Program Abstract: The goal of this program is to develop an understanding of the role that the 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. We are achieving this goal by developing atomic-scale 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 atomic 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. A further thrust of this program is to develop the of use electron tomography combined with Lorentz TEM to map the magnetic induction and magnetic vector potential in and around magnetic nanostructures, and to apply this to such structures in order to gain insights into their behavior.

Program Impact: The novel properties of nanoscale heterostructure materials depend strongly on their composition and nanostructure, with the chemical nature of the interfaces and surfaces being of critical importance. In addition, new technologies based on such nanostructures place ever-increasing demands for improved performance of materials. Providing materials to meet these challenges requires atomic-level knowledge of the interfaces and surfaces in order to predict and control their physical properties. In this program we are addressing this issue via atomic-scale three-dimensional chemical imaging of interfaces in nanostructures. To do this we are using electron tomography combined with electron energy loss spectroscopy (EELS) and transmission electron microscopy (TEM). The program is focusing on interfaces in oxide thin film heterostructures, and in particular on magnetic tunnel junction structures, multiferroic heterostructures and conducting oxide multilayer structures. The traditional 2D analysis of interfaces requires very accurate edge-on alignment and the results are only reliable for atomically flat interfaces. The heterostructures mentioned above exhibit roughness on a nano-scale and therefore require tomographic methods combined with analytical electron microscopy. In addition our continued development and application of vector field electron tomography is enabling us to contribute to an understanding of the three-dimensional magnetic structure in and around nanoscale magnetic structures such as magnetic vortices and nanoparticles. Our approach relies on combining the different expertise of the two PIs in a synergistic manner that has enabled the program to move forward more rapidly than would have been possible with a single-PI program, with developments both in the techniques that we are using and in the application of these techniques to novel materials systems.

FY 2009 Authorized Budget (New BA): $400K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff): A K Petford-Long (PI; 20%; 80% 58307), B Kabius (PI; 20%; 80% 58405), X Zhong (PD; 100%), Y Liu (PD; 100%).

Interactions: Internal: PECOH (58932), Interfacial Materials Group (58307), Electron Microscopy Center (58405), Center for Nanoscale Materials (58831). External: NIST, Northwestern University, Carnegie Mellon University, IBM, Canon-ANELVA.

Program Abstract:

Our goal is to investigate the synthesis of multiferroic oxide thin films and heterostructures, and to elucidate important compositional, microstructural and interfacial contributions to their novel behavior. The research program encompasses three themes that highlight exciting research areas. Firstly, through control of interfaces we seek to understand growth behavior in the synthesis of multiferroic oxide films. We also elucidate the contributions of interface and surface modification to factors such as domain behavior in ferroelectric thin films. Our second theme emphasizes understanding the mechanisms by which film properties are modified in heterostructures, through effects such as size confinement, charge transfer and band structure modification. We are developing this theme for traditional heterostructures and for novel systems composed of dissimilar materials, with a focus on laterally-confined nanostructures. Thirdly, we are developing a full understanding of the dynamic response in multiferroic nanostructures, including the physics underlying ferroelectric domain behavior, and ferromagnetic magnetization reversal mechanisms, in thin films and patterned oxide heterostructures. We are combining advanced materials synthesis, complementary *in situ* and *ex situ* characterization and property measurement, and computer simulations and theory to accomplish our research objectives.

Program Impact:

By combining advanced experimental tools and simulation, we have developed an unprecedented understanding of the impact of composition and microstructure, including interfaces, on materials behavior in functional oxide heterostructures. The interdisciplinary research currently conducted by members of the Interfacial Materials Group (IMG) in MSD-ANL, the Nanofabrication Group in the CNM-ANL, the X-Ray nanoprobe beam at the APS-ANL, and key collaborators from Universities, using a unique combination of materials design by density functional theory, film synthesis, fabrication of nanostructures, and analytical tools (e.g. the 30 nm X-ray nanoprobe beam at the APS and the combination of *in-situ* transmission electron microscopy (TEM)/piezoresponse force microscopy (PFM) for ferroic domain studies in the IMG) demonstrates the power of a multi-PI program to fulfill the materials by design vision. Our research provide insights that will guide the way in which ferroic nanostructures can be used for advanced technologies, such as new generations of low energy consumption non-volatile memories and high frequency devices, and integrated energy generation/energy storage systems, for example combining ferroelectric film-based photovoltaic devices with supercapacitors that have a giant dielectric constant. This addresses the DOE mission of advancing fundamental and applied science needed for the development of the new generation of renewable energy systems.

