using an ion beam to poke holes in thin films to produce structures that in turn are used to manipulate nanoscale matter. Manipulating matter on the nanometer scale is important for many electronic, chemical and biological advances, but available solid state fabrication methods do not reproducibly achieve nanometer scale dimensional control. Golovchenko and co-workers have discovered a method to fashion matter at these dimensions by means of low energy

ion beams. The processing reveals surprising atomic transport phenomena that occur in a variety of materials and geometries. They call their method "ion beam sculpting" and apply it to the problem of fabricating a molecular scale hole, or nanopore, in a thin insulating solid state membrane. This is schematically illustrated in the figure. Nanopores localize molecular scale junctions and switches and act as masks to create other small structures. Nanopores also function as membrane channels in all living systems. where they are extremely sensitive electromechanical devices that regulate electric potential, ionic flow and molecular transport across cellular membranes. They have used "ion beam sculpting" to fabricate an analogous solid state device: a robust electronic detector capable of registering single DNA molecules in aqueous solution. Such detectors may find utility in extremely rapid sequencing of DNA for medical diagnostics of genetic diseases and rapid drug design for large populations. This work was recently reported in Nature.



Simulating Porosity in Metal Castings. At a very different length scale, David Poirier at the University of Arizona (DMR-9901290) is simulating the formation of porosity in a nickel-base superalloy (IN718)

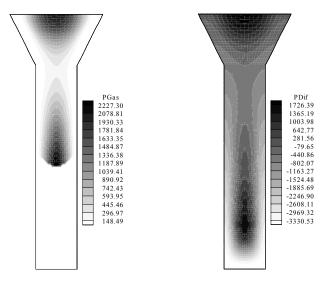
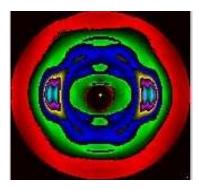


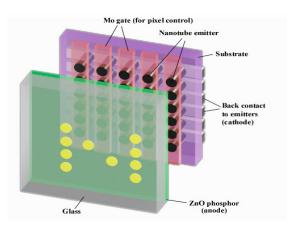
plate casting. Porosity evolves because the alloy contains gaseous impurities, hydrogen and nitrogen, which are dissolved as atoms in the melt. The concentrations of the atomically dissolved hydrogen and nitrogen are only 20 parts per million each, but as the casting cools and solidification proceeds they become more concentrated in the remaining liquid and generate hydrogen and nitrogen gases in their familiar molecular forms.. The total pressure of the hydrogen and nitrogen is shown as PGas (left). When the total pressure exceeds the pressure in the liquid, porosity occurs. In the figure (right), porosity is predicted where **PDif** is positive. Industry is interested in the simulator as a tool for making casting processes more energyefficient and cost-effective. Currently Pratt

and Whitney, a major producer of jet engines, and Howmet Castings are attempting to verify the simulation.



In-situ X-ray Scattering System. Prof. Benjamin Hsiao (SUNY Stony Brook) has developed an in-situ synchrotron wide-angle and small-angle X-ray scattering system, which allows him to study simultaneously and in real time the structural and morphological development in solidifying polymers. He has applied this to the understanding of shear-induced crystallization, to the study of orientational development during flow, to the isothermal crystallization of blends of different molecular weights, and to the analysis of crystallizing bio-absorbable polymers (DMR-9732653 and 0098104). His experimental system has been set up at Brookhaven National Laboratories and has been used widely in collaborative work with a large number of academic and industrial institutions.

Display Technology. R.P.H. Chang, NWU (DMR-0071737). A significant development involving the use of nanotubes in fabricating a flat panel screen display was the subject of a recent NSF Tip Sheet http://www.nsf.gov/od/lpa/news/tips/tipsrel.htm. It discusses the recent fabrication of a flat screen display using carbon nanotubes. The prototype screen uses hundreds of thousands of stationary nanotubes, which emit electrons to light up pixels on the screen. Unlike a standard CRT screen, in which one electron beam emitted from a hot filament beam moves rapidly back and forth to light the pixels, each pixel is lit by its own electron beam. The screen can be slim, the emission steady, and the resolution extremely is extremely high. Once nanotubes can be manufactured

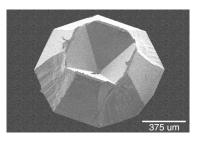


in bulk large screens could be fabricated very cheaply without expensive lithographic techniques.

