FWP Summaries

Materials Science Division

Argonne National Laboratory

December 2007

B&R Code	FWP	Title
KC020101	58931	Atomic Scale Elemental Imaging in Three-Dimensions
KC020103	58307	Interfacial Materials
KC020103	58930	Proximity Effects in Complex Oxide Heterostructures
KC020105	58502	Digital Synthesis
KC020201	58701	Neutron and X-ray Scattering
KC020201	58926	Synchrotron Radiation Studies
KC020202	58806	Dynamics of Granular Materials
KC020202	58906	Superconductivity and Magnetism
KC020202	58916	Emerging Materials
KC020202	58918	Magnetic Thin Films
KC020202	58920	Digital Synthesis (text combined with FWP 58502)
KC020203	59001	Condensed Matter Theory
KC020203	59002	Materials Theory Institute
KC020203	59003	Quantum Computation with Electron Spins
KC020301	57504	Nanostructured Thin Films
KC020301	57525	Nanostructured Biocomposite Materials for Energy Transduction
KC020301	58510	Molecular Materials
KC020301	58600	Directed Energy Interactions with Surfaces
KC020301	58601	Fundamental Studies of Electrocatalysis for Low Temperature Fuel Cell Cathodes
KC020301	58806-CD	Collective Dynamics, Self-Assembly and Mixing in Active Microparticle Ensembles

Laboratory Name: Argonne National Laboratory
B&R Code: KC020101

FWP and possible subtask under FWP: Atomic Scale Elemental Imaging in Three-Dimensions

FWP Number: 58931

Program Scope: This goal of this program is to develop an understanding of the role that interface morphology and composition play in determining the functional properties of nanostructured materials. In this program we are addressing this issue via atomic-scale three-dimensional chemical imaging of interfaces in nanostructures. To do this we are developing atomic-scale three-dimensional chemical imaging capabilities via the use of electron tomography combined with electron energy loss spectroscopy (EELS) and transmission electron microscopy (TEM). The eventual aim is to reconstruct the chemical distribution in a single nanostructure or in arrays of nanostructures at high resolution. Our approach is based on analytical transmission electron microscopy techniques such as EELS and energy filtering TEM (EFTEM), which are being coupled with advances in data reconstruction to improve resolution, sensitivity and validity of data interpretation beyond what is currently available.

Major Program Achievements (over duration of support):
Sample preparation techniques (focused ion-beam (FIB) milling and low-angle, low-energy ion sputtering) have been optimized to achieve flat samples, which are thin enough to allow high resolution for elemental mapping and structure imaging. The surface damage layers (damaged by the FIB Ga-beam) were removed with the low-angle, low-energy ion sputtering. The quality of the samples is high as required for EFTEM tomography experiments. Parallel to these efforts in sample preparation we have carried out software updates to our Tecnai F20 (200kV, FEG) to enable tomography. This includes installing programs for remotely controlling the specimen stage, microscope and CCD camera for acquisition of tilt series. A stage was purchased from Hummingbird Inc., which has been customized with a low-expansion shaft to minimize sample drift during the tilt experiments and this has proved very effective for the tomography experiments. Tests with this stage showed that the specified tilt range of ±80° could be achieved (compared to ±40° with conventional stages).

Cross-section samples of ultrananocrystalline diamond (UNCD) on Si and Pt/$PbZrTiO_3$/Pt/TaAlO/UNCD on Si were analyzed, and high-resolution TEM images, for atomic scale interface characterization, and EFTEM images, for elemental mapping with a resolution from 0.6nm to 1.0nm, were recorded. Chemical bonding information at the interfaces between the UNCD and the Si was obtained from the spectrum-image series, which enabled the differences between carbon sp^2 and sp^3 bonding to be imaged.

More recently we have been concentrating on analysis of 10 nm diameter TiO_2 nanoparticles. The three-dimensional structure of clusters of TiO_2 nanoparticles has been successfully reconstructed from tilt series of zero-loss EFTEM images. This was carried out using the "IMOD" software installed on a fast Windows-based system. In addition to studies of TiO_2 nanoparticles, the three-dimensional structure of clusters of Co nanoparticles has also been reconstructed.

Program Impact: Providing materials to meet the challenges of novel nanoscale structures requires atomic-level knowledge of the interfaces and surfaces in order to predict and control their physical properties. By contributing to a detailed understanding of the chemical origins of the physical properties of materials at the atomic scale, this program will aid both basic scientific knowledge of the materials and also lead to new designs for future nanotechnological applications.

Interactions: Internal: Electron Microscopy Center (ANL58405), Interfacial Materials Group (ANL58307), Center for Nanoscale Materials; External: Carnegie Mellon University.

Recognitions, Honors and Awards (fully or partially supported by this FWP or subtask):

Personnel Commitments for FY2007 to Nearest +/-10%:
A Petford-Long (20%) B Kabius (20%), X Zhong (postdoc, 100%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $0 **FY06 BA $**140K **FY07 BA $**400K

Laboratory Name: Argonne National Laboratory
B&R Code: KC020103

FWP and possible subtask under FWP: Interfacial Materials

FWP Number: 58307 (including FWP 58305 through Sept. 2005)

Program Scope: This program combines advanced materials synthesis, complementary *in situ* and *ex situ* characterization and property measurement techniques with computer simulations to elucidate the interfacial contributions to novel phenomena exhibited by thin film oxide heterostructures. The program is structured around three themes: interface control through understanding growth dynamics in complex oxide films, the contribution of interfaces when oxide films are incorporated in heterostructures and developing an understanding of domain behavior in ferroic nanostructures as a function of microstructure and composition. The complementary strengths of simulation and experiment provide fundamental insights into the mechanisms and interfacial driving forces that control composition and microstructure and thus overall film properties.

Major Program Achievements (over duration of support):
In situ studies of ferroelectric thin films: Using a unique integrated MOCVD film growth, x-ray scattering and fluorescence facility that we developed at the Advanced Photon Source in collaboration with G.B. Stephenson and P.H. Fuoss (ANL 58926), we observed ferroelectricity in epitaxial $PbTiO_3$ (PTO) films as thin as three unit cells at room temperature (the thinnest perovskite film to exhibit spontaneous polarization). Our studies also showed that 180° stripe domains form to compensate the depolarizing field in films grown on insulating substrates, and this has been extended to our recent discovery that for PTO films grown on conducting substrates, the polarization direction in monodomain films can be switched through control of the oxygen partial pressure above the film surface.
Atomistic simulation of ferroelectric perovskites: The first interatomic potentials capturing ferroelectricity in perovskites, including the full phase diagram, were developed and used to study solid solutions and heterostructures. The influence of epitaxial strain on polar properties of thin perovskite-ferroelectric films and superlattices was investigated with first-principles computational techniques, demonstrating for the first time that strong coupling between polarization and strain is not a universal feature of all perovskite-oxide ferroelectrics.
Studies of complex oxide phenomena at the micro and nanoscale: In collaboration with L. Ocola (CNM), we are investigating photovoltaic phenomena in transparent $ITO/LaNiO_3/Pb(Zr_x,Ti_{1-x})O_3/LaNiO_3/ITO$ capacitors grown on glass. First measurements have shown up to three orders of magnitude higher current out of the device upon sunlight illumination, with respect to the current measured without illumination, most likely as a result of efficient hole-electron pair separation resulting from the electric field induced in the polarized ferroelectric PZT layer.
Integration and patterning of oxide heterostructures: Integrating layers of piezoelectric $Pb(Zr_x,Ti_{1-x})O_3$ and ultrananocrystalline diamond enabled the development of piezoactuated diamond-based microelectromechanical-nanoelectromechanical system structures, opening new avenues for fundamental studies of the mechanical properties of these novel heterostructures.
In situ transport studies of tunnel junction structures at the nanoscale: We have developed a unique system for making nanoscale transport measurements whilst simultaneously imaging the same region in-situ in the TEM. This allows determining the structural and chemical origins of local changes to the transport properties in magnetic tunnel junctions.

Program Impact: By combining advanced experimental tools and simulation, we have developed an unprecedented understanding of the impact of microstructure including interfaces on material behavior in functional oxide heterostructures. We have established metal-organic chemical vapor deposition as a premier method for the fabrication of high-quality complex oxide films and have developed a sophisticated range of analysis tools for characterizing domain and transport behavior at the nanoscale.

Interactions: Internal: Synchrotron Radiation Science (ANL58926), Electron Microscopy Center (ANL58405), Conducting Oxide Heterostructures (ANL58930), Molecular Control of Synthesis (ANL57504), Advanced Photon Source, Center for Nanoscale Materials; External: 16 universities in the US, Argentina, Germany, and UK,; LBL, industry including INTEL, Seagate and IBM.

Recognitions, Honors and Awards (fully or partially supported by this FWP or subtask): Auciello: 2003 Hispanic Engineering Award, 2003 R&D 100 Award, 2006 Federal Lab Consortium Award.

Personnel Commitments for FY2007 to Nearest +/-10%: A. Petford-Long (Group Leader: 100%) O. Auciello (75% (25% CNM)), S. Nakhmanson (100%), G. Bai (100%), L. Thompson (80%), P. Baldo (50%), J. Eastman (30%), M. Tanase (postdoc, 50%).

