Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201010

FWP and possible subtask under FWP:
Studies of Nanoscale Structure and Structural Defects of Advanced Materials

FWP Number: MA-015-MACA

Program Scope:
To study crystal structure including defects, electronic structure and magnetic structure in technologically-important functional materials, such as superconductors and magnetic materials. Various electron-microscopy techniques, such as quantitative imaging, diffraction, spectroscopy, and phase retrieval methods including electron holography are developed and employed to study material behaviors. Computer simulations and modeling using density functional theory and molecular dynamics calculations are carried out to aid the interpretation of experimental data. New capabilities have also been developed to fabricate tailored microstructures via film deposition and TEM patterning.

Major Program Achievements (over duration of support):
Developed a novel quantitative diffraction technique PARODI (PArallel Recording Of Dark-field image) to accurately measure valence electron distribution in YBCO, Bi-2212 and MgB_2 superconductors and interfacial lattice displacement in Bi-2212 (1pm accuracy). Measurements of interfacial potential, charge and screening length in Ca doped YBCO tilt boundaries and Bi-2212 twist boundaries. *In-situ* magnetization and induction mapping in comparison with calculations in NdFeB magnets and artificially patterned magnetic nano-arrays. Developed a fast and stable algorithm that solves the longstanding problem of “phase unwrapping” inherent with holography and many other interferometric techniques. Spectroscopy study of hole states and symmetry near Fermi level in MgB_2.

Program impact:
Our unprecedented accuracy in measurement of charge distribution for crystals with a large unit-cell demonstrated the significant role electron microscopy can play in studying electronic structure of materials at the nanoscale. The PARODI technique we developed to study interfacial displacement was considered “the most accurate defect measurement” (PRL & Physical Review Focus, APS web-site). The fast “phase unwrapping” and the “symmetrization” methods we developed for holography and non-interferometry phase retrieval make real-time electrostatic and magnetic imaging a near-future reality.

Interactions:
Internal -- Materials Science groups, Condensed Matter Physics groups, Chemistry groups, Biology groups.
External -- SUNY-Stony Brook, Columbia, Princeton, Carnegie Mellon, U of Illinois-UC, Northwestern U, Arizona State, Ames National Lab, IBM, U of Oslo, U of Alberta, Delft Tech. U.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Y. Zhu -- 28 invited talks at national and international conferences since 1999; Program Committees, Microscopy Society of America, (1999, 2000, 2002); NSF national panel for Major Instrumentation for Materials Research, (2002); DOE review panel for National Center for Electron Microscopy and Center for Advanced Materials at LBL, (2000); Review Committee of “DOE 2000, Materials Microcharacterization Collaboratory”; Editorial Board of *MICRON*, *the International Research and Review Journal for Microscopy*; DOE/BES Chunky Bullet Competition Award, (2001); Symposium co-organizer for MSA, MRS and APS.

Personnel Commitments for FY2002 to Nearest +/- 10%:
Y. Zhu (75%); **V.V. Volkov** (100%); **M. Schofield** (100%); **L. Wu** (75%); **R. Klie** (post doc, 70%), **M. Beleggia** (post doc, 70%); **J. Bording** (post doc, 70%).

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $460K **FY01 BA** $1.5M (incl. capital) **FY02 BA** $1.6M (incl. capital)

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201030

FWP and possible subtask under FWP:
Mechanisms of Metal Environment Interactions

FWP Number: MA-010-MAEA

Program Scope:
Identification of dominant factors controlling kinetics of reactions between metals and their environments. Determine interactions as a function of metals properties, compositions of alloys, environment, and characteristics of electrified interfaces and interphases. Corrosion has been a major subject of study and included effect of alloy composition, characterization of properties of passive oxide films, role of environment composition, and the dependence on the electrochemical kinetics of corrosion reactions.

Major Program Achievements (over duration of support):
In situ studies led to implementation of a wide range of new scanning techniques and imaging methods, employing synchrotron x-ray and infrared approaches, and applications of novel experimental approaches. Synchrotron x-ray in situ methods have elucidated the structure of passive oxide films on iron and stainless steels, determined the chemistry, growth and dissolution characteristics of base metals and stainless steels, and salt film layers composition and growth within pits on stainless steels. Aluminum studies have employed novel visualization techniques for the study of the role of pH changes at corroding surfaces, used segmented electrodes to investigate the noise during pitting which contrast with the growth mechanisms of pits and passivity breakdown and repair with stainless steels. Demonstrated the extremely sensitivity of dissolution of aluminum passive film on anions, pH and temperature. Found major differences in the mode of oxide film growth on metals in organic media, compared with distinct similarities in aqueous solutions.

Program impact:
Has played a leading role in the development of in situ technique for study of corrosion mechanisms which are now being used by the corrosion community, e.g. current density mapping, x-ray absorption and fluorescence techniques, and imagining or visualization methods. Analogue experimental arrangements have been developed to control multiple variables participating in specific types of corrosion. Examples are artificial pits, segmented electrodes, and artificial passive films. Contributions to the understanding have been made to areas of corrosion that include pitting and crevice corrosion, passive film formation, chemical speciation, and stability of stainless steels and aluminum and its alloys.