FY 2009 Authorized Budget (New BA): $1987K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:

A.K. Petford-Long (PI, 80%), O. Auciello (PI, 75%), S. Nakhmanson (PI, 100%), S. Hong (PI, 100%), G-R. Bai (Technical Support Staff, 100%), L.J. Thompson (Scientific Associate, 100%), M. Tanase (PD, 40%), J. He (PD, 50%), R. Videtic (secretarial; 33%).

Interactions:

Internal: Synchrotron Radiation Studies (58926), PECOH (58932), Molecular Control of Synthesis (57504), the Electron Microscopy Center (58405), Nanomagnetic Materials (58918), the Center for Nanoscale Materials (58831) and the Advanced Photon Source.

External: 34 universities in the US, Argentina, Czech Republic, Spain, Singapore, Germany, UK and Korea: LBL, industry including Seagate, Canon, Samsung, Symetrix, Second Sight and Hewlett-Packard.

FWP Title: Proximity Effects in Conducting Oxide Heterostructures **Argonne National Laboratory**
FWP Number: 58932 **B&R Code: KC020103**

Program Abstract: This program creates and characterizes oxide thin film heterostructures that exhibit novel conduction (ionic, electronic, or mixed) or ferroelectric properties. By exploiting *proximity effects* induced by heterointerfaces through *space charge*, *elastic strain*, and *interfacial atomic structure*, we create new materials with controllable properties unattainable in bulk materials. These proximity effects are amplified in heterostructures when layer spacings are reduced below distances where electronic charges strongly interact or strain-fields overlap. The program is organized into three integrated themes that explore the relationships between synthesis, structure, and properties of oxide heterostructures possessing emergent conduction or ferroelectric behavior. One theme emphasizes ionic conductivity, specifically how proximity effects such as epitaxial strain and interfacial polarity can be manipulated to enhance oxygen transport. A second theme examines the interplay between ionic and electronic conductivity in oxide heterostructures. The third theme also focuses on the interplay between different phenomena, in this case between surface charge, epitaxial strain, conduction, and ferroelectric behavior in oxide heterostructures. The complex oxide materials that form the building blocks of the heterostructures of interest to this program include combinations of fast ion conductors (cubic-ZrO_2 and δ-Bi_2O_3), electronic conductors (In_2O_3), perovskite superlattices with potential for interface-enhanced *ionic* conductivity ($LaAlO_3/SrTiO_3$), and ferroelectrics ($PbTiO_3$ and $BiFeO_3$). Synthetically engineered heterostructures are assembled by atomic layer deposition, metal-organic chemical vapor deposition, and molecular beam epitaxy, techniques with the potential to provide precise control of each atomic plane in a growing heterostructure. We exploit the unique capabilities 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. First-principles calculations provide understanding of the factors that control strain, composition, and structure during growth, play a key role in identifying and elucidating charge transport mechanisms, and facilitate the development of predictive models for the design of oxide heterostructures with emergent properties.

Program Impact: The knowledge resulting from this program is furthering basic understanding of charge transport and interactions in oxide materials and has great potential to impact a wide range of energy-related technologies. Materials discovery, design, and synthesis are at the heart of the program and are the keys to the creation of materials with emergent behavior. Achieving the promise of new oxide heterostructures exhibiting emergent behavior driven by proximity effects requires the overlap of several key scientific directions. The program brings together scientists with considerable experience in complex oxide thin film synthesis, *in situ* synchrotron x-ray characterization of oxide thin film growth behavior and properties, conduction behavior, and first-principles electronic structure calculations. The scientific outcomes of the research include, among others, a fundamental understanding of how the structures of interfaces can be manipulated to cause emergent behavior.

FY 2009 Authorized Budget: $1.3M

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE: P. Baldo (Tech. Support Staff, 60%), J.A. Eastman (PI, 100%), D.D. Fong (PI, 100%), P.H. Fuoss (PI, 30%), H. Iddir (PD, 70%), D. Proffit (Student, 100% beginning 9/09), P. Zapol (PI, 20%).

