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

FWP and/or subtask Title under FWP: Studies of Nanoscale Structure and Structural Defects in Advanced Materials

FWP Number: MA-015-MACA

Program Scope:
The goal of this program is to study property sensitive nanoscale structure and defects in technologically-important materials such as superconductors, magnets, and other functional materials. Advanced quantitative electron microscopy techniques, such as coherent diffraction, atomic imaging, atomically-resolved spectroscopy, and phase retrieval methods including electron holography are developed and employed to study material behaviors. Computer simulations and theoretical modeling are carried out to aid the interpretation of experimental data. Fabrication of thin films with tailored microstructure and nano-assemblies to understand materials' electronic and magnetic response under applied stimulus is also incorporated.

Major Program Achievements (FY2007):
(1) Understanding the interplay between spin, charge, orbital and lattice ordering and local electronic inhomogeneity in strongly correlated and complex oxides, especially in multilayer systems; correlation between spins and electrons, interfacial bonding state and charge transfer during paramagnetic, ferromagnetic and anti-ferromagnetic phase transitions and their effects on properties. Materials studied: $YBa_2Cu_3O_7$, $La_{2-x}Sr_xCuO_4$, $LaMnO_3/SrMnO_3$, $Pr_{1-x}Ca_xMnO_3$, $La_{0.625-y}Pr_yCa_{0.375}MnO_3$, $CaCu_3Ti_4O_{12}$ etc.
(2) Studying the effect of crystal structure, incommensurate modulation, defects, and local strain on thermalelectric and dielectric properties. Materials : $Ca_3Co_4O_9$, $AgPb_{18}SbTe_{20}$, $BaTiO_3$ etc.
(3) Revealing magnetic reversal and switching behavior of magnetic elements and arrays, the effect of element shape, geometry, edge roughness, magnetic coupling with their neighbors, and magnetoresistance. Materials: Patterned Permalloy, Co and Ni films.
(4) Identifying structure-properties relationship of various nano-objects to understand their functionality and response under various stimulus such as magnetic field, electric bias and light. Materials : carbon nanotubes, functional nanowires and particles.

Program Impact: The impact of our work is the development of advanced imaging techniques that can be broadly applied to quantitatively characterize a variety of materials and their behavior. Applications to magnetic materials and strongly correlated electron systems including energy related materials are demonstrated.

Interactions: Internal—Oxide molecular beam epitaxy group, Correlated electron materials group, Neutron scattering group, Synchrotron x-ray diffraction group, Condensed-matter theory group; Center for functional nanomaterials; Center for data intensive computing, and Biology STEM group. External—Columbia University; Stony Brook University; Carnegie Mellon University; Yale University; ORNL; IBM; UC San Diego; University of Alberta, Canada; University of Oslo, Norway; and University of Bologna, Italy.

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
Y. Zhu – APS fellow (2006); Executive Editor (North America), Journal of Electron Microscopy (Oxford University Press); Program Committees and symposium co-organizer, MMM (2007), IMC16 (2006), MSA (2006), MRS (2005); Editorial Board of *MICRON*, Adjunct Professor at Dept. of Applied Physics and Mathematics, Columbia University; Dept. of Physics, and Dept. of Materials Science, Stony Brook University; J. Lau – National Research Council Postdoc Fellow (2005); M. Beleggia – Early Career Award (€1000), 2006, Italian Society of Microscopy Sciences (SISM). 35 invited talks in the last three years at major conferences excluding institution seminars.

Personnel Commitments for FY2007 to Nearest +/- 10%: Y. Zhu (75%), L. Wu (100%), V.V. Volkov (50%), M.A. Schofield (80%), M. Beleggia (80%), J. Zheng (100%) and J. Tao (100%, postdoc, starting June 07).

Authorized Budget (BA):
FY05 BA - $1,898K **FY06 BA** - $1,898K **FY07 BA** - $1,898K

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

FWP: Complexity from Simplicity: Quantum Criticality and Novel Collective Phases in Itinerant Ferromagnets

FWP Number: PM-009

Program Scope:
This project seeks to explicate the essential conditions under which magnetic order is possible, and the range of novel phenomena which occur when order is on the brink of instability, i.e occuring at zero temperature. These quantum critical phenomena are responsible for the functionality of many diffferent classes of advanced materials, and are examples of emergent behavior which results from complex and incompletely understood interactions among the mobile electrons in metals. The goal of this research project is to explore how minimal of a system is required to sustain these complex, many body states, and to determine whether even simple transition metal ferromagnets can host novel critical states, particularly superconductivity. The research we propose combines developing new synthetic infrastructure and approaches for these novel materials and the implementation of advanced measurement techniques, with extensive utilization of national research facilities. The training of students and postdocs is an integral goal of this research project, enabling the next generation of materials-inspired researchers.

Major Program Achievements (over duration of support):
Laboratory and research group were relocated from University of Michigan to Brookhaven. FWP submitted and under review. Completed two neutron scattering projects on Co/CoO core shell nanoparticles, showing that large exchange bias effect is controlled by induced interfacial moments which can be enhanced by selective oxidation. Inelastic neutron scattering experiment show that core is slowed by accelerating shell, as well as a new spin wave mode, perhaps unique to CoO nanoshells. Used small angle x-ray scattering experiments to demonstrate that there is an optimal core/shell dimension which maximizes exchange bias. Initiated project to synthesize transition metal Laves phase compounds. Have synthesized and characterized ten new compounds, one of which is a new superconductor.

Program impact:
Have completed first quantitative neutron scattering measurements of the magnetic structure and dynamics of compound nanoparticles.

Interactions:
Internal Collaborations: K. Nelson, Y. Lin, C. C .Kao (NSLS), W. Han and X. Teng (CFN), S. Wong, Y. Zhu and L. Wu (CMPMSD).
External: J. A. Borchers, Y. Qiu, and K. Kryczka (NIST), S. Inderhees, G. Strycker, and K. Sun(University of Michigan), J. Parise, P. Stephens, and C. Grey (Stony Brook University), C. Tulk (Oak Ridge).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
M. C. Aronson: Program Committees for International Conference on Low Temperature Physics, International Conference on Strongly Correlated Electron Systems, Neutron Advisory Board (Oak Ridge), Board of Governors Institute for Complex and Adaptive Matter (ICAM), Committee to Assess the Impact of the MRSEC Program (National Academy Board on Physics and Astronomy), Lee-Osheroff-Richardson Prize Committee, Neutron Scattering Society of America Prize Committee.