Authorized Budget (BA) for FY05, FY06, FY07:
FWP58307: **FY05 BA** $1,925 **FY06 BA** $1,735 **FY07 BA** $1,887
FWP58305: **FY05** joined to FWP 58307

Laboratory Name: Argonne National Laboratory
B&R Code: KC020103

FWP and possible subtask under FWP: Proximity Effects in Conducting Oxide Heterostructures

FWP Number: 58930

Program Scope: This is a provisional program, redirected in FY07 and pending approval by BES. The new program strives to create, characterize, and understand thin film oxide heterostructures that exhibit novel ionic, electronic, or mixed conduction properties. By exploiting *proximity effects* induced by heterointerfaces through *space charge*, *elastic strain*, and *interfacial atomic structure*, we are creating new materials with controllable properties that are unattainable in bulk materials. These proximity effects are systematically varied by judiciously selecting cation species with desired size and valence *for each atomic plane*, and are amplified in heterostructures when layer spacings are reduced below distances where electronic charges strongly interact or strain-fields overlap. Synthetically engineered heterostructures are assembled by atomic layer deposition (ALD), metal-organic chemical vapor deposition (MOCVD), and molecular beam epitaxy (MBE), techniques with the potential to provide precise control of each atomic plane in a growing heterostructure. We are exploiting the unique capability of *in situ* synchrotron x-ray techniques to determine depth-resolved atomic-level structure and film composition in *real-time*, in the near-atmospheric pressure, elevated temperature environments that are integral to growth and transport behavior. Multi-scale simulations are providing understanding of the factors that control strain, composition, and structure during growth, are playing a key role in identifying and elucidating charge transport mechanisms, and are facilitating the development of predictive models for the design of oxide heterostructures with emergent properties.

Major Program Achievements (over duration of support): Although the program has not yet been approved and thus has no formal achievements, we have explored promising research directions with initial studies on epitaxially-strained two-phase nanocomposite oxide heterostructures that phase-separate during growth to form nanolamellae, nanopillars, or nanodots embedded in single crystal thin film matrices. We have succeeded in creating epitaxial nanocomposites of yttria-stabilized zirconia (YSZ) nanolamellae embedded in a matrix of indium oxide (In_2O_3) on single crystal YSZ substrates. Synchrotron x-ray characterization has revealed that the two phases remain lattice-matched in the plane of the film during thermal cycling, but surprisingly, the out-of-plane thermal expansion of the YSZ component of the film is substantially smaller than that of both the substrate of the same material and the In_2O_3 film component, leading to a strain state in the film that is expected to substantially impact conduction behavior. Density functional theory calculations have revealed significant differences in the density of states in ZrO_2/In_2O_3 heterostructures compared with either bulk material. These simulations predict that the heterostructure band gap is reduced, leading to enhanced conductivity, while optical transparency is only slightly reduced. This demonstrates the possibility of creating improved transparent conductors based on oxide heterostructures.

Program impact: Reduction of heterostructure layer spacings below characteristic length scales associated with transport phenomena is expected to result in emergent properties not intrinsically found in the basic building blocks. By understanding and controlling space charge, strain, and interfacial structure, materials with enhanced ionic or electronic conduction properties can be created. The coupling of conduction behavior with other properties such as optical transparency or thermoelectric behavior is also of great importance, and insight into this coupling is obtainable through investigation of oxide heterostructures. I*n situ* x-ray techniques also provide a unique means of advancing understanding of growth processes during ALD, oxide MBE, and MOCVD.

Interactions: Internal: Synchrotron Radiation Science (ANL58926), Molecular Materials (ANL58510), Interfacial Materials (ANL58307), Electron Microscopy Center (ANL58405), Advanced Photon Source, Center for Nanoscale Materials; External: Pennsylvania State University, Northwestern University, Carnegie-Mellon University, University of Illinois-Urbana Champaign, Oakland University.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): The PIs have presented more than 35 invited talks at major national and international conferences in the past three years.

Personnel Commitments for FY2007 to Nearest +/- 10%: P. Baldo (50%), A. Bhattacharya (25%), J.A. Eastman (70%), D.D. Fong (100%), P.H. Fuoss (25%), H. Iddir (Postdoc, 100%), G.B. Stephenson (25%), L.J. Thompson (20%), P. Zapol (25%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA \$1,340K **FY06 BA** \$1,313K **FY07 BA** \$1,313K

Laboratory Name: Argonne
B&R Code: KC020105 and KC020202

FWP and possible subtask under FWP:
Digital Synthesis: A Novel Pathway to New Collective States in the Complex Oxides

FWP Number: 58502 and 58920

Program Scope:
In our program, we create, characterize, control and understand novel states of condensed matter at interfaces of complex oxides using *digital synthesis*. These strategies enable the realization and control of a new generation of interfacial systems whose singular characteristic is that they have no explicit chemical disorder. Ordered, undoped layers are stacked in integer sequences, and all charge transfer or doping takes place at ordered interfaces via charge reconstruction and polarizing electrostatic fields. Underlying this effort is our emphasis on connecting the microscopic reconstruction of magnetic, charge and orbital order at these interfaces to the emergent properties of the materials at macroscopic length scales.

Major Program Achievements (over duration of support):
The role of disorder upon the emergence of collective states forms a central theme of our research. We have observed signatures of enhanced antiferromagnetic ordering temperatures in digital superlattices of $(LaMnO_3)_m/(SrMnO_3)_{2m}$, where m=1-4, equivalent to $La_{1/3}Sr_{2/3}MnO_3$, where the *A*-site disorder has been eliminated. These were synthesized using ozone-assisted oxide molecular beam epitaxy (MBE).
We have observed a causal connection between emergent transport properties and the microscopic magnetic structure in double-exchange superlattices. Using polarized neutron reflectometry, we have determined the magnetic structure of digital superlatices of $(LaMnO_3)_{2n}/(SrMnO_3)_n$, and shown that the metal-insulator transition in these structures is related to the underlying magnetic structure, where the insulating state has strongly modulated ferromagnetic order, and the metal is a uniform ferromagnet. This is evidence for a Mott-transition driven by the distance between $LaMnO_3/SrMnO_3$ interfaces.

The transfer of holes from the antiferromagnetic insulator $SrMnO_3$ to $LaMnO_3$ is believed to be the underlying cause for the observation of ferromagnetic metallic behavior in $(LaMnO_3)_{2n}/(SrMnO_3)_n$ superlattices. Resonant x-ray scattering has enabled us to obtain the first direct evidence for interfacial charge reconstruction near the Fermi energy across a $LaMnO_3/SrMnO_3$ interface accompanying ferromagnetic ordering. This was achieved in $(LaMnO_3)_8/(SrMnO_3)_4$ superlattices.

Program impact:
This new program has generated interest due to the novel possibilities for creating new materials by tailoring the reconstruction of charge, spin and orbital degrees of freedom at interfaces. We have had five invited talks in FY07, and numerous contributed presentations at major international conferences. We have designed and commissioned a state-of-the art, ozone-assisted oxide MBE facility that is now being used to synthesize digital superlattices at Argonne's Center for Nanoscale Materials.

Interactions:
Argonne: Center for Nanoscale Materials, Materials Theory Institute and Advanced Photon Source.
External: LANSCE at Los Alamos, UIUC Departments of Physics and of Materials Science and Engineering, Department of Applied Science at College of William and Mary, and Northeastern University.

Recognitions, Honors and Awards (partly attributable to support under this FWP or subtask):
Sam Bader was awarded the 2007 APS David Adler Lectureship Award in the Field of Materials Physics.

Personnel Commitments for FY2007 to Nearest +/- 10%:
Anand Bhattacharya – PI (100% until July 2007, 25% afterwards); Sam Bader (10%); Steven May – Postdoc (100%)
External Subcontracts: Prof. James N. Eckstein, UIUC for $96,156.0; Prof. J.-M. Zuo, UIUC for $57,800.0; Prof. Laura Lewis, Northeastern University for $100,000.

Authorized Budget (BA) for FY05, FY06, FY07: Program began in late FY06.
FY05 BA $0 **FY06 BA** $720K **FY07 BA** $720K

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

FWP and possible subtask under FWP: Neutron and X-ray Scattering

FWP Number: 58701

Program Scope: Members of the Neutron and X-ray Scattering Group enable the Materials Science Division to pursue strong multidisciplinary research programs that combine state-of-the-art scattering capabilities with materials synthesis, theory, and other experimental tools. Worldwide neutron and x-ray scattering facilities are used but priority is given to research topics that anticipate the full capability of the Spallation Neutron Source. An important goal of the group is to strengthen the neutron user community in the US in preparation for the SNS, and we sponsor an annual summer school on neutron and x-ray scattering as a key part of our strategy. Group members also participate in the conception, design, and review of instrumentation for the SNS, and are responsible for a diffuse scattering instrument proposal funded as part of SING-II. More details are available at http://www.msd.anl.gov/groups/nxrs/.

Major Program Achievements (over duration of support): *Orbital Correlations, Frustration, and Self-Organization:* A comprehensive research program in layered manganites has provided the most detailed models of Jahn-Teller polaron correlations in any CMR compound. We are expanding this program to investigate the lattice dynamics and, in close collaboration with the Synchrotron X-ray and Theory groups, the electronic properties using Angle Resolved Photoemission in order to obtain a detailed understanding of the link between complex disorder and electronic excitations. We have also obtained new insights into spin-state transitions and the competition between long and short-range order in perovskite cobaltites and we continue a program to study the origin and influence of superstructures in the electron doped superconductors.