Interactions: Argonne collaborators: A. Bhattacharya (CNM), L.A. Curtiss (MSD), J.W. Elam (ES), R. Harder (XSD), M. Holt (CNM), S. Hong (MSD), B. Kabius (MSD), J. Maser (XSD), G.B. Stephenson (MSD); External collaborators: M.D. Biegalski (ORNL), C.B. Eom (U. Wisc.), H.N. Lee (ORNL), T.O. Mason (Northwestern U.), P.A. Salvador (Carnegie Mellon U.), S.R. Phillpot (U. FL), D.G. Schlom (Cornell U.), C. Thompson (NIU), S. Trolier-McKinstry (Penn. State U.).

FWP Title: Neutron and X-ray Scattering **Argonne National Laboratory**
FWP Number: 58701 **B&R Code: KC020201**

Program Abstract:
The Neutron and X-ray Scattering Group enables the Materials Science Division to pursue world-class multidisciplinary research programs that combine neutron and x-ray scattering with materials synthesis, characterization, and theory. Members of the group play lead roles in a variety of scientific programs that couple the strengths of the Materials Science Division in experiment and theory to advanced probes of the structure and dynamics of materials at DOE neutron and x-ray scattering facilities.

The present research areas are (1) *Orbital Correlations, Frustration, and Self Organization*, (2) *Magnetic Behavior in Constrained Geometries*, (3) *Behavior of Lipid Mixtures: From Lipid Rafts to Protein Crystallization*, and (4) *Structure/Property Relationships in Complex Oxides*.

The diversity of scientific topics reflects a broad range of expertise within the group and ensures that the group impacts a number of research areas within the Materials Science Division. A strong theme that permeates the group's research is the role of phase competition in enhancing material properties, whether produced by the balance of competing interactions within bulk materials, such as complex oxides or iron arsenides, or from proximity effects in magnetic and superconducting heterostructures. Phase competition also plays an important role in functionalizing multicomponent biomembranes, a process that is investigated in the program on lipid bilayers. Understanding the resulting physics requires a detailed knowledge of structure and dynamics that neutrons and x-rays can provide, especially when the complementary aspects of each probe are exploited.

When these scientific goals are hindered by limitations in existing instrumentation, the group uses their experience in scattering techniques to develop new methods that extend the capabilities of both neutron and x-ray scattering. The group is responsible for the design of a dedicated instrument at the Spallation Neutron Source to measure single crystal diffuse scattering, is developing a new more efficient method of measuring both single crystal inelastic neutron scattering on time-of-flight spectrometers using asynchronous crystal rotations and single crystal diffuse x-ray scattering using high-energy x-rays, and has demonstrated the feasibility of using neutron spin-echo to measure off-specular reflection from inhomogeneous surfaces.

Our group sponsors and helps direct the National School of Neutron and X-ray Scattering, a two-week course held each summer at Argonne and Oak Ridge National Laboratories. This is the only school in North America to provide graduate students with a comprehensive survey of both neutron and x-ray science, and includes experiments using advanced instrumentation at the Spallation Neutron Source and the Advanced Photon Source.

Program Impact:
The group plays a strategic role in linking the scientific programs within Materials Science Division in magnetism, superconductivity, and biomaterials to state-of-the-art probes of the structure and dynamics of materials at major DOE neutron and x-ray scattering facilities, such as the Spallation Neutron Source and the Advanced Photon Source. It leads the development of novel instrumentation and experimental techniques that extend the capabilities of major DOE neutron and x-ray scattering facilities and contributes to the education of graduate students through the National School of Neutron and X-ray Scattering.

FY 2009 Authorized Budget: $2,356K

Program Personnel Supported in FY2009:
R. Osborn (PI, 100%), U. Perez-Salas (PI, 100%), S. Rosenkranz (PI, 100%), S. G. E. te Velthuis (PI, 100%), R. Vitt (Technical Support Staff, 100%), J.-P. Castellan (PD, 100%), S. Garg (PD, 100%), A. Kimble-Hill (PD, 100%), Y. Liu (PD, 100%), F. Weber (PD, 100%), G. P. Felcher (STA 50%), O. Chmaissem (STA with Northern Illinois University, 25%), B. Dabrowski (STA with Northern Illinois University, 25%)

Interactions:
Research is performed in collaboration with Materials Science Division programs on Magnetic Thin Films (58918), Emerging Materials (58916), Nano- and Confined Materials (57502), Condensed Matter Theory (59001), Synchrotron Radiation Studies (58926), as well as with Biosciences Division, the Advanced Photon Source and over 70 researchers at US and foreign universities. The program sponsors and co-directs the National School of Neutron and X-ray Scattering each summer, and provides leadership of the Instrument Development Team for *Corelli*, a single crystal diffuse scattering diffractometer under construction at the Spallation Neutron Source.