Personnel Commitments for FY2007 to Nearest +/- 10%:
M. C. Aronson (50%), D. A. Sokolov (100%), M. S. Kim (100%), Y. Janssen (100%), K. Kim (100%), M. Feygenson (100%).

Authorized Budget (BA) for FY05, FY06, FY07:

FY05 BA $	FY06 BA $	FY07 BA $

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

FWP and possible subtask under FWP: Superconducting Materials

FWP Number: MA-012-MABA

Program Scope: This program studies the basic relationships between nanoscale structures and macroscopic properties of superconductors, providing the understanding of the fundamental physics and materials science required for their practical utilization. High temperature superconducting (HTS) cuprates, alloyed MgB_2, and superconductor heterostructures are systems receiving emphasis. Recently, the group has also established a successful synthesis and characterization facility for the study of correlated thermoelectric materials.

Major Program Achievements (over duration of support):
1) Dynamical layer decoupling in high-temperature superconductors (HTS) was discovered. The measurements of the anisotropic transport and magnetization properties of a stripe-ordered superconductor, $La_{2-x}Ba_xCuO_4$ (LBCO) at x=1/8, revealed a state of two-dimensional (2D) fluctuating superconductivity. This 2D fluctuation superconductivity exhibits unprecedented characteristics, including enhanced T_c of an order of magnitude higher than the value of 3D T_c, responsible for the bulk superconductivity. This finding suggests that stripe order in LBCO frustrates 3D superconducting phase order, but is fully compatible with 2D superconductivity. 2) Enhanced flux pinning in HTS $YBa_2Cu_3O_{7-\delta}$ (YBCO) films by nanometer-scale substrate surface roughness was demonstrated, which resulted in ~ 30% increase in critical current density J_c. 3) Strong *isotropic* flux pinning was observed for the first time in strong anisotropic HTS at liquid nitrogen temperatures. The very weak angular dependence of J_c around c-axis indicates that the pinning centers in record high-J_c YBCO thick films made on the magnetic substrates are *isotropic* and are not correlated to a particular direction or alignment. 4) Studies of structure, heat capacity, and transmission electron microscopy with electron energy loss spectroscopy were coordinated to probe the changes in superconductivity in MgB_2 when the Mg atoms are progressively replaced by Al. We obtained the first direct evidence for the filling of the hole states in the planar σ band, crucial for the high T_c in pure MgB_2, by the extra electrons donated by Al. Yet, superconductivity was not destroyed when there was sufficient Al to fill all of the hole states, but it persisted to much higher levels of Al doping. Using a two-band model of superconductivity, fits to the heat capacity data indicated that it is the π band that survives in the heavily doped regime, which is an inversion of the hierarchy of the bands in pure MgB_2.

Program Impact:
Results (1) may shed light on the mechanism of HTS, as well as lead to new strategies for increasing T_c. Results (2) suggest that nanoscale substrate surface roughness, magnetic coupling in superconductor/magnet heterostructures can be used to enhance the HTS performance. Results (3) suggest that it is possible to achieve very high J_c without using the additives to YBCO films, and this makes the process and application of HTS easier. Results (4) explain why the critical temperature in MgB_2 falls with dopant concentration.

Interactions:
Condensed Matter Physics and Material Science Department, Chemistry Department, Center for Functional Nanomaterials of BNL, Los Alamos Lab, Penn State University, UC San Diego, Brown University, University of Gottengen, Harvard University, Stanford University, University de Sherbrooke, SUNY at Stony Brook, University of Oslo, American Superconductors Inc., GM R&D Center, AIST-Japan.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
8 invited talks in FY07, CRADA with General Motors.

Personnel Commitments for FY2007 to Nearest +/-10%:
Q. Li (PI) 100%, L. Cooley (Co-PI) 30%, A. Moodenbaugh 50%, Q. Jie (Graduate student) 100%

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA - $729K **FY06 BA** - $714K **FY07 BA** - $714K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201050 + KC0202010

FWP: Molecular beam epitaxy and nano-structuring of perovskite oxide materials toward an understanding of strongly correlated systems.

FWP Number: MA-509-MACA
Subtask under FWP: Bulk Materials Synthesis and Characterization. **FWP Number:** PO-013

Program Scope:
Molecular beam epitaxy: We have developed a unique molecular beam epitaxy synthesis technique to synthesize atomically perfect thin films, multilayers, and superlattices containing cuprate high-temperature superconductors (HTS) and other complex oxides. This in turn enables fabrication of HTS heterostructures nanowires and nanodots of unprecedented quality.
Bulk Materials Synthesis: Exploratory synthesis and characterization of new materials; discovery of new phenomena associated with superconductivity, magnetism and correlated electron behavior. Development of new synthesis methods.

Major Program Achievements (over duration of support):
Molecular beam epitaxy: The new MBE laboratory, including a clean room, is fully functional at the peak performance; in the last year we have synthesized over 250 superconducting films, most of which are atomically smooth. All the films were characterized by RHEED, R(T) and/or χ(T) measurements and selected ones also by XRD, AFM and RBS. We have made two important discoveries: (i) colossal photo-induced expansion and (ii) interface superconductivity, both of which are expected to generate much follow-up research.
Bulk Materials Synthesis: Discovered colossal magnetoresistance (CMR) in doped nearly-magnetic semiconductor $FeSb_2$. Synthesized large high-purity crystals of quasi-2D heavy-fermion superconductors and discovered unconventional multi-band superconductivity. Discovered half-metallic ferromagnet Mn_4FeGe_3 for spin injecton in Ge. Developed in-situ decanting high-temperature-flux crystal growth method. Developed synthesis method of large intermetallic crystals and synthesized many previously unavailable materials at the quantum critical point for neutron scattering.

Program impact:
Our unique samples enable challenging experiments that deepen our understanding of correlated-electron materials and provide the scientific base for their optimization. Only few years ago, DOE panels expressed deep worries about US researchers at major facilities being totally dependent on samples synthesized in Japan or China. We are reversing this trend and now unique samples made at BNL are studied by many groups worldwide (including both Japan and China).