Magnetic Behavior in Constrained Geometries: Argonne scientists pioneered neutron reflectometry applying it to critical problems in polymer science and the magnetism of thin films and multilayers. Ongoing studies include exchange coupled superlattices and exchange bias in thin films. Recent projects have focused on understanding magnetic and electronic interactions at the interfaces between epitaxially grown complex oxide materials with different electronic and magnetic properties, such as ferromagnetic/superconducting superlattices.

Biological membranes: A new effort is being pursued to understand the structure/function relations of biological membranes using model biomembrane mimics which host biologically relevant membrane components. The understanding of lipid domain formation in lipid mixtures as well as understanding the phase diagram of lipidic mixtures which have potential in enabling membrane protein crystallization are the topics currently being pursued. This program will make effective use of new spin-echo techniques being developed by the group as well as existing facilities at the Advanced Photon Source.

SNS Instrument Concepts: Group members are developing two novel neutron scattering techniques, which are the basis for proposals to build dedicated SNS instruments. The first is Spin-Echo-Resolved Grazing Incidence Scattering, which is a new method for the study of biological and polymeric membranes. The second employs a correlation chopper to measure with high efficiency single-crystal diffuse scattering with elastic discrimination. A proposal to build an instrument based on this technique, *Corelli*, has been submitted and will be funded as part of the SING II project. Both methods promise to open up new directions in neutron scattering science.

Program Impact: Work of the group in many different science areas is recognized worldwide as leading the field and opening new research directions in neutron and x-ray scattering. Close interaction with materials synthesis, other experimental techniques, and theory is a particular strength of the group. The impact of research done by the group is demonstrated by 72 publications with 529 citations during 2004-2007.

Interactions: Group members collaborate with other groups in the Division and with a large number of scientists at universities and other national laboratories, as shown by over 200 coauthors on papers published 2004-2007.

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

J. D. Jorgensen: B. E. Warren Diffraction Physics Award (1991), C. E. Barrett Award in Powder Diffraction (1997), Among 100 most highly cited physicists (ISIhighlycited.com). G. P. Felcher: Humbolt Award, 1999, Fellow of the Neutron Scattering Society of America, R. Osborn & S. Rosenkranz: University of Chicago Distinguished Performance Award (2006). J. D. Jorgensen, G. P. Felcher & R. Osborn: Fellows of the American Physical Society

Personnel Commitments for FY2007 to Nearest +/-10%: R. Osborn (Group Leader) (100%), G. P. Felcher (100%), U. Perez-Salas (100%), S. Rosenkranz (100%), S. G. E. te Velthuis (100%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $2613K **FY06 BA $**2477K **FY07 BA $**2562K

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

FWP and possible subtask under FWP:
Synchrotron Radiation Studies

FWP Number: 58926

Program Scope: This program develops new capabilities using the nation's synchrotron radiation facilities and applies them to key problems in materials science. In particular, we aim to play a leading scientific role at the Advanced Photon Source (APS). X-ray scattering studies take advantage of the high brilliance APS x-ray source for in-situ studies of synthesis and structure of ultrathin films of complex oxides, and interfaces in electrochemical and catalytic systems. High-resolution angle-resolved photoemission is used to understand the nature of superconductivity in the High-T_c materials. Other thrusts focus on exploring science enabled by future facilities such as an x-ray nanoprobe, a high-energy photoemission facility, and a coherent, femtosecond x-ray source.

Major Program Achievements (over duration of support):
Vapor-Phase Epitaxy: We have used in situ x-ray scattering to understand the atomic-scale growth mechanisms and surface structures occurring during MOCVD growth of (In,Ga)N and $Pb(Zr,Ti)O_3$. Growth modes, surface reconstructions, and composition changes due to epitaxial strain relaxation have been mapped during growth.
Quasiparticles in High-T_c Superconductors. The nature of the carriers in high-T_c superconductors has been elucidated using angle-resolved photoemission. We have identified a particular point on the Fermi surface where the superconducting energy gap vanishes below T_c, and determined the nature of the excitations that dominate the properties of the system.
Nanoscale Ferroelectricity: The minimum system size needed to support ferroelectricity has long been a subject of debate. We have demonstrated ferroelectricity in the most confined perovskite system yet, $PbTiO_3$ films as thin as three unit cells. We have observed strong effects of electrical and chemical boundary conditions on polarization and surface structure
X-ray Studies of Catalysis Under Near Atmospheric Gas Pressure: Adsorption of CO is one of the most important issues in catalysis because of its poisoning of catalytic activity. Using innovative in situ x-ray techniques, we established the long-range-ordered nature of the CO overlayer on the Pt(111) surface under (near) atmospheric pressure of CO gas. A previously unobserved high-density structure was discovered, and a temperature-pressure phase diagram including the CO desorption boundary was determined.
Ultrafast X-ray Experiments: We have developed techniques for observing the interplay between electronic and structural dynamics on the femtosecond time scale using ultrafast x-ray pulses coupled with laser excitation. These studies using ultrafast x-ray pulses are providing part of the scientific basis for the next generation of accelerator-based x-ray sources.

Program Impact:
The Synchrotron Radiation Studies group publishes an average of 30 refereed articles every year, typically including 4 articles per year in Physical Review Letters, Science, or Nature. These articles are highly cited; based on citation rate, our average paper is in the top 1% of papers in materials science.

Interactions:
This project provides expertise in synchrotron techniques to collaborations with several Materials Science Div. groups, esp. FWP 59001 (Condensed Matter Theory), 58307 (Interfacial Materials) , 58930 (Proximity Effects in Complex Oxide Heterostructures, pending) and 58601 (Electroctalysis), other ANL Divisions (esp. CNM and APS), and with researchers at more than 30 universities, academic institutions, and industrial laboratories worldwide.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
J. C. Campuzano received the HENAAC Outstanding Technical Performance Award in 2007. Each year about two dozen invited talks are given by group members.

Personnel Commitments for FY2007 to Nearest +/- 10%:
Staff: J. C. Campuzano (50%), P. H. Fuoss (75%), N. Markovic (50%), H. You (70%), G.B. Stephenson (50%); Visiting Faculty: M. Bedzyk (10%); Postdocs: F. Jiang (50%), M. Pierce (100%), D. Hennessy (100%).

Authorized Budget (BA) for FY05, FY06, FY07:
FWP58926: **FY05:** **BA** $1,800K **FY06:** **BA** $1,660K **FY07:** **BA** $1,800K

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

FWP and possible subtask under FWP: Dynamics of Granular Materials

FWP Number: 58806

Program Scope: This program focuses on theoretical and experimental analysis of the physics of granular materials. We consider the experiments, the theory, and large-scale molecular dynamics simulations of partially fluidized granular flows in application to granular avalanches, effects of particles anisotropy on collective motion, and dynamic self-assembly of microparticles subject to electromagnetic field. New research directions were recently extended towards biological objects – self-organization and control of active bioparticles in confined geometries and physics of cytoskeleton formation.

Major Program Achievements (over duration of support):
Granular avalanche mobility and evolution induced by the presence of an erodible bed: Avalanche experiments on an erodible substrate are analyzed using the partial fluidization model of dense granular flows. The spreading of a circular cap of granular material over an erodible bed made of the same material was studied. Numerical results show that the presence of even a very thin layer of granular material lying on the solid bed strongly increases the mobility of granular flows. Furthermore, as the thickness of the granular layer increases, the dynamics of the flowing mass changes from a decelerating avalanche to a traveling wave. *Onset of swirling motion in a system of anisotropic particles*. Large-scale collective motion emerging in a monolayer of vertically vibrated elongated particles was studied. The motion is characterized by recurring swirls with the characteristic scale exceeding several times that of an individual particle. We developed a continuum model operating with the velocity field and local alignment tensor which is in qualitative agreement with the experiment. *Self-assembly and pattern formation in magnetically driven granular systems at liquid surface:* We developed and refined a new method based on ac magnetic field modulation to orchestrate the self-assembly of an ensemble of magnetic microparticles suspended on a liquid surface. With this method, we created a novel snake-like magnetic structure out of 40-90 micron sized magnetic particles. These structures are accompanied by four large-scale hydrodynamic vortices located at the opposite ends of the snake pattern. We performed detailed studies of these large-scale vortices and their relationship to the collective response of magnetic particles in an alternating magnetic field. We developed a model based on the amplitude equation for surface waves coupled to the equation for large-scale hydrodynamic mean flow.
Program Impact: Our phenomenological approach to non-equilibrium behavior, in general, and granular materials in particular, established it as a legitimate theoretical tool for the worldwide scientific community. • The manipulation of magnetic micro-particles provides a new means to create networks of conducting wires through self-assembly with application for transparent conducting electrodes for new generation of solar photovoltaic cells • Control of bio-objects by dynamic self-assembly constitutes a new approach which can be applied to the emerging bio-chip and biofilm technology • Understanding of physical mechanisms of cytoskeleton dynamics may result in the design of a new generation of biomolecular materials with unique mechanical properties.