Interactions:
Sandia National Laboratory, Nanostructure and Semiconductor Physics Department; Center for Synthesis and Processing, "The Science of Localized Corrosion;" Ohio State University, The Fontana Corrosion Center; Northrup-Grumman Corp., Pollution Prevention Programs; Honeywell Consumer Products Group; Imperial College, London, Department of Materials; Swedish Corrosion Institute; Swiss Federal Institute of Technology, Institute of Materials Chemistry and Corrosion.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Invited talks- 5 at Society Meetings, 2 at International Meetings, 4 at Universities and Research Institutes.

Personnel Commitments for FY2002 to Nearest +/- 10%:
H. Isaacs (research scientist, 90%); **R. Sabatini** (professional staff, 10%); **K. Sutter** (technical, 50%).

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $528K **FY01 BA** $495K **FY02 BA** $427K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201030

FWP and possible subtask under FWP:
Superconducting Materials

FWP Number: MA-012-MABA

Program Scope:
The task of this program is to study the basic relationships between nanoscale structures and macroscopic properties of advanced superconductors, providing both the basic data and understanding of the fundamental materials science required for their practical utilization. Emphasis is placed upon studies of high temperature superconducting cuprates, particularly $YBa_2Cu_3O_7$ (YBCO) and recently discovered MgB_2. This includes investigations of physical properties and of lattice defects, especially their role in altering superconducting properties, as well as of the kinetics of formation of these superconductors in practical conductors. Extensive use is made of transmission electron microscopy (TEM) and x-ray diffraction techniques at the National Synchrotron Light Source (NSLS).

Major Program Achievements (over duration of support):
- Clarification of the kinetic mechanisms for the nucleation and the growth process for thick $YBa_2Cu_3O_x$ films from the precursor in the so-call BaF_2 postdeposition reaction process.
- Theory and modeling of the mechanics and statistical thermodynamics of stress, point defects, and charge distributions lead to better understanding of grain boundaries and interfaces in cuprate superconductors
- Studies of correlation of electromagnetic properties and microstructure of high T_c grain boundaries, and probing superconducting order parameter symmetry in $Bi_2Sr_2CaCu_2O_{8+\delta}$ using bicrystal c-axis twist Josephson junctions.
- Processing and structural characterization of high density, high J_c superconducting MgB_2/Mg nano-composites and symmetry studies of the hole states near the Fermi level in the MgB_2 superconductor,
- A detailed structural/microstructural study of the "charge stripe" superconductor $La_{2-x}M_xCuO_4$ (M=Sr, Ba) leads to a better understanding of the relationships among superconductivity, charge stripes magnetism, and structure.

Program impact:
This group's longstanding program, concerned with the relationships among synthesis, micro- and crystal-structures, and properties of superconductors in experiments and theories, has been highly respected as one of the world leaders in this area. Recent investigations in properties and the crystal and electronic structure of grain boundaries in high T_c superconductors are seminal in the field. Also, our basic studies of nucleation and growth $YBa_2Cu_3O_x$ thick films are important for the fabrication of technological conductors.

Interactions:
This program has a very close and symbiotic relationship with Applied Superconductivity Programs in our Department and in the Magnet Group of Accelerator Department. Also, we collaborate closely with the members of the Condensed Matter Physics Group and of NSLS. In addition, we work with collaborators at various universities and other national laboratories as opportunities arise.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): Group members have given 28 invited talks in the past three years at national and international conferences/workshops including 1 plenary talk. Honors: 1 Fellow of the American Physical Society.

Personnel Commitments for FY2002 to Nearest +/- 10%:
Q. Li (88%), **A. R. Moodenbaugh** (56%), **M. Suenaga** (58%), **D. O. Welch** (29%), **H. J. Wiesmann** (19%), **L. Wu** (50%), **Y. Zhu** (25%).

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $1,502,000 **FY01 BA** $1,103,000 **FY02 BA** $999,000

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0204011 & KC0301045

FWP and possible subtask under FWP:
National Synchrotron Light Source Operations and Development

FWP Number: LS001

Program Scope: The National Synchrotron Light Source (NSLS) is a large user facility devoted to the production and utilization of synchrotron radiation, and the development of electron based radiation sources. From the far infrared to the gamma ray region, the NSLS provides a reliable and versatile tool for experimenters in many areas of Science and Technology including Chemical Sciences, Materials Sciences, Life Sciences, Geosciences & Ecology, Applied Sciences, Engineering, Atomic Physics, Medicine, and Nuclear Physics. The NSLS provides an integrated resource for synchrotron radiation research through the operation of its two electron storage rings, their associated injection system, and support of an extensive user science program involving both facility and user operated instruments. In addition there are ongoing development programs to improve the capabilities of the facility. In the case of the storage rings, the program emphasizes enhancements in stability, reliability, and lifetime of electron beams and to develop new insertion devices that allow manipulation of polarization, or enhancements in brightness. In parallel, the facility supports programs to develop new beamline instrumentation including beamline optics, monochromators and detectors that permit users to take full advantage of the unique research capabilities offered by the NSLS.