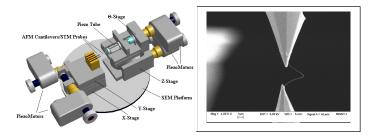
Neutron Scattering Studies of Nanodroplet Aerosols. Barbara Wyslouzil et al. (Worcester Polytechnic), Rinehard Strey (U. Cologne), Gerry Wilemski (U. Missouri-Rolla) & John Barker (NCNR/CHRNS) DMR-9986442.

Working at the DMR-funded Center for High-Resolution Neutron Scattering at NIST, this group has recently made the first definitive scattering measurements on the nucleation and growth of binary fluid nanodroplets. By continuously forming droplets *in-situ* by expansion in a supersonic nozzle inserted in the sample chamber, they have obtained data on the internal structure of the droplets needed to test current theories in atmospheric physics. For example, their measurements on deuterated alcohol/water mixtures clearly show that the alcohol concentrates in the surface regions of the droplets before they reach 100 nm in size, a result that will help refine realistic models for chemical reactions in the atmosphere.

Development of Nanocalorimetry. L.H. Allen and his colleagues at the University of Illinois at Urbana (DMR-9726458) have developed a calorimeter for nanoscale materials. This unique nanocalorimeter is over 1000 times more sensitive than conventional differential scanning calorimeters. The technique has been used successfully (1) to measure heat capacity of liquid/biological samples with droplets ranged in size from about 2 to 100 nL; (2) as a new in situ sensing tool for monitoring thin film growth via heat capacity measurements and scanning nanocalorimetry; and (3) to study



nanoscale calorimetry of isolated polyethylene single crystals. The Figure shows a silicon "bio-box" sample holder for nanoliter liquid samples. Initial exploration of this concept was supported by an SGER grant (DMR-9419604).



A New Tool for Nanotechnology. Rodney Ruoff, Tomasz Kowalewski James Huettner, and collaborators at Northwestern University (DMR-0196399) have developed a nanomanipulator (schematic left). The tool has been used inside a scanning electron microscope to pick up, mount, and tensile load carbon

nanotubes such as the individual multi-walled carbon nanotube shown attached between AFM cantilever

tips (right image). Studies on the breaking mechanism and tensile strength of multi-wall carbon nanotubes, the tensile strength of single wall carbon nanotube ropes, and "shell sliding," in which the outer shell of a multi-walled nanotube is displaced relative to the inner shell adjacent to it, have been reported in *Science* (287, 637 (2000)), *Phys. Rev. Lett.* (84, 5552 (2000), *Phys. Rev. Lett.*, 85, 1456 (2000) *Phys. Rev. Lett.*, 86(1), 88 (2001).), and *J. Phys. Chem. B*, 104, 8764(2000).

Gary Drobny, University of Washington (DMR-9616212) has developed solid state NMR as a tool unique in its ability to provide high resolution information on the structure and dynamics of biopolymers at materials interfaces. He has provided the first high resolution NMR structural and dynamical studies of proteins on inorganic crystal surfaces.

Leapfrogging the Microcircuit Pattern-size Barrier: X-ray Phase Masks for Next Generation Semiconductor Lithography. James W. Taylor, Lei Yang, and Franco Cerrina, Center for NanoTechnology, University of Wisconsin-Madison. jwtaylor@nanotech.wisc.edu. With support from DARPA, scientists at the Center for NanoTechnology (CNTech) have used radiation from the Synchrotron Radiation Center (SRC) at the University of Wisconsin (DMR-0084402) in a unique way for a new approach to next generation lithography. The Bright Peak Enhanced Phase Mask (BPEXPM) approach uses the X-rays from the storage ring to demonstrate printing of 50 nm to 30 nm features that correspond to the years 2007 and 2011 in the International Technology Roadmap for Semiconductors. Prof. Taylor and his colleagues have found a new way to apply the principle of phase masks to enhance the intensity that is produced from a mask structure that can be fabricated with normal semiconductor processing. The new lithographic approach truly opens the possibility for leapfrogging the Roadmap in the fabrication of microprocessor and low-density microcircuit applications. It also opens the field to higher-speed microwave communication devices.