Interactions: UC San Diego; U. of Kansas; LANL; Northwestern U.; Hebrew U. of Jerusalem, Israel; CEA Saclay, Fr.; ESPCI, Paris, France; U. of Arizona, Cambridge University, UK, Georgetown University, DC, University Paris VII, France

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): 4 papers published and 4 in press (with FWP58806-CD), including 1 Physical Review Letters, and 2 Physical Review E, 6 high-profile invited talks on international conferences, including plenary lecture at Traffic and Granular Flows and lecture course (Aronson) , Invited talk at the APS March Meeting (Snezhko), 7 invited colloquia and seminars; one patent license on novel technique for creation of conducting networks was filed. "Magnetic snakes" was featured in many popular science websites and science blogs and news, including Argonne news, Eureka, Sciencedaily, Physorg, Zdnet, Nanitenews, Physicsnewsandpress, Redtram, Magneticsmagazine, Maroon.uchicago, Azonano, Newscientist and many others. The chunky bullet on magnetic snakes was submitted to DoE-report to Congress.

Personnel Commitments for FY2007 to Nearest +/-10%: I. Aronson (50%), W. Kwok (15%), A. Snezhko (50%), Maxim Belkin (50%), D. Rosenmann (10%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $500K **FY06 BA** $465K **FY07 BA** $482K

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

FWP and/or subtask Title under FWP: Superconductivity and Magnetism

FWP Number: 58906

Program Scope: This program makes in-depth experimental and theoretical investigation of fundamental phenomena in novel superconducting and hybrid superconducting/magnetic materials at all length scales. Using nanotechnology tools for physics, we engineer novel structures whose small dimensions and electronic tunability facilitate the exploration of new phenomena and devices arising from confinement, proximity, and collective effects which could dramatically alter the physical properties and response to external fields and currents. We maintain leading programs in synthesis, experiment and theory, deriving strong benefit from their synergy.

Major Program Achievements (over duration of support):

Hybrid superconductors • Developed mesoscopic ferromagnet (permalloy)-superconductor (MoGe) bilayer structures to explore magnetic field-enhanced superconductivity and vortex pinning. Discovered anisotropic transport properties associated with the magnetic interaction of Abrikosov vortices with magnetic domains. Observed commensurate vortex phases with STM and magneto-optics. • Magnetically intercalated Nb(Co, Mn)$_x$Se$_2$ crystals to probe coexisting order parameters (charge density waves (CDW), superconductivity and magnetism) at the nanoscale by correlating real-space STM studies with momentum space ARPES and diffuse X-ray scattering measurements. Observed dramatic broadening of CDW peaks with < 1% cobalt intercalation and effective pinning of Abrikosov vortices by magnetic impurities in NbCo$_x$Se$_2$. • Developed theory of low-temperature noise and kinetics in SINIS junctions based on nonequilibrium sub-gap state distribution (with FWP59002).

Mesoscopic and nanosuperconductors • Synthesized NbN nanowires and nanoribbons with T_c~11K by direct transformation of NbSe$_3$ nanoscale precursors, a new platform for 1-D transport, quantum and thermal phase slips. Observed pronounced resistance oscillation with magnetic field in NbSe$_2$ and NbN nanowires attributable to the commensurability of a 'few-row' vortex lattice. • Observed unique single flux quantum behavior in controlled-shape type I superconducting Pb mesocrystals made using novel electrochemical deposition. A large barrier to flux entry/exit due to induced supercurrents leads to a remarkably large 'inherent' pinning at low temperatures.

HTSC and vortex physics • Demonstrated an upper limit to the irreversibility line in YBCO crystals resulting from a vortex line tension transformation [*Nature Physics 2, 402 (2006)*]. • Explored the fundamental transformation of a first order three-dimensional melting transition to higher order in the presence of 'countable' discrete defects induced by high energy heavy ion-irradiation. Preliminary results point to a threshold of defect density responsible for an abrupt higher order transition rather than a gradual smearing of the first order transition. • Developed theory which showed that Josephson oscillations in intrinsic Josephson-junction (IJJ) stacks with laterally modulated coupling, resonantly excite an internal cavity mode leading to synchronized oscillations of the entire stack resulting in powerful electromagnetic emission in the terahertz frequency range. • Developed quantitative theory of the high-frequency response of Josephson vortex lattice which provides consistent description of experimental results.

Novel materials • Synthesized the newly discovered 11.6K graphite intercalated superconductor CaC$_6$ and its isotopic variants to characterize its superconducting phase diagram, its isotope effect and its superconducting gap (FWP58916), and for neutron (FWP58701) and muon-spin relaxation experiments.

Emerging areas in THz emission and plasmonics • Guided by our theoretical study, experimentally achieved coherent continuous-wave THz-radiation with power of up to 0.5 μW from IJJ stacks in BSCCO. Our result introduces an entirely new method for generating THz (Science **318**, 1291 (2007), with FWP58916) • Developed nanostructures for coherent generation and subwavelength focusing of plasmons in noble metal films and demonstrated its advantages over conventional Surface Enhanced Raman Spectroscopy techniques. • Used phase control of the focused plasmon beam to create a nanoscale plasmon multiplexor which can be used in future nanophotonic chips • Developed patentable ultra-fast response H$_2$ sensors based on nano-granular Pd films.

Program Impact: THz emission from superconductors (Science318,1291,2007)); Surface plasmons inLaser Focus World (2005), Science 311, 189 (2006) and Virtual Journal of Nanoscale Science & Technology (2007).

Interactions: Our collaborations extend within MSD, CHM, BIO, MTI, CMT, CNM, APS and worldwide.

Recognitions, Honors and Awards: Editorship Physica C (W. K. Kwok); NHMFL program/user committee (U. Welp); Patents for Magneto-optic Current Sensor (#6,630,819), Near-field Magneto-optical Microscope (#6,972,562), Superconducting MEMS (# 6,638,895), H$_2$ sensors (#7,171,841), THz patent filed (ANL-IN-07-051, ANL-IN-05-066); 2006 R&D 100 and Micro/Nano 25 Award on H$_2$ sensors; V. Vlasko-Vlasov elected APS Fellow

Personnel Commitments for FY2007 to Nearest +/- 10%: W. Kwok (30%) G. Karapetrov (75%) A. Koshelev (30%) M. Iavarone (50%) V. Vlasko-Vlasov (20%) V. Vinokur (20%) U. Welp (60%) D. Rosenmann (20%) Z. Xiao (20%)

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

FY05 BA $940K **FY06 BA $**889K **FY07 BA $**1140K

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

FWP and/or subtask under FWP: Emerging Materials

FWP Number: 58916

Program Scope: The Emerging Materials effort explores the fundamental science of complex materials that exhibit collective electronic, magnetic and structural behaviors, with an emphasis on low-dimensional systems. Current and planned research concentrates on phase competition and short-range order, new geometrically frustrated magnets, exotic magnets, superconductors and quantum critical materials. Synergy between properties measurement and materials synthesis stands as the cornerstone of our activity, driving a feedback loop that energizes the program. We employ both exploratory and strategic synthesis to expose new science in both unknown and previously-discovered materials. Our high-quality crystals grown by zone, flux and vapor transport methods are in high demand worldwide. Looking forward, we plan to expand the scope of our materials synthesis activities by growing our own program, through strategic connections with local universities, and through DOE system-wide initiatives in materials design, discovery, and growth. This enhanced synthesis capacity will enable our own program and our network of collaborators to address an expanding portfolio of condensed matter challenges.

Major Program Achievements (over duration of support):

- Our decade-long search for THz radiation from BSCCO superconductors reached a spectacular success. Using the idea of a cavity resonance (A.E. Koshelev), we sculpted resonant cavities in BSCCO crystals and observed a 10,000-fold increase in far-field detected power at 0.85 THz (with Superconductivity and Magnetism group).
- Using high-pressure techniques, we have extended the doping range of $La_{1-x}Sr_xCoO_3$ to x=0.25. Spanning the full range of the phase diagram from diamagnetic insulator to ferromagnetic metal, our crystals are the centerpiece of a nationwide collaboration to understand the spin, lattice, and charge behavior of this system.
- Synthesis of $YBaCo_4O_{7+}$ material demonstrates that long-range magnetic frustration can be manipulated with small O sublattice perturbations. The addition of as little as 0.1 O to the antiferromagnetic parent compound (T_N~110 K) destroys long-range order down to at least 1.4 K. Future activities include chemical substitutions and single crystal diffuse scattering to model the frustrated magnetism.
- High-pressure synthesis has delivered new materials for exploration of magnetism, transport and lattice effects. These include the first complete solid solution in the low-dimensional $Ca_{1-x}Na_xV_2O_4$ system and a new high-pressure phase in the negative thermal expansion material ZrV_2O_7. Future plans focus on developing crystal growth capabilities at high pressure.
- Coulomb interactions push electron states near the Fermi level to higher energies. We measured the energy range, confirmed an essential part of theory and established the validity of Abrikosov's intuitive approach.
- Our rapid response to the discovery of superconducting CaC_6 shows a large energy gap and Ca isotope effect implying it is either a strong-coupled superconductor or has significant anisotropy.
- The surprises in the bilayer manganite phase diagram, a very narrow compositional range of stability for orbital order and lack of the coexistence seen by others, emphasizes the need for scrupulous control of composition. Crystals grown in our group were essential for mapping out this highly composition-dependent phase space.

Program Impact: Our program boasts >334 publication citations (for papers in the past three years). Our world-renown synthesis effort addresses the most exciting science and often drives the research agenda of internal and external collaborators. Our tunneling and anisotropic transport programs are at the cutting edge of research worldwide. In three years, our research has produced over 64 refereed papers with 16 in high visibility journals (PRL, Nature or Science), 25 in PRB, and 39 invited talks (8 at major international conferences).