Major Program Achievements (over duration of support): Each of the NSLS storage rings continue to operate for more than 5000 hours each year, with reliability greater than 95%, and availability of more than 100% of scheduled time. More than 2500 users each year take advantage of the capabilities of the NSLS as part of their research program.

Program impact: Nearly two thirds of our users are from the Northeast US making the NSLS a valuable regional source, although 16% of our users come from foreign countries, comprising our next largest constituency. NSLS contributes to the development of a technically trained workforce for the Nation as nearly one thousand students (not including Ph.D's) receive part of their training by performing experiments at the facility each year. Beyond that, the NSLS contributes to the Industrial Competitiveness of the Nation as more than 60 U.S. corporations use the facility to enhance their competitive position. The NSLS provides a valuable resource and the research of its users continues to have high visibility and impact as noted in the DOE review of the NSLS held in July 2001. In fact a selection of 20 high impact publications had more than 700 citations at that time.

Interactions:
Users from over 400 institutions perform experiments at NSLS.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Recent recognition includes the induction of four NSLS Users to the National Academy of Sciences. There are too many other individual achievements among our staff and users to enumerate in the available space.

Personnel Commitments for FY2002 to Nearest +/- 10%:
62.7 Scientific and Professional Full Time Equivalents (FTE)
89.9 Support FTE (152.6 FTE Total)

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $32,111,000 **FY01 BA** $34,720,000 **FY02 BA** $34,611,000

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC020201

FWP and possible subtask under FWP:
Neutron Scattering

FWP Number: PO-010

Program Scope: Study of cooperative phenomena in complex solids by elastic and inelastic neutron scattering. Phenomena such as structural and magnetic phase transformations, magnetic structure, charge-density-wave order and elementary excitations such as spin-waves and phonons are investigated in systems such as high-temperature superconductors, strongly-correlated transition-metal oxides, low-dimensional and quantum-disordered antiferromagnets, ferroelectrics, piezoelectrics, and shape-memory alloys. Experiments utilize national and international neutron facilities, and single-crystal samples grown at BNL.

Major Program Achievements (over duration of support):
High-Temperature Superconductivity: Discovery and characterization of magnetic order and fluctuations in cuprates; discovery of stripe order in certain cuprates; discovery of interstitial order in oxygen-doped cuprates.
Ferroelectrics: Identification of new structural phase in $Pb(Zr_{1-x}Ti_x)O_3$; characterization of overdamped optical modes and atomic displacement pattern corresponding to polarized nano-domains in relaxor ferroelectrics.
Quantum magnetism: Characterization of dimensional crossover in systems of coupled quantum-spin chains; first observation of magnetic-field induced order in a quantum-disordered system.
Crystal growth: First successful growth (in high-pressure oxygen) of superconducting $La_{1.85}Sr_{0.15}CaCu_2O_6$; growth of new metallic but nonferromagnetic oxide, $Y_{0.5}Sr_{1.5}NiO_{4-\delta}$.

Program impact:
Results on charge-stripe correlations in cuprates have stimulated new theories of the mechanism for high-temperature superconductivity. Identification of structure and polarization direction in optimized piezoelectric $Pb(Zr_{1-x}Ti_x)O_3$ (PZT) has led to predictions of improved performance in atomically-tailored materials.

Interactions:
Internal---Physics Department: Center for Neutron Science, X-ray Scattering Group, Powder Diffraction Group, Electron Spectroscopy Group, Theory Group; Materials Science Department: Superconductivity Group, Electron Diffraction Group
External---Massachusetts Institute of Technology; University of Delaware; University of Toronto, Canada; Johns Hopkins University; Rutgers University; Iowa State University; Oak Ridge National Laboratory; National Institute of Standards and Technology; Institute for Solid State Physics, University of Tokyo, Japan; Kyoto University, Japan; Tohoku University, Japan; Oxford University, UK; Rutherford-Appleton Laboratory, UK; Laboratoire Léon Brillouin, France; CEA/Grenoble, France; Forschungszentrum Karlsruhe, Germany; Institute for Low-Temperature Physics, Ukraine

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Past recognition: 1 member of the NAS and former recipient of the Buckley prize; 3 Fellows of the APS;
1 Presidential Early Career/DOE Young Investigator Award (2001).
10 invited talks in FY02.
S.M. Shapiro---Divisional Associate Editor, Physical Review Letters, 1999-2001
G. Shirane---On list of most-highly-cited physicists, at http://isihighlycited.com
J.M. Tranquada---Divisional Associate Editor, Physical Review Letters, 2002; Chair, SNS-HFIR User Group Executive Committee, 2002; Organizing Committee, American Conference on Neutron Scattering, 2002.