Interactions:
Internal: TEM (Zhu), XRD (Hill, Billinge), ARPES (Valla), surface crystallography (Pindak, Wilkins), NSLS (Kao, Nelson, Frenkel), CFN (Warren), Chemistry (Adzic, Vukmirovic, Khalifah), Neutron Scattering (Zaliznyak) External: LANL (Balakirev, Migliori, Conradson); NHMFL (Boebinger, Tozer, Popovic); LBL (Freelon, Birgenau); Urbana (Abbamonte); Cornel (D. Muller); UC Berkeley (Dynes, Cybart), Akron (Djordjevic); Miami (Clayhold); EPFL, Switzerland (Pavuna); PSI, Switzerland (Morenzoni, Suter); Konstanz Germany (Demsar); Belgrade, Serbia (Radovic, Popovic); Bar Ilan, Israel (Yeshurun); Technion, Israel (A. Keren); Johns Hopkins (Broholm, Chien, Armitage), Columbia (Uemura), Princeton (Ong), Maryland (Paglione), Brown (Mitrovic), Notre Dame (Eskildsen), Liege (Hermann), Sherbrooke (Taillefer), Toronto (Wei, Julian, Kim), ETH (Degiorgi), UC San Diego (Maple), Ames (Canfield, Bud'ko), Univ. of Tokyo (Nakatsuji), Chinese Academy of Sciences Beijing (Wang), Yonsei Univ. Seoul (Lee), UC Irvine (Fisk), Northwestern (Ketterson), ISIS (Stock), Sao Paolo (Pagliuso), CBPF Rio de Janeiro (Saitovich), TU Budapest (Simon), Simon Fraser (Broun), UBC (Damascelli), ASU (Porter)

Recognitions, Honors and Awards (partly attributable to support under this FWP:
Member, Editorial Board, The International Journal of Superconductivity.
Chair, HTS Thin Films Workshop, Tsukuba, Japan, 2007.
Member, The International Advisory Board, five international conferences (Japan, Serbia, USA, Montenegro, Australia)
Guest Editor, J. Superconductivity (special issue honoring Nobel Laureate V. L. Ginzburg).
20 invited (including several keynote) talks at conferences in 2006-7 and a number of invited seminars and colloquia.

Personnel Commitments for FY2007 to Nearest +/- 10%:
I. Bozovic (100%), G. Logvenov (100%), V. Butko (100%), A. Gozar (100%) A. Bollinger (100%), C. Petrovic (100%), R. Hu (student) 100%, R. Huang (student) 100%.

Authorized Budget (BA):
FY05 BA - $1,615,000 **FY06 BA -** $1,737,000 **FY07 BA - $1,737,000**

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201050

FWP and possible subtask under FWP:
Synthesis and Characterization of Individual Carbon and Perovskite Oxide Nanotubes
FWP Number: MA-507-MAAA

Program Scope:
Synthesis of carbon and perovskite oxide nanomaterials, individual nanomaterial characterization, and modeling are combined to provide insights toward correlating nanomaterial structure with function.

Major Program Achievements (over duration of support):

- Advances in the synthesis of novel nanomaterials including the development of solid-state synthesis techniques for high-quality oxide nanomaterials. A primary example this year has been the generation of single-crystalline perovskite $BaZrO_3$ submicron-sized particles, synthesized using a simple, scaleable molten salt method, wherein the effects of different experimental processing parameters, such as the identity of the salt, annealing temperatures, overall reaction times, cooling rates, and the chemical nature of the precursor, were primarily analyzed in determining their impact upon the purity, size, shape, and morphology of as-obtained products. Moreover, the role of additional factors such as heating rate, amount of salt used, molar ratios of precursors, and surfactant was also deduced. In addition, the evolution of particle morphology from predominantly cubes to solely spheres has been demonstrated by increasing annealing/reaction times at suitable annealing temperatures, all other parameters being equal. Rationally controlling perovskite oxide shapes is of great importance due to their strongly structure-dependent physical properties.
- Developed sensitive spectroscopic tools to determine the electroluminescence emission spectra from individual carbon nanotubes in-situ at a probe station where simultaneous transport studies are performed. Developed techniques for structural determination of the nanotube under probe. Developed a Fourier-transform photoconductivity spectroscopy to examine the low energy photoexcitations in single nanomaterials.
- Investigated the biocompatibility, specificity, and activity of a ligand-receptor-protein system covalently bound to oxidized single-walled carbon nanotubes (SWNTs) as a model proof-of-concept for employing such SWNTs as biosensors. SWNTs were functionalized under ambient conditions with either the Knob protein domain from adenovirus serotype 12 (Ad 12 Knob), or its human cellular receptor, the CAR protein, via diimide-activated amidation. Demonstrated that SWNT-CAR complexes in a FET structure can serve as electronic biosensors for detecting environmental adenoviruses.

Program impact

- Development of a host of functional nanostructures using (a) cost-effective, nontoxic precursors; (b) relatively few numbers of reagents; (c) few reaction steps with minimization of waste and power consumption; (d) high-yield processes with little if any volatile and toxic byproducts; (d) room temperature (or low temperature) synthesis under ambient conditions, if at all possible; and (e) efficiency of scale-up.
- We have shown that NEXAFS spectroscopy can be used to determine the surface orientation and the extent of order in vertically aligned carbon nanotube arrays grown on a substrate which provided for a complementary, more nuanced determination of local surface order as compared with SEM analyses.
- Discovered new method of optical emission from a single carbon nanotube. Spectroscopic studies of individual carbon nanotubes showed that the electroluminescence spectra depend on the length and diameter of the carbon nanotube. First simultaneous spectroscopy and direct structural determination on same nanotube, showed chiral dependence of metallic tube energy splitting.
- Provided proof-of-concept for the development of a simple, efficient, sensitive, fast-response, and real-time miniaturized nanotube FET biosensor based on the conductivity change of a single SWNT by adding a discrete CAR domain to the nanotube.

Interactions:
National Synchrotron Light Source, State University of New York at Stony Brook, Argonne National Laboratory, Columbia University, IBM Yorktown Heights, NIST, University of Pennsylvania, Princeton University.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
S.S. Wong – Alfred P. Sloan Foundation Fellowship - 2006.

No. of Invited Talks (National and International Meetings): 11 in FY07

Personnel Commitments for FY2006 to Nearest +/- 10%:
S.S. Wong (50%); J. Misewich (10 %)

Authorized Budget (BA) for FY05, FY06, FY07:

FY05 BA $422K **FY06 BA $414K** **FY07 BA $414K**

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 synchrotron x-ray scattering. The Group also develops instrumentation and maintains and operates beamlines at the National Synchrotron Light Source, and at the Advanced Photon Source (APS). Particular emphasis is placed on the investigation of novel electronic ground states and excitations. Current research is focused on strongly correlated electron systems and organic electronic materials.

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 of electronic ordering and excitations in strongly correlated systems. Efforts in the field of liquid interfaces have led to significant discoveries such as surface freezing and surface-induced layering in liquid metals. The X22 beam lines have been among the premier x-ray scattering lines at the NSLS. The group played a leading role in the construction, and operation, of the Complex Materials Consortium-Collaborative Access Team (CMC-CAT) at the APS and the construction of a new sector dedicated to inelastic x-ray scattering (IXS-CDT), which became operational in FY07.