Interactions: Internal: Intense Pulsed Neutron Source; Advanced Photon Source; Center for Nanoscale Materials, and Electron Microscopy Center. External: Universities and laboratories worldwide. In the past three years, about 450 samples have been sent to over 37 unique collaborations, demonstrating the scope of outreach and impact that our program delivers.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
John Mitchell received Argonne Distinguished Performance Award in 2006
David Hinks has notably achieved an h-index of 60: 60 publications over his career with 60 or greater citations each.

Personnel Commitments for FY2007 to Nearest +/- 10%:
Staff: K.E. Gray (group leader) 70%, J.F. Mitchell 100%, H. Zheng 100%, D.G. Hinks (part-time staff) 50%
Postdoc: T. Varga (100%), Visiting Scientist: Qing'An Li (100%), L. Ozyuzer (30%). Graduate students: D. Mazur (80%), C. Kurter (100%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05: BA $1,349K **FY06: BA $** 1,245K **FY07: BA $**1,345K

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

FWP and possible subtask under FWP: Magnetic Films

FWP Number: 58918

Program Scope: Our goals are to create, explore and understand novel nanomagnetic materials and phenomena. Our interests include the physical, chemical and metallurgical properties of artificially layered superlattices, sandwiches, wedges, ultrathin films, surfaces, and includes lithographic patterning and self-assembly. The task is to identify fundamentally new phenomena associated with the competition between spatial and magnetic length scales and proximity effects. We want to understand the ultimate limits of miniaturization, and to work to transform the art of nanomagnet fabrication into a science. We tailor properties via preparation conditions and manipulation of dimensionality for structures grown via sputtering, molecular beam epitaxy, and novel patterning and templating strategies. We explore exchange-coupled heterostructures and those formed with superconductors, insulators and antiferromagnets. We utilize surface magneto-optic Kerr effect (SMOKE), wideband microwave resonance, and synchrotron probes, and operate Brillouin and Raman scattering facilities. We study basic magnetization dynamics, magneto-transport, and magneto-optic phenomena. The new phenomena that we explore extend our basic understanding of nanostructured magnetic materials and lay the foundations for emergent technologies.

Major Program Achievements (over duration of support):

Magnetization Reversal Dynamics: We investigated the influence of geometric shape on the magnetization reversal dynamics in -patterned permalloy arrays. Using synchrotron-based, time-resolved magnetic imaging, we observed that upon applying a reversed magnetic field the location where the reversal nucleates depends on shape. For rectangular shapes the reversal can start at the end, while for tapered structures reversal occurs in the center of the structure and then slowly spreads out. The different locations for the reversal onset can be understood within a model based of local instability regions, which provides insight in how to optimize for fast reversals.

Nonlinear, Driven Vortex Dynamics: We explored the response of the vortex translational mode to high *rf* driving fields in arrays of circular and elliptical permalloy pancakes that are 40-nm thick. Above a critical value of the driving field, the resonant mode splits into two peaks that differ in frequency by as much as 25%. Micromagnetic simulations provide limited insight into the resultant anharmonic potential by showing that for large driving fields two stable solutions exist that differ by their phase lag with respect to the driving field.

Organic Spintronics: We assessed published claims that spin-polarized transport and the giant magnetoresistance (MR) effect can exist in thick Alq3-based spin valves. We systematically studied the temperature-dependent charge- and magneto-transport in spin-valve and unipolar devices where the Alq3 thickness is beyond the tunneling limit. We demonstrate that charge transport in Fe/Alq3/Co spin valves is by holes only and is unstable at large current densities due to cationic degradation. Our results are consistent with known properties of Alq3, but are in stark contrast to some recent reports in that we observe no MR. We show that hole transport in Alq3 from magnetic electrodes is limited by interfacial injection, thus spin-polarized injection from metal electrodes is prevented due to impedance mismatch. The findings challenge basic premises of the field of organic spintronics.

Origin of Recoil Hysteresis in Exchange Springs: In two-phase nanocomposite magnets, the openness in the recoil loops are usually attributed to a decoupling of the soft and hard phases. Our element-specific magnetic measurements on bilayer Sm-Co/Fe exchange springs reveal that open recoil loops are present not only in the soft Fe layer, but also in the hard Sm-Co layer, and that the Fe- and Sm-specific remanence curves are similar to each other. The experiments and micromagnetic modeling reveal that the observed open recoil loops can originate from magnetic-anisotropy variations in the Sm-Co. Thus, routine open-recoil loop measurements on nanocomposites do not provide straightforward information about the extent of interphase exchange coupling.

Program Impact: The laterally confined nanomagnet program, started in mid-FY01, was a winner of the DOE-BES competition entitled: Complex Systems: Science of the 21st Century. We (i) helped lead the theme on Electron and Magnetic Materials and Devices at Argonne's new Center for Nanoscale Materials, (ii) coordinated the DOE CSP project on Nanocomposite Magnets for ten years, and (iii) provide novel samples to a broad user community at the DOE synchrotron and neutron sources and electron microscopy centers.

Interactions: Our collaborations extend within MSD, CNM, BIO, MCS, CHM, IPNS, XSD-APS and worldwide.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
2007 APS Adler Award (SB); 2003 UC-ANL Distinguished Performance Award (JSJ); 2001 AVS Thornton Award (SB); since 2001 a group total of over 120 invited talks and 40 invited participations as co-organizer or program/advisory committee member of major meetings (*i.e.* APS, AVS, ICM, ICMFS, MMM, INTERMAG, MRS, IUMRS, SRMS, DOE, NSF.)

Personnel Commitments for FY2007 to Nearest +/- 10%: S. D. Bader (70%), F. Y. Fradin (40%), M. Grimsditch (STA), J. S. Jiang (100%), A. Hoffmann (80%), V. Novosad (100%), J. Pearson (100%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $1,620K **FY06 BA** $1,590K **FY07 BA** $1,590K

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

FWP: Condensed Matter Theory

FWP Number: 59001

Program Scope:
Condensed matter theory research programs in MSD are currently carried out in the areas of superconductivity, spectroscopy, magnetism, and nanoscience. More detail is available at http://www.msd.anl.gov/groups/cmt/

Major Program Achievements:
Superconductivity: Reproduced the phase diagram of the cuprates by a model where the pseudogap temperature T* is due to pair formation, and the superconducting transition is a percolation threshold.

Spectroscopy: Found a universal `hourglass' dispersion of the spin excitations in cuprates using linear response theory for a d-wave superconductor. Predicted x-ray circular and linear dichroism spectra in cuprates using a multiple scattering formalism. Discovered an anomalous dispersion in photoemission autocorrelation spectra of cuprates due to many-body interactions. Demonstrated that STM Fourier spectra in cuprates are coherent at energies beyond the gap due to vertex processes. Modeled the Fermi arc in the pseuodgap phase of cuprates by assuming fluctuating pairs above the superconducting transition. Proposed that magnetic stripes are responsible for the recent observation of magneto-oscillations in the cuprates. Demonstrated that the optical sum rule violations observed in the cuprates is a cut-off effect due to the finite frequency range of the optical integral.

Magnetism: Calculated the dynamic spin susceptibility of bilayer manganites using linear response theory, and related this to nesting properties of the Fermi surface.

Nanoscience: Predicted the evolution of the electronic structure of quantum wires as their thickness increases, and their resulting magnetic properties. Found a linear temperature dependence of the resistivity of the wires due to electron-electron interactions. Calculated the spectral function of the electrons of quantum wires using a new bosonization approach.

Program Impact:
Work, particularly in the areas of superconductivity, spectroscopy, and mesoscopics, is recognized world-wide, with numerous invited talks given by Drs. Abrikosov, Matveev, and Norman. The collaboration on photoemission in cuprate superconductors with Campuzano's group in the past years has led to 53 publications. Dr. Norman has 31 papers and Dr. Matveev has 13 papers with over 50 citations. Dr. Abrikosov is the author of many highly cited papers in physics, as well as two well-known books.

Interactions:
This program involves collaborations with ANL Materials Science programs on Superconductivity and Magnetism (58906), Synchrotron Radiation Studies (58926), Neutron and X-Ray Scattering (58701), and Emerging Materials (58916); and with programs at the University of Illinois-Chicago, Northwestern University, Ohio State University, University of Washington, University of Wisconsin-Madison, Columbia University, Yale University and Ames Laboratory. Also, collaborations exist with the University of Toronto (Canada), SPhT-Saclay (France), University of Geneva, Paul Scherrer Institute (Switzerland), RIKEN, and Hokkaido University (Japan).

Recognitions, Honors and Awards: Dr. Abrikosov is a member of the National Academy of Sciences and the Royal Society of London. He received the Nobel Prize in Physics in 2003, and has received many honorary degrees as well. Dr. Norman received the University of Chicago Distinguished Performance Award in 1999. Both are Fellows of the American Physical Society. Dr. Matveev is a Sloan Fellow.