Personnel Commitments for FY2002 to Nearest +/- 10%:
J. M. Tranquada (group leader) (90%), G. Gu (100%), S. M. Shapiro(50%), G. Shirane(50%), G. Xu (50%), I. Zaliznyak (100%); Post-docs: M. Hücker (100%), H. Woo (100%)

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $1835k **FY01 BA $**1807k **FY02 BA $**1706k

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202010

FWP and possible subtask under FWP:
Condensed Matter Physics--X-ray Scattering

FWP Number: PO-011

Program Scope:
The X-ray Scattering Group carries out basic studies of the structural, electronic and magnetic properties of condensed matter systems using x-ray synchrotron radiation. As members of various Participating Research Teams, the Group also develops instrumentation, maintains and operates three beamlines at the National Synchrotron Light Source (NSLS), and oversees the development of two insertion device beamlines at the Advanced Photon Source (APS). Particular emphasis is placed on investigation of surface and interfacial phenomena, including thin films, on electronic and magnetic structure and phase behavior, and on electronic excitations in solids. Recently, steps have been taken to move into materials synthesis, particularly polymer-assisted synthesis of nanomaterials.

Major Program Achievements (over duration of support):
The program has played a significant role in developing and applying resonant x-ray scattering techniques to the study of condensed matter systems, including especially the study of magnetic phenomena and more recently electronic ordering and excitations in strongly correlated systems. Efforts in the field of liquid interfaces have led to significant discoveries such as surface freezing, surface-induced layering in liquid metals and the phase behavior of Langmuir films on liquid mercury.

Program Impact:
The Group's longstanding programs concerned with x-ray resonant phenomena and magnetism, and with liquid and soft interfaces have been seminal in stimulating related efforts worldwide, and remain among the leading programs in these areas today. The group has played a leading role in the construction, and operation, of the Complex Materials Consortium-Collaborative Access Team (CMC-CAT) at the Advanced Photon Source and has, with others, led the creation of a CAT dedicated to inelastic x-ray scattering (IXS-CAT). Efforts in soft condensed matter have led to the creation of a new FWP aimed at understanding nanotemplating phenomena.

Interactions:
The Group typically collaborates with 40-50 PIs per year, together with an approximately equal number of students and post docs. This includes significant internal BNL collaboration, both within Condensed Matter Physics and more widely (in particular, the NSLS, Chemistry and Materials Science Departments) together with external collaborations with universities, other national laboratories and foreign institutions.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):

FY02

Brookhaven Science and Technology Award (Ocko)

Fellow of AAAS (Gibbs)

24 invited talks in FY02

Previously

1 Goldhaber Fellow

1 Wohlfarth Award

1 Significant Achievement in Solid State Physics

1 Presidential Early Career Award

2 Fellows of the APS

1 Brookhaven Engineering Award

Personnel Commitments for FY2002 to Nearest +/-10%:

John Hill (Group Leader),

Doon Gibbs (50%),

Ben Ocko,

Elaine DiMasi (20%),

Tianbo Liu (70%),

Young-June Kim (20%, Research Associate),

Christie Nelson (20%, Research Associate) – left 2/1/02,

Kazu Tamura (20% Research Associate) –left 4/1/02,

Stephane Grenier (20% research associate) - arrived 2/1/02.

Authorized Budget (BA) for FY00, FY01, FY02:

FY00 BA $1,199,000 **FY01 BA $**1,120,000 **FY02 BA $**1,030,000

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202010

FWP and possible subtask under FWP:
Condensed Matter Physics—Soft Matter and Biomaterials

FWP Number: PO-034

Program Scope:
The Soft Matter and Biomaterials effort is a joint project initiated by researchers in the BNL Physics and National Synchrotron Light Source Departments, and by several university collaborators. The primary goal of the program is to investigate the nanoscale confinement and assembly in soft matter, liquids and biomaterials through the use of patterned templates. We will examine how the templates, having well defined nanoscale chemical or surface height structures, modify the structure, phase behavior, and nucleation of liquids, liquid crystals, proteins, and biomaterials. Using state-of-the-art structural probes that are compatible with the liquid/vapor environment, we will extend current descriptions of liquid, liquid crystalline, and bulk soft-matter and biomaterial phases to the nanoscale. New methods for creating large scale templated surfaces will be developed and potential applications in sensors and photonic devices will be explored.

Major Program Achievements (over duration of support):
In the few months that this program has been funded, there have been several significant administrative achievements:

1. Dr. Oleg Gang has accepted a position as a Goldhaber Fellow and will join the group in the fall. Two post-doc positions were advertised and a soft matter and biomaterials review committee is in the process of interviewing candidates for these positions.
2. The first semi-annual organizational meeting was held at Univ. of Mass.-Amherst in September to chart the scientific goals of the team and explore new collaborative projects. The BNL members of the research team meet semi-monthly to track progress and discuss project needs.
3. As part of the BNL-Center for Functional Nanomaterials 'Jump-Start' program, a facility to measure Grazing Incidence Small Angle X-Ray Scattering was proposed and incorporated into the program. These facilities will serve an extended community of CFN users who are interested in characterizing thin organic films. We anticipate that new collaborations will result operation of this user facility.

Program Impact:
As a result of this program, a new soft matter and biomaterials research group was established within BNL. The group currently includes members from three BNL departments: Physics, the NSLS, and Instrumentation. We anticipate the inclusion of members from Chemistry and Materials Science as the effort grows in scope. This group has been an active participant in developing the infra-structure of the new Center for Functional Nanomaterials. In particular, Ocko has served as one of the CFN Thrust Leaders in Thin Organic Films and Pindak has served as Interim Associate Director. This group is equally active in developing new end-stations within the NSLS for soft matter and biomaterials general users. These efforts include the development next year of a new Small Angle X-ray Scattering (SAXS) End-Station (Yang), a Low Energy Resonant Scattering End-Station (Pindak), and a Grazing Incidence SAXS End-Station (Ocko, DiMasi).