Program impact:
The Group's longstanding programs concerned with x-ray resonant phenomena, and inelastic x-ray scattering have been seminal in stimulating related efforts worldwide, and remain among the leading programs in these areas today. Efforts in soft condensed matter led to the creation of a new FWP aimed at understanding nanoscale confinement and the role of self-assembly in soft materials. Work in inelastic x-ray scattering led, with others, to the creation of the IXS-CDT at the APS. Highlights in FY07 include the observation of dynamics of orbital domain walls using soft coherent x-ray scattering techniques and the investigation of the phonon spectra in a new class of organic, graphite-based, superconductors.

Interactions:
The Group typically collaborates with ~20 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 Materials Science and more widely 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):
6 invited talks in FY07
Previously:
2 Goldhaber Fellows, 1 Wohlfarth Award, 1 Significant Achievement in Solid State Physics, 1 Presidential Early Career Award, 3 Fellows of the APS, 1 Fellow of AAAS, 1 Brookhaven Engineering Award, 1 Brookhaven Science and Technology Award, Editorial Board Member, J. Phys. Condens. Matter.

Personnel Commitments for FY2007 to Nearest +/- 10%:
John Hill (Group Leader) (50%), Ben Ocko (100%), Mary Upton (50%), Stuart Wilkins (100%), Scott Coburn (50%, Engineer), Bill Schoenig (100%, technician), Members of the Soft Matter Group (Fukuto and Checco) are also members of the x-ray scattering group, but received no salary support from this FWP.

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $1,525,000 **FY06 BA** $1,496,000 **FY07 BA** $1,496,000

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

FWP and possible subtask under FWP: Neutron Scattering

FWP Number: PO-010

Program Scope: Elastic and inelastic neutron scattering are used to investigate phenomena such as high-temperature superconductivity, charge and spin ordering in doped Mott insulators, low-dimensional and quantum-disordered antiferromagnism, and ferroelectricity. Experiments utilize national and international neutron facilities, especially instrumentation developed and supported by BNL, and single-crystal samples grown at BNL.

Major Program Achievements (over duration of support):
High-Temperature Superconductivity: Discovery of charge and spin stripe order in certain cuprates; discovery of universal magnetic spectrum for cuprates; discovery of 2D superconductivity coexisting with stripe order.
Doped Mott insulators: Discovery of stripe order in $La_{2-x}Sr_xNiO_{4+\delta}$ and measurement of associated spin waves; checkerboard charge plus magnetic order in $La_{0.5}Sr_{1.5}MnO_4$, $La_{1.5}Sr_{0.5}CoO_4$.
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: Growth of very large crystals of $La_{2-x}Ba_xCuO_4$ and $Bi_2Sr_2CaCuO_{8+\delta}$ enabling detailed studies of magnetic excitations in superconductors.
Instrument development: Concept for HYSPEC at the SNS; US-Japan cold triple-axis spectrometer at HFIR

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---Condensed-Matter Physics & Materials Science Dept.: X-ray Scattering Group, Materials Synthesis and Characterization Group, Electron Spectroscopy Group, Theory Group, Superconductivity Group; Center for Functional Nanomaterials: Electron Microscopy Group
External---University of Delaware; Johns Hopkins University; Rutgers University; Virginia Tech; Oak Ridge National Laboratory; National Institute of Standards and Technology; Institute for Solid State Physics, University of Tokyo, Japan; Institute for Materials Research, Tohoku University, Japan; Japanese Atomic Energy Agency; Oxford University, UK; Rutherford-Appleton Laboratory, UK; Laboratoire Léon Brillouin, France; CEA/Grenoble, France; Hahn-Meitner Institute, Berlin, Germany; Forschungszentrum Karlsruhe, Germany; IFW Dresden, Germany

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
2 Fellows of the American Physical Society; 1 Fellow of the Neutron Scattering Society of America;
1 Fellow of the American Association for the Advancement of Science.
15 invited talks at national and international conferences in FY07.
I. Zaliznyak and S.M. Shapiro---Principle investigators for HYSPEC instrument development team
J.M. Tranquada---Sustained Research Prize, Neutron Scattering Society of America, 2006; Divisional Associate Editor, Physical Review Letters, 2001-2007; member, Basic Energy Sciences Advisory Committee, 2008; member, Neutron Scattering Science Advisory Committee, ORNL.

Personnel Commitments for FY2008 to Nearest +/- 10%:
J. M. Tranquada (group leader) (100%), G. D. Gu (100%), M. Hücker (100%), B. Winn (stationed at ORNL, 100%), G. Xu (100%), I. Zaliznyak (100%), K. Mohanty (100%)

Authorized Budget (BA) for FY05, FY06, FY07: (including Neutron Instrument Development and User Support)
FY05 BA $1836K+$550K **FY06 BA** $1650K+$400K **FY07 BA** $2,250K

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 Group's primary focus is on the electronic structure and dynamics of condensed matter systems. The group carries out studies on a range of materials including strongly correlated systems. A special emphasis is placed on studies of High Tc superconductors and related materials. The primary techniques used include High-Resolution Photoemission and Infra-Red Spectroscopy or Optical Conductivity. The experiments are carried out both within the laboratories in the Condensed Matter Physics and Materials Science Department and at the National Synchrotron Light Source. The emphasis is on the study of the low energy excitations and the nature of the interactions of the latter with their environment. The group has also established a successful pulsed laser deposition facility for the study of thin films. Future plans involve studies of nanoscale systems and will involve close collaboration and work within the newly created Center for Functional Nanomaterials. The group is also heavily involved in the development of new spectroscopy capabilities.

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. The group has recently been involved in detailed studies of $La_{2-x}Ba_xCuO_4$ and reported important new insights into the physics of the pseudogap phase, and demonstrated a scaling law relating the superfluid density to the product of the normal state conductivity and the superconducting transition temperature for the high Tc superconducting cuprates. The group was also the first to identify the kink or mass renormalization observed in the nodal direction of the high Tc materials. Further the group has introduced the method of analysis in photoemission involving Momentum Distribution Curves (MDC).

Program Impact:
Using the techniques of photoelectron spectroscopy and optical conductivity, the group has had a major impact in the areas of high Tc superconductivity, magnetic thin films and multilayers and surfaces. This is evidenced by the large number of citations and by the number of invited talks at major international and national conferences.