Personnel Commitments for FY2007 to Nearest +/- 10%: A. Abrikosov (100%), K. Matveev (100%), M. Norman (100%), I. Paul (100%), J. Rech (100%), V. Vinokur (50%), A. Koshelev (50%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $1,100K **FY06 BA** $1,350K **FY07 BA** $1,650K

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

FWP and subtask Title under FWP: Materials Theory Institute

FWP Number: 59002

Program Scope: This program carries out forefront investigations via assembling national and international visitor research teams with complementary expertise tailored to most important emerging problems in the field of materials sciences. The extensive visitor programs attract and bring together world-leading scientists for collaborative joint projects in direct support of DOE's mission. The visits can last from a few days to several months. The program main thrust is on the physics of nanostructured materials and hybrid systems, quantum phase transitions, and soft condensed matter. The research projects are developed in close collaboration with MSD's experimental programs. Current research is focused along the following major themes: (1) Quantum phase transitions in low-dimensional and disordered structures; (2) Quantum charge and spin transport in hybrid and disordered materials; and (3) noise and decoherence effects in nanodevices.

Major Program Achievements (over duration of support):
A theory of glassy effects in disordered Coulomb systems and their manifestation in memory effects, low-frequency noises in disordered hopping insulators. Disordered hopping insulators are building blocks for low-loss sensors and detectors and understanding their transport properties is of prime importance. The main feature of these systems is their non-ergodic behavior. We have developed a model allowing for a description of non-ergodic slow relaxation in interacting hopping systems under the non-stationary variation protocol for gate and bias voltages. We have shown that the experimentally specific observed long time behavior of such systems is due to formation of "polaron cloud" around the sites belonging to hopping clusters. These polarons are formed by either by the structural defects or by the rare so-called "chessboard" electronic clusters which re-arrange via many-electron transitions. The effects of slow relaxation put fundamental limit to sensitivity of the dc operated sensors and detectors.

Other theoretical achievements: a theory of Kondo-shuttling in a nanoelectromechanical single-electron transistor was developed • a microscopic theory of phase slips in thin superconducting wires • a theory of the time dependence of thedecorence of charge and flux qubits due non-Gausian electromagnetic noise of the environment.

Program Impact: Maintains global collaborative network: MTI – BNL – LANL – UofC – Northwestern University – University of Wisconsin – UCSD – Ruhr University – Köln University – TU Delft – Chalmers University – Oslo University – A F Ioffe Institute – CRTBT-CRNRS (Grenoble) carrying out joint projects on nanophysics and soft condensed matter physics, exchanging visits and conducting a chain of International Workshops on Nanophysics in US and Europe. Created the program on properties of nanostructured materials which is recognized as one of the world-leading programs as evidenced by the numerous applications for participation in the Argonne Fall Workshops on Nanophysics. Advisory Committee recruited new active members to propose and design novel research topics and joint projects on the most demanding subjects, involving a wide community of researchers into DOE projects and exposing ANL achievements to the scientific community. New collaborations with University of Minnesota, Columbia University, and Tulane University (New Orleans) were established. During the period of October 1, 2006 – September 30, 2007 the program activity resulted in 29 publications (including 4 PRLs, 1 APL, and 17 PRBs).

Interactions: Internal: Condensed Matter Theory, Emerging Materials, Magnetic Films, Synchrotron Radiation Studies (MSD). External (In addition to listed above): Princeton University; Syracuse University; University of Florida; Harvard; Leiden University; Helsinki Technological University; Weizmann Research Institute, Israel; Tel Aviv University, Israel; Hebrew University, Jerusalem, Israel; Coherentia-INFM, Rome, Italy; Landau Institute, Moscow; Institute for Microelectronics, Nizhny Novgorod, Russia.

Recognitions, Honors and Awards (at least in some part attributable to support this FWP or subtask):
Editorship Central European Journal of Physics [2003-present – V. Vinokur].

Personnel Commitments for FY2007 to Nearest +/- 10%: Postdocs A. Glatz (100%) and Igor Beloborodov (20%), short term visitors including (among others) Peter Silvestrov (Ruhr University), Frank Hekking (Grenoble), Alexander Mel'nikov (Nizhni Novgorod), Nikolai Kopnin (Helsinki), Yuri Galperin (Oslo), Ken Elder (Oakland University)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $250K **FY06 BA $**250K **FY07 BA $**250

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

FWP and possible subtask under FWP: Quantum Computation with Electron Spins

FWP Number: 59003

Program Scope: One of the most exciting phenomena at the nano-scale is that of quantum phase coherence and its application to quantum computing because of the powerful potential in areas of large database searches, large number factorization, and quantum mechanical simulation of physical systems The grand challenge is to develop scalable arrays of quantum bits (qubits) and the logic gates of a quantum computer. In this research program we develop electron spin resonance (ESR) techniques, scanning tunneling microscopy-ESR (STM-ESR) and radio frequency-single electron spin transistor techniques to manipulate and measure single electron spins in arrays of nanoscale quantum dots in order to form the scientific underpinnings of an electron spin quantum computer. We focus on endohedral nitrogen in C_{60}, which has a long spin phase coherence time, as the qubit. We also make use of biological processes to attach C_{60} to DNA networks to form the array of interacting qubits, and advanced lithographic processes to form address gates and the readout tunnel junctions necessary for a quantum computer.

Major Program Achievements:
A key task is to prepare the qubits of endohedral nitrogen in C_{60}. Using a new C_{60} effusion cell combined with a Kaufman ion source we have increased the production rate of endohedral N in C_{60} by 2 orders of magnitude as determined by ESR measurements of the narrow 3 line hyperfine split spectra of N^{14} in N@C_{60}. A new mass spectroscopy detector for the automated preparatory HPLC chromatography system has been put into operation. Work is in progress to separate inactive C_{60} from N@C_{60}.

Synthetic procedures to functionalize C_{60} have been developed and the fullerene derivative has been successfully utilized to accomplish the covalent linkage between fullerene and PNA adapter. Excessive fullerene-PNA conjugate was applied to scaffolding DNA template to achieve the patterning of C_{60}. Development of different imaging methods to visualize the clean network of patterned fullerene is in process.

The new STM with both pico-ampere sensitivity for single molecule tunneling spectroscopy and a highly sensitive radio frequency receiver for ESR detection of single electron spins is being used with a novel high speed signal digitizer to study single spins systems such as DPPH and N@C_{60} on Au (111). We have also studied spins system deposition on Au (111) as binary mixtures with 1-10 phenantroline. We are currently trying to reduce the size of the DPPH clusters inserted into ordered 1-10 phenantroline superstructures.

Program Impact:
A number of presentations on the research in this program were made, including the March APS meeting, NanoTX07, at the Beijing National Lab for Molecular Sciences, and at the BES Review of the CNM. Papers have been published in J. Appl. Phys, and submitted to Review of Scientific Instruments and to IEEE Transaction on Nanotechnology.

Interactions:
Our collaborations extend within 3 groups in MSD and within CNM, CHM, BIO and Northwestern University.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP):
Dr. Fradin is a fellow of the American Physical Society.

Personnel Commitments for FY2007 to Nearest +/- 10%:
F. Fradin (60%), J. Schlueter (0%), O. Auciello (0%), C. Liu-postdoctoral appointee (0%), P. Messina-postdoctoral appointee (100%), L. Zhang-postdoctoral appointee (0%), T. Rajh (0%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $400K **FY06 BA** $377K **FY07 BA** $400K

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

FWP and/or subtask Title under FWP: Nanostructured Thin Films

FWP Number: 57504

Program Scope: The Nanostructured Thin Films Program is an integrated effort involving synthesis, characterization, and computer simulation. Research within the program is on fundamental science related to the synthesis and characterization of nanostructured carbon materials, and also quantum chemical computational studies of the new materials. Work is focused on the transport properties including thermal and electrical conductivity of nanocrystalline diamond and composites involving diamond either at ANL or via collaborations with leading researchers at other national labs, and universities. The work is also focused on functionalization of nanocrystalline diamond with biomolecules. The program exhibits a high degree of world leadership in advancing characterization of nanostructured diamond materials using a variety of techniques including state-of-the-art electron microscopies and synchrotron-based techniques, and in so doing leverages many of the unique resource available only at ANL. The program also supports a computational methods development effort that is used in these programs as well as others, and is recognized worldwide.

Major Program Achievements (over duration of support):
Major new advances have been achieved at Argonne and with collaborators in other laboratories in understanding and utilizing the properties of ultrananocrystalline diamond (UNCD) films including:

- An understanding of the remarkable n-type electronic conductivity of UNCD films was achieved on the basis of a formalism that relates the insulator-metal transition to a critical carrier concentration associated with the width of the sp2 bonded carbon sheath surrounding diamond "nanowires"
- Discovery of giant magnetoresistance that can be interpreted as arising from a transport mechanism characteristic of a low-dimensional disordered metal which can potentially lead to superior thermoelectric properties
- Grafting of multifunctional polymers onto UNCD surfaces enabling large loading capacity for biomolecules
- Functionalization of UNCD with dense collagen films mixed with dexamethasone which powerfully suppressed inflammatory gene expression. This startling result may find important applications for implant coatings.

Major advances in the area of theory and modeling included include:

- A new type of defect in carbon nanotubes has been predicted that can be used to modify their reactivity for making new composites and their electronic properties for thermoelectrics
- Calculations have predicted the formation of diamond/carbon nanotube composites having a covalent interface
- Quantum chemical methods development work has resulted in Gaussian-4 theory, which has a new level of accuracy that will have many applications in materials chemistry and other fields.

Program Impact: This program is widely recognized as a leading program in the world on nanostructured diamond materials. The work has lead to numerous invited talks and publications including articles in Nature-Materials, Advanced Materials, Langmuir, Physical Review Letters, and several in Applied Physics Letters. The program has organized major international diamond conferences over the last three years.