Interactions:
This is a joint project among researchers in three BNL departments: Physics, the National Synchrotron Light Source, and Instrumentation, as well as university researchers at the University of Massachusetts-Amherst, the University of Florida, the State University of New York at Stony Brook, Harvard University, and Case Western Reserve University. As part of the BNL Nanocenter Jumpstart Program, we anticipate hosting General Users of both the NSLS and Center for Functional Materials (CFM).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP/subtask):
Brookhaven Science and Technology Award – B. Ocko. Earlier two Fellows of the APS

Personnel Commitments for FY2002 to Nearest +/-10%:
Ben Ocko (25%) Oleg Gang (100%)

Ron Pindak (25%)	Harvard Student (50%)
Lin Yang (25%)	Univ. of Mass Student (100%)
Elaine DiMasi (25%)	Case Western Student (50%)
Tianbo Liu (25%)	3 additional post-docs (to be hired)

Additional personnel commitments anticipated for FY2003:

Authorized Budget (BA) for FY00, FY01, FY02:
FY02 BA $750,000

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC

FWP and possible subtask under FWP:
Powder Diffraction; from January 1, 2003 on, Materials Synthesis and Characterization

FWP Number: PO-013

Program Scope:
Synthesis and physical characterization of bulk, thin films and nanoparticles of metal oxides using ceramic and soft-chemical routes as well as various deposition techniques. Structural characterization using high-resolution synchrotron and neutron powder diffraction using X7A at the National Synchrotron Light Source as the main facility; high-pressure crystallography using diamond anvil cells; pair-distribution function (pdf) analysis of nanomaterials;

Major Program Achievements (over duration of support):
First structural confirmation of pressure-induced hydration in a nanoporous material. (JACS 124, 5466 (2002)
Discovery of nonreversible pressure-induced hydration. (Nature in press)

First determination of compressibility and combined theoretical study on the behaviour of the new superconductor MgB2 (PRB 63, 220505(R))

First structural characterization of room temperature electride in nanoporous material using pair-distribution function analysis (PRL 89(7), 075502)

Program impact:
Opened up and advanced novel field of pressure-induced hydration in framework structures (i.e. zeolites, pyrochlores). A patent application entitled "Pressure-Induced Swelling in Microporous Materials" is being filed.
This group remains one of the leaders worldwide in high-resolution powder diffraction.
Continuing improvement of total scattering experiments and pdf data analysis

Interactions:
Dept. of Chemical Engineering U. Delaware (D. Buttrey)
Physics Dept. Penn State University (T. Egami, W. Dmowski)
Chemistry Department University of Birmingham, UK (J.A. Hriljac)
Chemistry Dept. University of Oslo Norway (P. Karen)
Chemistry dept. University of Sydney, ,Australia (B. Kennedy)
ChevronTexaco (R Medrud, A. Bard)
Geoscience and Chemsitry Dept. SUNY Stony Brook (J. Parise)
Dept. of Physics and Astronomy Michigan State University (S. Billinge, V. Petkov)
Chemistry Dept. Ohio State University (P. Woodward)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
2002 Van Valkenburg Award to Yongjae Lee
2002 Sidhu Award of the Pittsburgh Diffraction Society to Yongjae Lee
2001 Barrett Award to Dave Cox (emeritus)
Popular Mechanics 2002 Design and Engineering Award for novel metal hydride battery electrode to Tom Vogt in collaboration with Jim Reilly, John Johnson, Gordana Adzic from BNL Materials Science.

No. of Invited Talks: 2 +

Personnel Commitments for FY2002 to Nearest +/- 10%:
Tom Vogt (Group Leader) 100%
Yongjae Lee (postdoc on LDRD) 10%
Beatriz Noheda (Assistant Physicist, now at University of Delft) 75%
Al Langhorn (senior technical specialist) 100%
Sharon Smith (33%)

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA 300 k$ **FY01 BA** 450k$ **FY02 BA** 430k$

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP:
Structure-Sensitive Properties of Advanced Permanent Magnet Materials: Experiment and Theory

FWP Number: MA-410-MABA

Program Scope: This program elucidates the relationships linking the microstructure of advanced permanent magnetic materials to their magnetic properties, with the ultimate goal of understanding how the microstructure may be manipulated and organized into desirable architectures by suitable nonequilibrium processing methods. The scope of the research has expanded to include basic studies of related magnetic alloys in their nanocrystalline, nanocomposite and amorphous forms. Examples of materials under study include $Nd_2Fe_{14}B$, CoPt and the multiphase bulk amorphous glass Nd-Fe-Al. Extensive collaboration with other DOE laboratories (including subcontract to INEEL), academia, and industry is a strong component of the research.