Interactions:
The Group collaborated with approximately sixty faculty, together with associated students and post docs. This includes significant internal BNL collaboration, both within Condensed Matter Physics and Materials Science Dept. and more widely (in particular, the NSLS, and CFN) 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):
3 Fellows of the APS
1 Fellow of the Institute of Physics, U.K.
1 Fellow of the AAAS
2001 Brookhaven Science and technology Award
11 Invited talks at National and International meetings in FY07

Personnel Commitments for FY2007 to Nearest +/-10%:
Peter D. Johnson (Group Leader, 50%)
Christopher Homes (95%)
Tonica Valla (100%)
Weidong Si (100%)
Hongbo Yang (75%-Research Associate)
F. Loeb (85%)
Jon Rameau (100% - Student)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA - $1,660K **FY06 BA - $1,660K** **FY07 BA - $1,660K**

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

FWP and possible subtask under FWP: Atomistic Transport Mechanisms in Reversible Complex Metal Hydrides
FWP Number: BO-130

Program Scope:

This research program has two major objectives: i) the development of a comprehensive, quantitative understanding of the fundamental, atomic-scale mechanisms underlying the facile reversible hydrogen storage in titanium-doped sodium alanate ($NaAlH_4$), the only complex hydride allowing reversible hydrogen storage known to date; and ii) the utilization of this basic knowledge for a rational search for novel complex hydride storage materials with properties superior to those of $NaAlH_4$. In contrast to previous research on bulk compounds with complex microstructures and reaction pathways, the present program is based on the use of well-defined model systems and a suite of state-of-the-art surface experiments to achieve a quantitative understanding of the important reaction mechanisms at the atomic scale. This approach generates data on systems accessible to first-principles calculations, and allows an unprecedented level of interaction between experiment and theory. Key questions to be addressed include: i) the mechanism of hydrogen dissociation on Al surface doped with Ti; ii) the identification of the predominant carrier of mass transport, and measurements of its diffusion kinetics; and iii) the microscopic reaction mechanisms and their rate-limiting step as NaH and Al react to Na_3AlH_6 and $NaAlH_4$ in the presence of hydrogen.

Major Program Achievements (over duration of support):

As a key step toward understanding the beneficial effects of Ti dopants in $NaAlH_4$, the mechanisms of interaction of hydrogen with Ti-doped Al(111) surfaces have been established by scanning tunneling microscopy (STM) and density-functional theory (DFT). Ti is kinetically stabilized in surface sites as a disordered Ti-Al alloy with particular short-range order. The suppression of nearest-neighbor pairs of Ti atoms produces a large population of second-nearest neighbor Ti-pairs, which our calculations predict to dissociate adsorbing H_2 molecules with little or no activation barrier, in contrast to the free Al surface where the activation energy exceeds 1 eV. This finding explains why hydrogen storage in $NaAlH_4$ can be made reversible by small amounts of Ti doping. Once H_2 is dissociated by a Ti-atom pair complex, atomic-H needs to diffuse onto the free Al surface to regenerate the catalytic site, i.e., enable further dissociative H_2 adsorption. High-resolution STM movies show that this process proceeds readily through hops between specific H-binding sites, identified by DFT calculations as local minima in the potential energy landscape around the Ti-complex. Transition-state calculations confirm that the regeneration of the catalytic site is endothermic by few 1/10 eV, i.e., will be possible at or near room temperature.

IR spectroscopy, together with STM and theory, shows the evolution of surface alanes (AlH_3, Al_2H_6, etc.) as dissociated H interacts with Al. Etching of Al steps by H leads to a population of small alanes with high diffusion mobility. At higher temperatures, these mobile small alanes agglomerate to form larger oligomers. Together with hydrogenation experiments on bulk materials, which show that AlH_3 can react with NaH to form $NaAlH_4$ without a catalyst, these findings identify alanes as the primary carrier of mass transport during the hydrogen storage reaction.

Our work on new hydrogen storage materials, finally, has concentrated on crystalline AlH_3 as a promising system with 10 wt. % hydrogen capacity. Crystal structures and thermodynamic properties of several AlH_3 phases have been determined. Liquid-phase routes toward the regeneration of AlH_3, again using Ti as a catalyst, have been explored, inspired by our results on Ti-catalyzed H_2 dissociation from experiments on model systems.

Program impact:

The impact of this project will be to provide a fundamental understanding of the atomic-scale processes enabling the reversible storage of H_2 in complex metal hydrides. This understanding will provide the basis for the development of new higher performance hydrogen storage materials.

Interactions:

Yves Chabal, Rutgers University; Cristian Ciobanu, Colorado School of Mines; BNL-CFN; BNL Chemistry; and BNL Materials Science & Condensed Matter Physics.

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

Ewald Wicke Award, 2006, presented at the International Metal Hydride Symposium to Jason Graetz.

Personnel Commitments for FY2007 to Nearest +/- 10%:

P. Sutter (20%), J. Muckerman (20%), J. Graetz (50%), E. Muller (80%), J. Flege (20%), Y. Chabal (Contract), C. Ciobanu (Contract).

Authorized Budget (BA): FY05, FY06, FY07:

FY05 BA - $700K **FY06 BA** - $700K **FY07 BA** - $700K

Laboratory Name: Brookhaven National Laboratory
B&R Code KC0202020

FWP and possible subtask under FWP:
Spectroscopic Imaging STM Studies of Atomic Scale Electronic Structure in Transition Metal Oxides

FWP Number: PM-007

Program Scope:
Spectroscopic Imaging Scanning Tunneling Microscopy (SI-STM) allows the energy-resolved density-of-electronic-states (*LDOS(E)*) of complex electronic materials to be imaged with atomic-resolution. Since, one is essentially imaging the electronic wavefunctions; SI-STM is being developed under this FWP as a key tool for development and study of advanced magnetic/electronic materials, because it reveals directly the impact on atomic-scale electronic structure of dopant profiles, crystalline disorder, electron lattice interactions and electronic/magnetic phase transitions.

Major Program Achievements (over duration of support):

1. Combined ARPES and STM imaging of electronic structure of striped LBCO at 1/8 doping. 'The Ground State of Pseudogap in Cuprates: $La_{1.875}Ba_{0.125}CuO_4$ '(**Science** 314, pp. 1914 – 1916 (2006)).
2. Discovery of spatial structure of the electronic glass occurring at low doping in cuprates – direct evidence for nanostripes. 'An Intrinsic Bond-Centered Electronic Glass with Unidirectional Domains in Underdoped Cuprates' (**Science** 315., pp. 1380 – 1385 (2006)).
3. Discovery of quasiparticle interference and measurement of superconducting energy gap in a new cuprate 'Quasiparticle interference and superconducting gap in $Ca_{2-x}Na_xCuO_2Cl_2$ ' (**Nature Physics,** Online 28 October 2007 | doi:10.1038/nphys753).
4. Direct imaging of impact on cuprate superconductivity of varying inter-atomic distances within individual crystal unit-cells in $Bi_2Sr_2CaCu_2O_{8+\delta}$.
5. Discovery and parameterization of the evolution of the electronic excitation spectrum with strongly diminishing hole-density in $Bi_2Sr_2CaCu_2O_{8+\delta}$.
6. Discovery of Quasiparticle Extinction in $Bi_2Sr_2CaCu_2O_{8+\square}$.