Related Project URL: http://www.msd.anl.gov/groups/nxrs/

FWP Title: Synchrotron Radiation Studies **Argonne National Laboratory**
FWP Number: 58926 **B&R Code: KC020201**

Program Abstract: This program addresses fundamental challenges in materials science and pioneers new capabilities at the Nation's synchrotron radiation facilities. Our approach is to develop novel x-ray experimental techniques that take advantage of the unique capabilities of synchrotron sources, and to apply these techniques to obtain fundamental understanding of synthesis processes, functional mechanisms, transformation dynamics, and structure-property relationships in key materials. We play a leading scientific role at the Advanced Photon Source through in-situ x-ray scattering and imaging studies of synthesis and ferroelectricity in ultrathin complex oxide films and of interfaces in electrochemical and catalytic systems, and through ultrafast studies of materials transformation mechanisms. At the Wisconsin Synchrotron Radiation Center and at a new high-energy angle-resolved photoemission facility we are developing at APS, the program plays a leading role in the study of electronic structure of high-T_C superconductors and other complex oxides. We also participate in the development of future x-ray facilities and explore the science they enable, such as x-ray nanoprobes, in-situ interface scattering instruments, and a coherent, femtosecond source.

Program Impact: The research in this program addresses fundamental science directly related to DOE missions and develops new capabilities to provide deep insight into those problems. For example, themes we address that are identified in the DOE Grand Challenge Workshops on Basic Research Needs include:

- *Size effects on materials structure linked with new functionality and properties in nanoscale systems*
  We are developing new x-ray imaging techniques using synchrotron capabilities and exploiting them to explore the physics and chemistry of nanoscale materials.
- *How charge carriers and chemistry can be manipulated at interfaces*
  Our time resolved x-ray studies of ferroelectric interfaces and catalytic materials examine these problems in important materials.
- *Atomic scale mechanisms and dynamics of catalysis under realistic operating conditions*
  Our studies of catalysis use the unique properties of synchrotron radiation to explore these mechanisms under the extreme operating conditions of practical energy conversion systems.
- *How remarkable properties emerge from complex electronic and atomic correlations*
  The advanced photoemission techniques we develop provide insight into strongly correlated systems.
- *Dynamics in systems far from equilibrium*
  We use ultrafast x-ray techniques to explore the structural evolution of metastable materials.

The Materials Science Division at Argonne is a particularly suitable location for this program because of our proximity to the Advanced Photon Source (for hard x-ray studies) and the Wisconsin Synchrotron Radiation Center (for soft x-ray studies). As resident users at these facilities, we are well positioned to lead long-term programs to develop instrumentation and techniques that bring the powerful capabilities of the synchrotrons to bear on important but difficult scientific problems. In addition, through collaborations, we directly provide knowledge in performing and interpreting synchrotron measurements needed for other scientists to take full advantage of these capabilities. Having experts on synchrotron techniques located within MSD provides an important bridge between the scientific interests of staff and visitors to Argonne, and the powerful capabilities of the local synchrotron sources. Because the techniques and equipment developed by the program are located at national user facilities, they become available to the scientific community in a straightforward manner as a user group grows. Training of outside researchers and students in the new techniques often occurs initially through our collaborations.

FY 2009 Authorized Budget: $1800K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:
Juan-Carlos Campuzano (PI) 50%; Paul Fuoss (PI) 60%; G. Brian Stephenson (PI) 80%; Hoydoo You (PI) 60%; Daniel Hennessy (PD) 100%; Matthew Highland (PD) 50%; Marie-Ingrid Richard (PD) 20%; Michael Pierce (PD) 100%.

Interactions: Work in this program is highly collaborative. In FY09 we have coauthored publications with A. Rappe (U. Penn.), M. Toney (SSRL), C. Thompson (Northern Illinois U.), and D. Schlom and S. Trolier-McKinstry (Penn. State U.). We collaborate with synergistic programs in MSD such as Conducting Oxide Heterostructures, Interfacial Materials, Energy Conversion Materials, Molecular Materials, and Condensed Matter Theory (DOE/BES), and the Solid-State Energy Conversion Alliance (DOE/FE).