Major Program Achievements (over duration of support): Elucidated effects of intergranular interactions in nanocrystalline magnetic materials. Experimental and computational results indicate that formation of multi-grain "interaction domains" in nanoscale magnetic materials significantly alters the nature of the magnetic reversal, below:

Manipulation of Interphase Exchange in Magnetic Nanocomposites: Results concerning magnetic reversal in $L1_0$-type CoPt/Co thin film bilayers indicate the ability to tailor the response of the magnetic "exchange-spring" by careful manipulation of the nanoscale interface between the two magnetic phases.

Processing-Induced Internal Stress in Magnetic Nanocomposites: Quantitative analysis of synchrotron XRD data from rapidly-solidified nanocomposites of $Nd_2Fe_{14}B$ and α-Fe indicates the presence of significant local strain within the material that affects the global magnetic response. From analysis of the data it is postulated that the exchange field emanating from the high Curie temperature α-Fe fosters stabilizes the magnetic state of the nanoscaled $Nd_2Fe_{14}B$ and thereby produces an elevation of its lower Curie temperature.

Program Impact: Challenged long-standing assumptons about structure-property relationships in permanent magnets: Presented comprehensive results that support the (unfortunate) idea that high coercivity and high remanence are mutually incompatible in nanoscale magnets by virtue of intergranular exchange interactions.
Promoted the idea that "amorphous" materials are not truly amorphous on an atomic scale and contain angstrom-sized nuclei that are extremely challenging to detect. These quenched-in nuclei ultimately determine both the as-processed magnetic properties as well as the devitrification pathways.

Interactions: Brookhaven National Laboratory*:* Y. Zhu (Materials Sci. Dept.): advanced electron microscopy; J. Hill (Physics Dept) and C. C. Kao (NSLS): spectroscopy

National Laboratory Collaborations: Core Participant in DOE Centers for Excellence in Synthesis and Processing: "Isolated and Collective Phenomena in Nanocomposite Magnets."; Ames Laboratory (R. W. McCallum, M. J. Kramer: solidification studies in melt-spun $Nd_2Fe_{14}B$ & ferromagnetic bulk amorphous glasses);

U. S. Academic Collaborations: Carnegie Mellon University (K. Barmak: reversal studies in model bilayer systems; S. Majetich: nanoparticles; M. McHenry: general student exchange), SUNY Stony Brook (R. J. Gambino: magnetic nanocomposite films, S. Sampath: thermal spray products; J. Parise: nano-oxides);

Industrial Collaborations*:* Magnequench International, Inc. (B. M. Ma: general structure/ property relationships in $Nd_2Fe_{14}B$-based nanocrystalline magnets);

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Five invited presentations (BNL) since FY 2000.
Program Committee: Magnetism and Magnetic Materials Conference: 1999, 2000, 2001. (L. H. Lewis)

Program Chair: INTERMAG 03, Boston, MA 2003
Invited article: "The New Future of Magnetism", The World & I,/The Washington Times (Sept. 2001) (Lewis)

Personnel Commitments for FY2002 to Nearest +/- 10 % @ BNL
L. H. Lewis (BNL, experimental studies, 90%), **D. O. Welch** (BNL, theoretical studies, 25%), **D. Crew** (BNL, post-doctoral associate, 1999-2000, 100%), **C. Harland** (BNL, post-doctoral associate, 2001-2002, 100%)

Authorized Budget (BA) for FY00, FY01, FY002 @ BNL:
FY00 BA: $531,000 **FY01 BA:** $509,000 **FY02 BA** $445,000

Laboratory Name: Brookhaven National Laboratory

B&R Code: KC0202020

FWP and possible subtask under FWP:
Condensed Matter Physics—Electron Spectroscopy

FWP Number: PO-016

Program Scope:

The Electron Spectroscopy Program conducts experimental studies of the electronic and magnetic properties of surfaces and thin films, and further examines how such properties influence the physical behavior of materials. The program places a special emphasis on developing new spectroscopic techniques based at the National Synchrotron Light Source. In particular, new experimental capabilities in angle resolved photoemission and infrared spectroscopy allow detailed studies of correlated systems. Research topics include: (a) high resolution photoemission studies of complex oxides, (b) infrared studies of correlated metals including ultra-thin films and oxides, (c) spin-polarized valence-band photoemission studies of magnetic surfaces. The work in this program falls within the Complexity and Nanotechnology Initiatives of the DOE.

Major Program Achievements (over duration of support):

The program has established one of the leading spectroscopy groups in the world working in the area of strongly-correlated electrons. In particular the group, using the techniques, photoelectron spectroscopy and optical conductivity, has had a major impact in the areas of high Tc superconductivity, magnetic thin films and multilayers and surfaces.

Program Impact:

That the group has had a major impact in characterizing the electronic structure of correlated systems as evidenced by the large number of citations and b y the number olf invited talks at major international and national conferences.