Program impact:
Fundamental new understanding of the pseudogap state, striped state, electronic cluster glass state and quasiparticle interference in cuprates.

Interactions:
Dr. T. Valla, Dr. I. Bozovic, Dr. G. Gu, Dr. A. Tsvelik: BNL
Prof. D.-H. Lee LBNL.
Dr. A. V. Balatsky, LANL.
Prof. P. Hirschfeld University of Florida.
Prof. S. Uchida Tokyo University, Japan.
Dr. H. Eisaki AIST, Tsukuba, Japan.
Prof. H. Takagi RIKEN, Tokyo, Japan.
Prof. A. P. Mackenzie St. Andrew's University, Scotland

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Physics Today Story: Dec 2007, pp, 17.
17 Invited talks at National and International meetings in FY07

Personnel Commitments for FY2007 to Nearest +/- 10%:
Dr. Jinho Lee (BNL) 100%, Dr. K. Fujita (Cornell) 100%.

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $0 **FY06 BA $0** **FY07 BA $410K**

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC020203

FWP and possible subtask under FWP: BES Detailee / Materials Science and Engineering

FWP Number: NC-004

Program Scope: Support for Dr. James W. Davenport to serve as a detailee in the Office of Basic Energy Sciences in Germantown, Maryland at the rate of one quarter time for FY 07 beginning December 1, 2006 and half time for FY 08. He will be based at Brookhaven National Laboratory, but spend the detailee assignment partly at Germantown, partly at Brookhaven, or on travel as requested by BES.

To assist with the oversight of university grant research and various research coordination and planning activities, planning and reporting on workshops, and participation in site reviews as requested.

Major Program Achievements (over duration of support):

Program impact:
Assist with University Grant Program

Interactions:

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

Personnel Commitments for FY2007 to Nearest +/- 10%:
J. W. Davenport 25%

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $0 **FY06 BA $0** **FY07 BA $114,000**

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC-02-02-030

FWP and possible subtask under FWP: Electronic Properties of Transition-Metal-Compound Nanotubes
FWP Number: PM-002

Program Scope:

The emphasis of our research program is on electronic properties of transition-metal-compound nanotubes. The main topics are:

- Theoretical study of low-energy electronic structure and excitations of TMO- and TMD-nanotubes.
- Nano-scale many-body effects in strongly correlated bulk materials
- Theoretical development of advanced first-principles based numerical methods for strongly correlated systems

Major Program Achievements (over duration of support):

Discovery and Identification of the important role of nano-scale disorder in $CaCu_3Ti_4O_{12}$ and their potential role in explaining the record-high dielectric properties (in collaboration with BNL-CFN TEM group).

Observation and Analysis of inter-layer collective charge excitation (previously predicted by the PI) in MgB_2 and its unusual long lifetime into the continuum at large momenta (in collaboration with NSRR X-ray group at Spring-8).

Explaining the small charge disproportion of half-doped manganites and reconcile it with the 3+/4+ picture of charge-orbital ordering. Quantification of electron and lattice interactions for orbital and charge order in manganites.

Investigation of material dependence of high-T_c cuprates, identification of essential roles of apical oxygen atoms, and discovery of a novel super-repulsion effect that weakens the strength of local pairing.

Investigation of localization of carriers in the crossing of nano-wires (in collaboration with U. of Utah group).

Discovery and Explanation of magnetic memory effects in ultrathin paladium and platinum nanowires (in collaboration of CFN synthesis group)

Analysis of charge excitations in arrays of carbon nanotubes (in collaboration with X-ray group)

Explanation of gapless CDW in dichalcogenides, and initial investigation of electron-phonon interactions and their implications in the nanotube geometry.

Development of bi-orthogonal wavelet based minimization method for O(N) DFT calculation of nano-materials

Construction of a systematic technique of quantitatively mapping out the relevant interactions in strongly correlated system, based on first-principles Wannier functions.

Development of dynamical linear response theory of LDA+U functional and implementation in local Wannier functions.

Development of a new "super-atom" technique to derive low-energy effective Hamiltonian in strongly interacting multi-orbital system.

Development of real-space method for the study of local excitons ideal for study of excitons in nano-materials; formulation of two-particle effective hopping approach to describe exciton propagation.

Devised a new model Hamiltonian for hole-doped copper oxide superconductors intermediate between 1 and 3 band Hubbard models which will enable detailed comparisons with STM spectral functions distinguishing between Cu and O sites using time dependent density matrix renormalization group methods.

Program impact:

Provided many insights into nano-scale behavior of strongly correlated systems and their excitations.

Interactions:

Internal: CFN TEM group (Y. Zhu), CFN synthesis group (W. Han), CMPMSD X-ray group (J. Hill)

External: University of California, Irvine (Prof. S.R. White), Harvard University (Prof. E. Demler), ORNL (B.C. Larson), NSRR, Taiwan(Y. Q. Cai), University of Illinois Urbana-Champaign (Prof. P. Abbamonte), University of Wisconsin (Prof. A. Chubukov), University of Erlangen- Nürnberg (Prof. O. Pankratov), University of Utah (Prof. D. Mattis), Tamkang University, Taiwan (Prof. H.-C. Hsueh), University of Tennessee (Prof. A.G. Eguiluz)

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

No. of invited Talks: 17 (Wei Ku); 3 (Weiguo Yin) [over lifetime of FWP]

Personnel Commitments for FY2007 to Nearest +/- 10%:

Wei Ku (principle investigator) 10%	Chi-Cheng Lee (postdoc) 30%	Yucel Yildirim (postdoc) 10%
Weiguo Yin (assist. physicist) 100%	Tom Berlijn (SBU student) 100%	William Garber (postdoc) 30%
S. White (UC Irvine) 10%	Shiu Liu (UCI student) 30%	

Authorized Budget (BA) for FY05, FY06, FY07:

FY05 BA 0 K **FY06 BA 410 K** **FY07 BA 410 K**

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202030

FWP and possible subtask under FWP:
Condensed Matter Theory
FWP Number: PO-015
Program Scope:
The emphasis of our research program is on strongly correlated electron systems and on statistical mechanics of complex systems. Our main topics include:
Theoretical studies of quantum and classical condensed matter systems with extensions to nano-systems.
Development and application of advanced *ab initio* methods in physics of strongly correlated systems.
Understanding the statistical and dynamical properties, noise and fluctuations in complex (particularly biological) systems and their underlying networks.
Major Program Achievements (over duration of support):
Development of a phenomenological theory of the pseudogap state in copper oxide superconductors. Application of this theory to LBCO. Description of the first ever observed Bereziskii-Kosterlitz-Thouless transition in a bulk material.Testing of a semi-numerical method combining exactly solvability with a numerical renormalization group for the calculation of spectra and wave functions of coupled of quasi-one-dimensional strongly interacting systems (including quantum dots, coupled chain systems and perturbed integrable systems). Development of a technique to compute the exact finite temperature behavior of response functions in one dimensional spin chains. Demonstration of the exact solvability of a number of quantum dot systems.
Discovery and explanation of strong anisotropy of local excitons in NiO and CoO, establishing a new utilization of non-resonant X-ray scattering in the study of sub-nano-scale excitations. Observation of the inter-layer collective charge excitation (previously predicted by Wei Ku) in MgB_2 and analysis of its unusual long lifetime. Developed a Wannier picture reconciling 3+/4+ picture with small charge disproportion in half-doped manganites, and quantifying the essential rule of electron interactions in charge ordering. Uncovered material dependence of high-T_c cuprates, identified crucial roles of apical oxygen atoms, and discovered a novel "super-repulsion" that weakens local pairing.
Noise and fluctuations in protein binding networks were quantified using the Fluctuation-Dissipation Theorem. The propagation of small perturbations was elucidated using an analogy with current flow in disordered conductors. Two novel algorithms aimed at 1) prediction and verification of indirect interactions and 2) detection of the dominant direction of information flow in densely interconnected regulatory networks were developed and optimized.
A new low frequency regime of coherent semiclassical dynamics of persistent current qubit was analyzed and a model describing experimental data was developed. Dirac vacuum reconstruction in the vicinity of a charged impurity and its implications for transport measurements was analyzed.
Program impact:
Provided numerous insights into behavior of strongly correlated systems and properties of complex networks.
Interactions:
Internal: Electron Spectroscopy, X-ray Scattering, Neutron Scattering, Powder Diffraction, CFN, CSC, Biology Dept.External: Columbia U. (B. Altshuler and I. Aleiner), ETH Zurich (T. M. Rice), MIT (L. Levitov, T. P. Orlando, Dr. W. D. Oliver), U. Wisconsin (A. Chubukov), ICTP and SISSA, Trieste, Italy (V. Kravtsov, A. Nersesyan), Stony Brook U. (A. Abanov), U. of Dusseldorf (R. Egger, Dr. de Martino), Rutgers U. (S. Lukyanov), Niels Bohr Institute, (K. Sneppen,, S. Krishna), Ariadne Genomics (I. Mazo, Y. Ispolatov, A. Yur'ev, E. Kotelnikova), U.. of Paris (B. Roehner, G. Shlyapnikov, P. Azaria), U. of Fribourg, Switzerland (Y.-C. Zhang, M. Blattner), U. of California, Irvine (Prof. S.R. White), ORNL (B.C. Larson), NSRR, Taiwan(Y. Q. Cai), Harvard U. (E. Shakhnovich, S. Zhang), Boston U. (S. Redner. P. Chen), J.-S. Caux (U. of Amersterdam), A. Ludwig (UCSB). H. Saleur (Saclay/USC), A. Gogolin (Imperial College), F. Essler (Oxford U.), M. J. Bhaseen (Cambridge U.), M.Katsnelson (U. Nihmegen)
Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
One Fellow of American Physical Society; 2006 Brookhaven Science and Technology Award (Tsvelik)
No. of invited Talks: 30 (A. Tsvelik), 23 (S. Maslov), 12 (R. Konik), 25 (W. Ku), 5 (A. Chitov) [over lifetime of FWP]
Personnel Commitments for FY2006 to Nearest +/- 10%:
A.M. Tsvelik (group leader) 100%; S. Maslov 70%; K-K Yan (student) 90%; Wei Ku 90%; R. Konik 100%; D. Voljia (student) 100%; A. Chitov 100%; S. Reyes (student) 100%; D. Walker (student) 100%
Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA 1,450 K **FY06 BA 1,450 K** **FY07 BA 1,450 K**

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0203010

FWP and possible subtask under FWP: Biology-inspired programmable assembly of functional nano-structures.

FWP Number: MA-114-MAEA

Program Scope:
There is a great demand for developing approaches for a large scale assembly with nanometer precision. Our approach utilizes a strategy of a bio-programmable assembly, in which biomolecules with highly selective interactions, like DNA and proteins, guide an assembly of inorganic nano-components. The main approaches are based on (i) adopting the addressable, "key-lock" interactions of biomolecules to nano-environments; (ii) understanding and incorporation of diverse physical interactions, entropic effects, and energetic landscapes of biomolecules; (iii) and developing methods for tailoring biomolecular structures. Our research strategy combines the development of methods for the assembly of nano-architectures with exploration of their microscopic structures using electron and atomic force microscopies, x-ray and light scattering, and optical spectroscopy.

Major Program Achievements (over duration of support):
1. Our studies of DNA functionalized micron and nano-sized particles has been focused on the development of novel approaches to regulate interaction between DNA functionalized particles. We developed new approach for tuning the interactions between particles. Our theoretical estimation is in agreement with experiment. This approach allows a gradual change of the assembly rate or aggregate sizes for fixed physical conditions by incorporation of non-hybridizing "neutral" DNA strands into particle's shell.
2. DNA hybridization was utilized as a reversible, chemically weak and a highly selective way to assemble nanoparticles on surfaces. We studied in-situ the assembly kinetics of the DNA-capped nanoparticles on surfaces covered with complementary DNA, as well as the structural changes with temperature in the resulting 2D DNA/nanoparticle system. Using high energy x-ray reflectivity, the microscopic structure of the 2D particle assembly was probed directly, while AFM and SEM were used to confirm the local particle's arrangement at the surface.
3. By tailoring the design of the DNA shell the interparticle potential was modulated and the formation of 3D nanoparticle assemblies with crystalline long range order was discovered using synchrotron based SAXS measurements. The crystalline assemblies are thermodynamically reversible and temperature-tunable, with body centered cubic lattices, where particles occupy only ~4% of the unit cell. The DNA design and thermodynamic pathway leading to the crystallization of particles has been explored, thus, opening the way for creation of new classes of nanoscale metamaterials.
4. We investigated the biocompatibility, specificity, and activity of a ligand-receptor protein system covalently bound to oxidized single-walled carbon nanotubes (SWNTs) as a model proof-of-concept for employing such SWNTs as biosensors. SWNTs were functionalized under ambient conditions with either the Knob protein domain from adenovirus, or its human cellular receptor, the CAR protein. We confirmed the biological activity of Knob proteins immobilized on the nanotube surfaces using its labeled conjugate antibody. In addition, current-gate voltage (I-V) measurements on a dozen nanotube devices explored the effect of protein binding on the intrinsic electronic properties of the SWNTs

Program impact:
Understanding the assembling of nano-materials in ordered and pre-designed structures will enable a broad array of applications in energy and environmental security.