Interactions: This program has extensive collaborative relationships within the Materials Science Division and throughout the world. We also make substantial use of major user facilities at ANL such as the Intense Pulsed Neutron Source, the Electron Microscopy Center, the Laboratory Computing Center, and Center for Nanoscale Materials.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
2000 MRS Medal (Gruen); 2003 R&D 100 Award, ISI Highly Cited Researcher in Chemistry, 1980-1999 (Curtiss)

Personnel Commitments for FY2007 to Nearest +/- 10%:
L. A. Curtiss (40%), D. M. Gruen (100%), P. Zapol (10%), P. Redfern (10%), P. Bruno (Fermi Scholar)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $924 K **FY06 BA $**925K **FY07 BA $**825K

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

FWP and possible subtask under FWP: Nanostructured Biocomposite Materials for Energy Transduction

FWP Number: 57525

Program Scope:
This program involves the synthesis and characterization of nano- or meso-structured materials that either mimic or exploit biomolecules to store and transduce energy. The program involves three integrated tasks focused on developing biomolecular materials for energy transduction. Specifically, these include the synthesis of biomimetic soft materials (complex fluids, ionogels) for organizing a variety of biomolecules (e.g., soluble and membrane proteins) or nanoparticles (semiconductors or metals), synthesis of hard materials (rigid mesoporous inorganic frameworks, ferroelectric thin films, carbon nanostructures) tailored for enhanced electronic transport or photon-induced processes and the integration of these soft and hard materials to from robust, functional biocomposites.

Major Program Achievements (over duration of support):
Developed three families of thermoresponsive soft nanostructures whose supramolecular architecture and physical properties can be altered by modest changes in temperature. Demonstrated the utility of these materials in controlling the collective properties of encapsulated guests (host-mediated energy transduction). Materials proven as biomimetic and biocompatible soft tunable frameworks for the stable encapsulation of water soluble and membrane proteins.

Developed ionic-liquid–based gels whose nanostructure can be tuned by controlled addition of water. Demonstrated that these ionogels can serve as templates, directing the particle morphologies of nanoparticles photochemically synthesized within them to yield previously unattainable particle shapes and thus, novel optical properties. Synthesized polymerizable ionic liquids that form liquid-crystalline, polymeric hydrogels and organogels. Used ionic liquid polymers to fabricate an organogel with optical properties (plasmons) tunable from the visible to NIR.

Demonstrated that biotic – abiotic integration can be achieved by tailoring the biomolecule – inorganic interface. Two functional composites have been created. In the first, an array of membrane proteins, bacterial photosynthetic reaction centers (RCs), have been asymmetrically surface-coupled and “hardwired” to metal electrodes, demonstrating that they can function as components to create a photobioelectronic device. In the second system, viruses (phage display) have been used to identify peptides that selectively bind to an inorganic (perovskite) ferroelectric. Data suggests that the electric field polarizablity of the surface-tethered peptides can provide the basis of a biomolecular switch

Program Impact:
Hybrid soft-hard materials that can stabilize active biomolecules have been synthesized, thereby laying the groundwork for the assembly of functional, protein-based materials.

Interactions:
Internal: Condensed Matter Physics and Scattering Science sections of MSD, CNM, APS, and Bioscience. External: Northwestern University, University of Puerto Rico, University of Chicago, University of Wisconsin- Madison

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Named 1 of “20 people you don’t know who are changing the world” by iBIO (the Illinois Biotechnology Industry Organization). - M. Firestone; James Flack Norris Award for Physical-Organic Chemistry, Professor Michael R. Wasielewski

Personnel Commitments for FY2007 to Nearest +/- 10%:
M. A. Firestone (100%), P. Zapol (20%), L. E. Iton (100%, STA), P. Laible (30%), S. Adiga (50%, Post-doc), C. Burns (100%, Post-doc), S. Grubjesic (100 %, Post-doc), M. R. Wasielewski (subcontract to Northwestern University).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $675K **FY06 BA** $650K **FY07 BA** $650K

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

FWP and possible subtask under FWP: Molecular Materials

FWP Number: 58510

Program Scope: World-class fundamental research on materials with the aim to develop new chemistry for synthesizing molecular and nanoscale building blocks to create macroscopic materials that have unique architectures, and ultimately to create new materials that have novel functional properties. The program successfully integrates expertise in synthesis, physical characterization, and computer simulations to address some of the most challenging problems in materials chemistry. The research encompasses two related thrusts. The first is the tailoring of molecular framework architectures through supramolecular chemistry. The second involves the control of size, shape, and functionality of nanoscale building blocks such as nanoparticles, nanowires, and nanotubes and the integration of these units into materials with desired properties. In addition, a computational component provides theoretical insight into various aspects.

Major Program Achievements (over duration of support):

Major accomplishments in framework materials includes:

- Successful synthesis of the first bifluoride-bridged coordination polymer, which has a magnetically ordered state below 1.5 K that is stabilized by linear hydrogen bonds.
- We have identified superconducting fluctuations above the superconducting transition temperature in an organic superconductor that lies near the Mott insulating region of the phase diagram. This discovery provides a strong link between this class of superconductors and the high T_c cuprates.
- A new ultramicroporous metal organic framework material has been synthesized with triazole linkers that has potential for separation of impurities from H_2 and for development of new catalytic materials.

Major accomplishments in synthesis of nanomaterials:

- Single-walled carbon nanotube (SWNT) networks decorated with palladium nanoparticles were found to be an ultra-sensitive transducer toward hydrogen in air.
- AAO/Al nanowell thin film structures have shown intense interference colors that can be controlled by the surface coating. This new thin film material may have uses for surface protection, permanent colors with no pigments, and potential chemical sensing.
- Semiconductor PbSe nanoparticles have been deposited over SWNT network electrochemically to develop new composite materials for solar energy harvesting
- Experiments on Co and FePt nanocrystals have demonstrated that both the ligand type and the concentration of ligand affect the formation of particles, resulting in different sizes and shapes.

Major accomplishments in computational studies include:

- Computational studies have revealed new insight into the shapes of nanoparticles and their phase transitions, and into the catalytic properties of supported metal clusters.

Program Impact: The synthesis effort is leading to new and exciting nanostructured materials with potential for applications in sensors, catalysis, photonics and advanced electronic and magnetic materials. Our unique capabilities in the design, synthesis, and characterization of new materials have led to close interaction with other groups in the Materials Science Division, as well as the worldwide scientific community. We have also been closely involved with the development of new lab-wide initiatives on hydrogen, catalysis, solar energy, solid state lighting, the Center for Nanoscale Materials, and a Crystal Growth Facility.

Interactions: Collaborations with other groups in MSD, as well as other divisions at the Lab. Over 50 collaborations with national and international research facilities, such as the University of Chicago, Northwestern University, University of Illinois (Chicago and Urbana-Champaign), Northern Illinois University, Indiana University.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Numerous publications in the past three years including papers in Nature and Physical Review Letters, as well as many invited talks. Organized symposia and workshops. Several of our papers have been selected for feature articles and for journal covers. Organic superconductor research was named one of the 100 top scientific discoveries funded by the DOE Office of Science.

Personnel Commitments for FY2008 to Nearest +/- 10%: H. Wang (90%), J. Schlueter (90%), U. Geiser (25%), L. Curtiss (20%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA \$1150K **FY06 BA** \$900K **FY07 BA** \$900K

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

FWP and/or subtask Title under FWP: Directed Energy Interaction with Surfaces

FWP Number: 58600

Program Scope: The interaction of directed energy sources such as energetic ions, electrons, and photons with surfaces provides the basis for modifying, patterning and analyzing surfaces and nanoscale materials. This program investigates the fundamentals of these complex interactions over a wide range of conditions using several unique, world-class methods developed in our laboratory. These uniquely sensitive tools for trace analysis are also providing, for the first time, mass based analysis of materials with nanometer scale lengths.

Major Program Achievements (over duration of support):
Major new advances have been achieved at Argonne both for understanding and utilizing laser and energetic ion with surfaces. In the area of atomic and elemental studies:

- Using both experiment and modeling, a detailed understanding of the diffusion of Mg in samples irradiated with excesses of energetic protons has been developed. The effect is a significant redistribution of the Mg. Understanding the synergistic effects of multiple mass energetic ion implantation and temperature on the diffusion of impurities in materials following energetic ion implantation by multiple masses is both largely unexplored and crucial for the development of "extreme" materials capable of with standing harsh radiation environments.
- Irradiated nanomaterials have been demonstrated to "Self Heal" radiation damage. Tungsten aerogel materials created using Argonne discovered Atomic Layer Deposition synthesis when irradiated with energetic protons spallate forming radionuclides. At high temperature, these radionuclides evaporate at high rates (due to the short diffusion distances to the surface) essentially healing the damage.

Molecular analysis of surfaces is significantly more difficult than elemental analysis. In this period we have demonstrated two unique properties energetic surface interactions that can ameliorate this difficulty.

- Threshold single photon ionization (SPI) of desorbed neutral molecules that proceeds by localized ionization of a chemical tag bound to a molecular analyte. We have demonstrated both the optimal nature of these "ionophores" and used them to investigate the quorum sensing behavior of biofilms. The resulting lateral images have (by several orders of magnitude) the highest lateral resolution ever demonstrated.
- By launching acoustic waves in a solid material we have demonstrated that intact intermediate mass molecules can efficiently be desorbed into the gas phase. We have for the first time demonstrated that the velocity distributions of these molecules are far higher than can be generated by the surface wave itself. A new mechanism is suggested.