Interactions:

The Group collaborated with approximately twenty faculty, together with associated students and post docs. This includes significant internal BNL collaboration, both within Condensed Matter Physics and more widely (in particular, the NSLS, Chemistry and Materials Science Departments) together with external collaborations with universities, other national laboratories and foreign institutions.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):

<u>FY02</u>

BNL Science and Technology Award
(Johnson)

13 invited talks in FY02

<u>Previously</u>

2 Fellow of the APS
1 Fellow of the Institute of Physics, U.K.

Personnel Commitments for FY2002 to Nearest +/-10%:
Peter D. Johnson (Group Leader),
Myron Strongin (100%)??
Christopher Homes (100%)??
Tonica Valla (100%) ??
Jiufeng Tu (50%) ??
Zikri Yusof (20%, Research Associate) – left 7/02??
Tim Kidd (20% Research Associate) - arrived 7/02??

Authorized Budget (BA) for FY00, FY01, FY02:

FY00 BA $	**FY01 BA $**	**FY02 BA $**

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202020

FWP and possible subtask under FWP: Soft X-ray Magnetic Speckle

FWP Number: LS007

Program Scope: Development and application of soft-x-ray speckle for x-ray imaging and x-ray photon correlation spectroscopy (XPCS) to characterize novel nano-scale functional materials, including magnetic, strongly correlated oxides, soft and bio-materials, with element-specificity and nanometer spatial resolution, as well as to elucidate the equilibrium and non-equilibrium dynamics of these systems.

Major Program Achievements (over duration of support): This FWP was redefined in FY02. Previously it supported the hard x-ray microfabrication effort as part of the sustainable technology initiative. That program has evolved to provide two exposure stations on the NSLS x-ray ring. These beamlines are currently the subject of negotiations with Sandia National Laboratory and Honeywell Federal Manufacturing (Kansas City Plant) as partner users who will provide for the operation and maintenance of the program. With this effort under way, the FWP was redirected to establish a new program in x-ray photon correlation spectroscopy at the NSLS.

Under the new program, a reconstruction algorithm based on multiple-wavelength anomalous diffraction (MAD) was developed. Specifically, large resonant enhancement and strong polarization/magnetization dependence of the scattering amplitudes of 3d transition elements near the L absorption edges and the 4f rare earth elements near the M absorption edges are used to provide the missing phase information and the necessary redundancy to reconstruct magnetic domain pattern from magnetic speckle patterns.

Experimentally, first observation of magnetic speckles from a Co/Pt multiplayer sample was made with both linearly and circularly polarized x-rays. Imaging reconstruction using observed magnetic speckle is in progress. A new experimental station with larger detector array was designed and commissioned. The new end station using transmission geometry will allow easier sample exchange, alignment of the system, improved spatial resolution, and better sample cooling/heating.

Program Impact: Provided a new photon-in-photon-out, nanometer spatial resolution, and element specific imaging tool to characterize a wide range of nano-scale functional materials. This new capability is particularly important for the study of materials under high magnetic fields.

Interactions:
Internal: BNL Physics department and Materials department.
External: Department of Physics, Stony Brook University; Department of Materials Science and Engineering, Massachusetts Institute of Technology; Department of Physics, University of Oregon; Argonne National Laboratory; Lawrence Berkeley National Laboratory; and IBM.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
3 Invited talks in international and domestic conferences in 2002:5th International workshop of Synchrotron Radiation Theory Network; International Materials Congress; Second annual emerging information technology conference- Nanotechnology, MEMS, System-on-Chip, and Bioinformatics.

Personnel Commitments for FY2002 to Nearest +/-10%:
Chi-Chang Kao (Senior Scientist) 10%
Cecilia Sanchez-Hanke (Assistant Scientist) 20%
Onur Mentes (Student) 100%

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $175,000 FY01 BA $160,000 FY02 BA $147,000

Laboratory Name: Brookhaven National Laboratory

B&R Code: KC-02-02-030

FWP and possible subtask under FWP:
Condensed Matter Theory

FWP Number:
PO-15

Program Scope:
Theoretical study of quantum and classical condensed matter systems, with extensions to nano systems. The emphasis of our research is on strongly correlated electron systems (low-dimensional and frustrated magnets, disordered electrons) and on statistical mechanics of complex systems and their underlying networks. Development and application of advanced non-perturbative techniques in physics of strongly correlated systems.

Major Program Achievements (over duration of support):
For the first time the possible existence of spin-1/2 neutral excitations (spinons) in more than one dimension was demonstrated for models with realistic interactions. Also, for the first time, expressions for the temperature dependence of the electronic spectral function in 1D Mott insulators was obtained. The theory of the metal-Mott-insulator transition was suggested based on a combination of a non-perturbative scheme and the Random Phase approximation. The theory contains a small parameter, which makes it unique among the theories of Mott insulator transitions, and allows a rigorous treatment. It predicts the existence of a metallic state with a small Fermi surface close to the transition.

A statistical algorithm aimed at detecting statistically significant topological patterns in complex networks was developed. It compares wiring patterns in a given network with its properly randomized counterpart and detects statistically significant deviations of one from another. This algorithm was applied to protein interaction and genetic regulatory networks in yeast Saccharomyces cerevisiae. It was found that links between highly connected proteins are systematically suppressed in favor of links between highly connected nodes and those of low connectivity. Such correlation pattern is beneficial for the cell since it decreases the likelihood of biologically undesirable cross talk and enhances the overall robustness of a network by localizing the effects of deleterious perturbations.