Interactions:
Internal: BNL-Biology, BNL – MSD/CMP, BNL-Medical
External: University of Michigan, University of Illinois, Stony Brook University, University of Pennsylvania.

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

Personnel Commitments for FY2007 to Nearest +/- 10%:
Oleg Gang (PI) 17%; Daniel van der Lelie (PI): 10%; Zhang (professional) 30%; Mathew Maye (postdoc) 15%; Huiming Xiong (postdoc) 40%

Authorized Budget (BA):
FY05 BA - $360K **FY06 BA** - $345K **FY07 BA** - $345K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0203010

FWP and possible subtask under FWP: Condensed Matter Physics and Materials Science—Soft Matter
FWP Number: PO-034
Program Scope: The primary goal of the group is to understand the effects of nanoscale confinement and the role of self-assembly in soft materials through the use of patterned templates and well-defined interfaces. We use synchrotron x-ray scattering, scanning probe and optical microscopy techniques to study fundamental properties of complex fluids, simple liquids, macromolecular assemblies, liquid crystals, polymers, and biomolecular materials. The challenges are (1) to understand liquids under nano-confinement, (2) how templates and confinement can be used to direct the assembly of biomolecular materials, nanoparticles and diblock copolymer thin films, (3) to understand the fundamental interactions which give rise to similar self-assembly behaviour for a wide variety of systems, (4) how the order correlates with function.

Major Program Achievements:

- First verification of shape and size dependent wetting of ethanol on chemically nanopatterned (50-300 nm) lines prepared by oxidation nano-lithography under controlled equilibrium vapor conditions (PRL, 2006). Extended studies, using improved AFM environmental cell, to cyclohexane drops.
- Demonstrated that AFM can be used to investigate the real time flow of liquids on chemical patterns.
- Utilized AFM to measure changes in morphology and hygroscopicity as a function of the relative humidity for sodium chloride aerosols (50-200 nm) deposited on substrates with differing surface energy.
- Demonstrated the ability to laterally confine and orient diblock copolymer thin-films by using chemical patterns prepared using oxidation nano-lithography. Extended studies to both filled and unfilled patterns.
- Carried out first wetting studies using GISAXS on e-beam prepared topographical patterns with 35 nm features.
- Demonstrated that the reported "hydroscopic gap", observed at methyl-terminated surface solid interface, originates from the low electron density of the methyl group & possibly from water layering and not from water depletion.
- Observed apparent optimal charge density for creating ordered arrays of tobacco mosaic virus (TMV) at buried substrate/lipid/buffer interfaces. Also found substrate fluidity to be critical for developing structural order.
- Lipid monolayer-assisted 2D assembly of aligned TMV rods observed with GISAXS and Brewster angle microscopy (BAM) at the solution-vapor interface.
- GISAXS and BAM study demonstrated the existence of a threshhold surface biotin density for 2D crystallization of streptavidin on a biotinylated lipid monolayer at the solution-vapor interface.
- Obtained FRAP results that suggests different lateral diffusion coefficients in the two "monolayer" leaflets of the same substrate-supported bilayer.
- Completed x-ray reflectivity study of liquid crystal surfaces coated by fluorocarbon wetting films to demonstrate complete wetting and induced smectic layering at a nematic-fluorocarbon liquid interface.

Program Impact: The Group's work has clearly demonstrated the important role that nanopatterned surfaces and templates play in controlling the behavior of liquid, and the assembly of biomolecular materials and polymer films. Studies confirm long-standing theoretical prediction on the effects of the Disjoining pressure on the shape and size of nanodrops. Recognized by invited talk at the Int. Stat Phys (theory) Conf. The x-ray work at buried liquid interfaces is helping to provide a structural basis for a wide array of interdisciplinary problems ranging from protein crystallization to molecular electronics. Electro Pen Nanolithography provides a new method for chemically patterning surfaces.
Interactions: The researchers in the group have significant scientific overlap and interactions with scientist at the National Synchrotron Light Source and the Center for Functional Nanomaterials and with university collaborators.
Recognitions, Honors and Awards (at least partly attributable to support under this FWP/subtask):
Invited Talks 5, Antonio Checco received the Pierre Favard 2005 award for the best PhD thesis in Microscopy between 2002-2005. This award is given by the French Society of Microscopy. Brookhaven Science and Technology Award and APS Fellow– B. Ocko.

Personnel Commitments for FY2007: Masa Fukuto(100%), Antonio Checco (100%), Lin Yang (.05%), Suntao Wang (.8%), Tommy Hoffman (100%), Sumit Kewalramani (10%), Htay Hlaing (20%), Ron Pindak (.02%), Brandon Chapman (.08%).

Authorized Budget (BA): FY05 BA - $655K **FY06 BA** - $630K **FY07 BA** - $630K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0203010

FWP and possible subtask under FWP:
BES Detailee / Materials Chemistry and Biomolecular Materials

FWP Number: PM-008

Program Scope: Support for Dr. James McBreen to serve as a detailee in the Office of Basic Energy Sciences in Germantown, Maryland at the rate of one half time for one year beginning July 1, 2007. He will be based at Brookhaven National Laboratory, but spend the detailee assignment in Germantown or on travel as requested by BES.

To assist with the processing of proposals for university grant research and various research coordination and planning activities, planning and reporting on workshops, and participation in site reviews as requested.

Major Program Achievements (over duration of support):

Program impact:
Assist with University Grant Program

Interactions:

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

Personnel Commitments for FY2007 to Nearest +/- 10%:
J. McBreen 50%

Authorized Budget (BA) for FY05, FY06, FY07:

FY05 BA $0 **FY06 BA $0** **FY07 BA $161K**