Program Impact: Directed Energy sources represent an important method for analyzing, patterning and modifying nano-materials. The instruments and fundamental studies here quantify the limits of these techniques for nano-material modification, functionalization and analysis. The trace analysis capability developed under this FWP leads the world for trace analysis at nanoscale dimensions, both in terms of lateral and depth resolution and in terms of trace detection levels.

Interactions: Collaborative publications with a wide range of University (including University of Chicago, Washington University St. Louis, California Institute of Technology, University of Newcastle) and National Labs (ANL, SNL, and LLNL) have appeared in the last few years. Further, our unique tools are applied in collaborative research on problems of particular importance to DOE. This work includes studies of OLED solid state lighting studies funded by EERE.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
2001 Energy 100 Award (One of the best 100 scientific accomplishments of the 20th Century; DOE-BES)

Personnel Commitments for FY2007 to Nearest +/- 10%: M.J. Pellin (25%), M.R. Savina (50%), I. Veryovkin (50%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $ 520 K **FY06 BA $**520 K **FY07 BA $**520 K

Laboratory Name: Argonne National Laboratory
B&R Code: KC20301

FWP and possible subtask under FWP:
Fundamental Studies of Electrocatalysis for Low Temperature Fuel Cell Cathodes

FWP Number: 58601

Program Scope:

This program focuses on fundamental, molecular-level study of the surfaces of electrocatalysts for the fuel cell cathode and the reactions occurring on them. The electrocatalysts include catalysts of platinum and platinum alloys. We investigate in-situ electrocatalytic systems with varying degrees of complexity, ranging from single crystals, to designed nano-arrays, to real fuel cell catalysts, and to single nanoparticles. The basic knowledge obtained from this study can be used to guide the development of future electrocatalysts. We use the advanced surface-science and x-ray techniques, complemented by electrochemical techniques, scanning probe microscopy, and theoretical modeling to investigate the mono- or sub-monolayer sensitive molecular orientation and short- and long-range structures of oxygen and oxygen-containing molecules, reaction intermediates, poisons, spectators, and the chemical states of surface atoms of the electrocatalyst itself, in addition to the kinetic parameters of the reaction.

Major Program Achievements (over duration of support):
We discovered that Pt_3Ni bimetallic single crystal surfaces exhibit unprecedented increases in catalytic activity of the oxygen reduction reaction; a nearly ten-fold increase compared to pure Pt surfaces and nearly ninety-fold increase compared to conventional carbon-supported nanoparticle catalysts. The increase is attributed to the modified electronic properties of a Pt monolayer skin formed on the single crystal surface. We studied one- and two-dimensional arrays of platinum nanoparticles for their oxygen reduction reaction (ORR) and dissolution reaction. 1) We discovered the catalytic activity of Pt nanoparticles to be considerably enhanced by the simultaneous exposure of two distinct crystallographic faces, each catalyzing a separate reaction in the ORR sequence. Density-functional theory and tight-binding methods are used to theoretically model the enhanced catalytic activity of faceted nanoparticles. 2) The dissolution reactions of the Pt nanoparticles were found to be sensitive to the crystallographic orientations of the exposed facets. 3) Studies of Se-modified Ru nanoparticles, highly active in the oxygen reduction reaction while tolerant to methanol crossovers, demonstrated that the major factor governing the activity of Se/Ru catalysts is the incomplete coverage and non-uniform distribution of Se atoms on the Ru surface that expose 2-fold Ru sites to oxygen molecules. It was also found that a delicate balance of oxygen affinities between Ru and Se contributes to the high activity.

Program Impact:
The observed increase in oxygen reduction activity of bimetallic Pt alloys provides possibilities of radical redesign of electrocatalysts. Hydration and dehydration and the cooperative crossover reaction mechanism have a potential for wide applications in understanding a variety of catalytic activities. A new x-ray technique developed during our studies enables us to investigate low-Z elements at interfaces that are typically invisible to hard x-rays capable of penetrating through electrolyte or other media burying the interfaces.

Interactions:
Internal --- Center for Nanoscale Materials (J. Greeley), Chemical Engineering Division (D. Myers), Electron Microscopy Center (D. Miller and N. Zaluzec).

External --- Marc Koper (University of Leiden), Helmut Bonnemann (Max Plank Institute) and Jens Norskov (University of Lingby), Christopher Lucas (University of Liverpool), A. Wieckowski (U. of Illinois at Urbana), P. Ross (Lawrence Berkeley Laboratory).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Four plenary lectures (NM) and several invited talks (NM,HY,VS) at international conferences.

Personnel Commitments for FY2007 to Nearest +/- 10%:
N.M. Markovic (30%), H. You (30%), V. Stamenkovic (100%), D. Myers (10%), G. Karapetrov (10%), P. Zapol (10%), 1 Postdoc (E. Cavar), 3 Students (D. Strmcnik, D. van der Vliet, D. Tripkovic)

Reorganization for FY2008: Proposed Renewal Budget: $1460K; N.M. Markovic (80%), V. Stamenkovic (80%), P. Paulikas (80%), K.-C. Chang (50%), H. You (30%), G. Karapetrov (10%), P. Zapol (10%), 4 postdocs, 3 students

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $ 760K **FY06 BA $ 960K** **FY07 BA $960K**

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

FWP and possible subtask under FWP: Biohydrodynamics

FWP Number: 58806-CD

Program Scope: This program focuses on theoretical and experimental analysis of the physics of active biological objects such as bacteria, motor proteins interacting with biofilaments and cytoskeleton dynamics. We consider the experiments, the theory, and large-scale molecular dynamics simulations of swimming bacteria on thin film geometry, interaction of microtubules with molecular motors and static crosslinks, and constitutive relation for cytoskeleton dynamics.

Major Program Achievements (over duration of support):
*Self-organization and control, and manipulation of active bioparticles***:** We initiated a new research direction which applies the theoretical and experimental aspects of dynamic self-assembly found in granular matter to the self-organization of active bio-organisms such as *Bacillus subtilis* and *E. coli.* The self-organization takes the form of coherent structures with sizes that are many times larger than those of the individual bacteria. We investigated the emergent collective behavior in dense bacterial colonies confined in a thin liquid film of controlled thickness and developed a new method to control the density of the bacteria colony by transmitting electric current, enabling studies of the scale of the emergent dynamic structures as a function of cell concentration. We developed a continuum mathematical model of this phenomenon to demonstrate that the primary mechanism of self-organization is associated with the shear flow induced deflection of bacteria orientation. In new sets of experiments, we focused on high-resolution non-invasive three-dimensional imaging techniques based on optical coherence tomography. Using this technique, we studied the density distribution of bacteria in thin free-standing films in the presence of oxygen gradients and related the observed spontaneous density fluctuations with the onset of bio-convection. In the future, we plan to study the rheology of bacteria-laden fluids in confined geometries. Our preliminary experiments indicate that the effective viscosity of living bacterial suspensions can be remarkably decreased by increasing the concentration of bacteria. The experimental studies will be combined with theoretical modeling, including molecular dynamics type simulations of elementary “swimmer” particles in a thin fluid film geometry. New generation of experiments with magnetotactic bacteria *Magnetospirrilium* which can be controlled and manipulated by external magnetic field has been initiated. *Effects of motors and crosslinkers on micromechanics of cytoskeleton*: we considered the effects of finite flexibility on the interaction of two microtubules with dynamic molecular motor and static crosslinkers. On the basis of numerical solution to nonlinear elasticity equation, we showed that the flexibility enhances the tendency of microtubules to align. We demonstrated that even a small amount of crosslinkers can lead to a nontrivial macroscopic behavior: the oriented state exhibits a transverse instability in contrast to the isotropic instability that occurs without crosslinkers, similar to recently observed structures in actomyosin.

Program Impact: Control of bio-objects by dynamic self-assembly constitutes a new approach which can be applied to the emerging bio-chip and biofilm technology and targeted drug delivery. Understanding of underlying principles leading to the onset of highly-organized collective motion in dense bacterial suspensions sheds a new light on enhanced mixing and transport in microscopic biological systems.

Interactions: UC San Diego; Northwestern U.; Hebrew U. of Jerusalem, Israel; CEA Saclay, Fr.; ESPCI, Paris, France; U. of Arizona, Cambridge University, UK, University of Wisconsin, Madison, Tel Aviv University, Israel.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Four papers published and 4 in press (with FWP58806), including 1 Physical Review Letters, and 1 Physical Review E, 5 high-profile invited talks on international conferences, 5 invited colloquia and seminars; one patent license for novel bacteria concentration technique was filed . “Bacterial crowd control” technique was featured on many popular science websites and science news and blogs including Argonne news, Eureka, Sciencedaily, Physorg, Medicalnewstoday, Bio-medicine, Biologynews, Nanowerk, Innovations-report, Sciencenewsdaily, Secure.bluehost, Newscientist and many others.

Personnel Commitments for FY2007 to Nearest +/-10%: I. Aronson (50%), W. Kwok (15%), A. Snezhko (50%), Maxim Belkin (50%), D. Rosenmann (10%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $0K FY06 BA $524K **FY07 BA $**524K