Program impact:
Provided many insights into behavior of strongly correlated and complex systems, most notably the stripe theory of superconductivity of Emery and Kivelson.

Interactions:
Princeton University (Prof. B. L. Altshuler)
ETH Zurich (Prof. T. M. Rice)
Abdus Salam ICTP, Trieste, Italy (Prof. V. Kravtsov, Dr. A. Nersesyan)
SUNY at Stony Brook (Prof. A. Abanov)
MIT, Cambridge (Prof. L. Levitov)
University of Minnesota, Minneapolis (Prof. L. Glazman)
University of Pierre and Marie Curie, Paris (Prof. P. Azaria)
Niels Bohr Institute, (Prof. K. Sneppen)
Nordita, Copenhagen (Dr. K. Eriksen)
Institute for Theoretical Physics, University of Fribourg, Switzerland (Prof. Y..-C. Zhang)
Weizmann Institute (Prof. U. Alon)
Rockefeller University (Dr. M. Elowitz)
NEC Research Institute, Princeton (Dr. C. Tang)
ITP, Santa Barbara (Prof. A. Zee)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Dr. V. Emery – Buckley Prize, elected a Fellow of the American Academy of Arts and Sciences.
No. of Invited Talks: 43, of which 16 were invited conference talks.

Personnel Commitments for FY2002 to Nearest +/- 10%:

A.M. Tsvelik (group leader) 90%
S. Maslov 100%
F. H. L. Essler 60%
R. Watson (retired in February) 32%
B.L. Altshuler (visiting scientist from Princeton Univ.) 5%
A.A. Nersesyan (visiting scientist from ICTP) 20%
T. M. Rice (visiting scientist from ETH) 10%
B. Naroznhy (postdoc) 10%
M.J. Bhaseen (postdoc) 0%
V. Perebeinos (postdoc) 10%
S. Carr (student)

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $800 **FY01 BA $971** **FY02 BA $1082**

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP:
Synthesis and Structure of Conducting Polymers

FWP Number: MA-114-MAEA

Program Scope:
Use the results of our spectroscopic studies to guide the design and synthesis of new functional groups and ion-conducting polymers with enhanced ion dissociation and cation transference. The approach, at BNL, is to modify the solvent chemistry to enhance anion-solvent interactions by adding new Lewis acid compounds, to the solvent. The compounds form complexes with anions, dissociate the ion pairs, and free the cations. Therefore, the number of charge carriers, the conductivity, and the Li^+ ion transference number are all increased significantly. Characterization includes electrochemical and conductivity studies and the use of a wide array of spectroscopic techniques, such as x-ray absorption spectroscopy (XAS), to elucidate ion-ion and ion-solvent interactions.

Major Program Achievements (over duration of support):
XAS and Raman studies: XAS and Raman spectroscopy were used to study ion-ion and ion-polymer interactions in both liquid and polymer non-aqueous electrolytes. Both spectroscopies indicated a high degree of ion pairing. EXAFS of polymer electrolytes gave quantitative information on the ion pairing and confirmed a very high degree of ion pairing in polymer electrolytes. Furthermore, in many cases, ion pairing increased with increasing temperature. The results indicated that the ion pairing is due to the inability of Lewis base polymers, such as PEO, to accommodate anions.

A new synthetic approach: BNL has synthesized a new family of anion-complexing additives based on Lewis acid boron compounds with various fluorinated aryl or alkyl groups. The compounds can be boranes, borates or boronates. These have electron deficient boron sites that interact strongly with anions and break up the ion pairs. The result is improvement in electrolyte conductivity and Li^+ ion transference. Work is underway to incorporate these complexing agents into the polymer backbone.

Program impact:
The program has developed a totally new approach to the synthesis of non-aqueous electrolytes, based on the incorporation of Lewis acid entities in the electrolyte to accommodate anions. Other groups are now using this approach, particularly in Japan. Prior to this, the main approach was the use of salts with highly delocalized charge on the anions. However, this leads to unstable salts. The new anion complexing agents have attracted the attention of many organizations including IBM, Merck, Honeywell, Duracell, Panasonic, Mitsubishi Chemical and Daikin Corp.

Interactions:
University collaborations include SUNY Stony Brook, Northeastern University and Polytechnic University in USA, Saga University in Japan, and University of Sao Paulo, in Brazil.
Industrial collaborations include Gould Electronics, Inc., FMC Corp., 3M Corp., and Gillette (Duracell).
Government Laboratory interactions include SNL, ARL, NRL and PNNL.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
J. McBreen - Elected Fellow of The Electrochemical Society (2001); Co-organizer MMC-9 (9^{th} IUPAC Meeting on Metal Macrocyclic Complexes), August 19-23, 2001, Brooklyn, NY.
H. S. Lee, X. Q. Yang, J. McBreen – 6 US patents on anion complexing agents.
X. Q. Yang, J. McBreen – 15 invited presentations since 1999.

Personnel Commitments for FY2002 to Nearest +/- 10%:
J. McBreen (project leader, 30%); **X. Q. Yang** (25%); **H. S. Lee** (100%); **X. Sun** (20%).

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $456,000 **FY01 BA** $408,000 **FY02 BA** $425,000