FWP Title: Superconductivity & Magnetism **Argonne National Laboratory**
FWP Number: 58906 **B&R Code: KC020202**

Program Abstract: This program makes experimental and theoretical investigations of novel superconducting and magnetic materials important for the fundamental physics and applications of innovative materials. We maintain leading programs in both experiment and theory, with each deriving strong benefit through close mutual cooperation. The purpose of this program is to discover novel physical phenomena associated with superconductivity and its interplay with magnetism and to decisively determine their origins to promote use-inspired innovations. Our program explores the novel behavior of superconductivity from the macroscopic to the nanoscale under various controlled environments using a wide range of sophisticated characterization tools. Our present goal focuses on (i) unveiling the microscopic mechanism of vortex pinning and vortex dynamics which determine the electromagnetic properties of superconductors at all length scales, from bulk critical current to novel confinement phenomena found at the nanoscale, (ii) probing the rich competing phenomena at the interface of superconductivity and magnetism in unique hybrid bi-layer structures, (iii) exploring the intriguing superconductivity discovered in ferrous pnictide superconductors and (iv) developing the physics of coherent THz electromagnetic wave generation by intrinsic Josephson junctions.

Program Impact: This program comprises a strong synergy between synthesis, characterization, theory and simulations that are typically not available in a single investigator University environment. Furthermore it makes full use of site located DoE facilities such as the Center for Nanoscale Materials, the Electron Microscopy Center and the Argonne ATLAS heavy-ion accelerator. The program has led to numerous high-impact results in the area of superconductivity, including the determination and characterization of the first-order vortex melting transition in high-temperature superconductors (HTS), the discovery of twin boundary pinning in HTS, the publication of a seminal review article on vortex physics with over 3000 citations, the development of the Bose glass theory and significant contribution to the understanding of novel multi-band superconductivity in MgB_2 by coupling extensive thermodynamic and scanning probe spectroscopy studies of the superconducting gap structure with theory. More recently, the program achieved the first sizeable THz emission from a mesoscopic HTS through an in-house (FWP 58916) and international collaboration, developed the theory of crossing vortex lattices in highly anisotropic superconductors and elucidated new dynamic vortex behavior in hybrid superconducting/ferromagnetic structures. It was also quick to respond and contribute to the understanding of the phase diagram of the newly discovered high T_c ferrous pnictide superconductors through novel micro-calorimetry measurements on single crystals.

This program has maintained leading projects related to superconductivity in both experiment and theory, with each deriving strong benefit through close mutual cooperation. We built an extensive experimental characterization capability which includes state-of-the-art magneto-transport, SQUID magnetization, micro-calorimetry, micro-Hall probe magnetometry and magneto-optical imaging. On the theoretical side, we emphasize the analytical derivation of measurable properties from basic assumptions, the phenomenological description of complex behavior that occurs in disordered systems and at phase transitions, and the numerical simulation of systems that cannot be treated analytically because of strong non-linear effects or unusual boundary conditions. The critical mass of leading scientists, new ideas and innovative measurements enables the synergy of synthesis, characterization, theory and simulation to produce results whose output is often greater than the sum of its parts.

FY 2009 Authorized Budget (New BA): $1340K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:
W. –K. Kwok (PI 50%), A. E. Koshelev (PI 30%), V. Vlasko-Vlasov (PI 75%), U. Welp (PI 50%), Z. Xiao (PI 50%), H. Claus (STA 50%), M Metz (Secretary 75%), A. Belkin (student 75%), R. Xie (student 50%).

Interactions: This effort enjoys strong collaborations with ANL materials science programs on Molecular Mats. (58510), Emerging Mats. (58916), Dynamics of Granular Mats. (58806), Magnetic Thin Films (58918), MTI (59002), Directed Energy Interaction with Surfaces (58600), and the EMC (58405); with other ANL Divisions including the APS, the CNM, PHY, NE, CSE and MCS; with other DOE Labs including LANL, Ames, and BNL; with university programs at Notre Dame; Iowa State; NHMFL; Western Michigan; U of I at Urbana-Champaign; U of I at Chicago; Texas A&M; U. of Colorado, UC-San Diego; U. of Tokyo; Tsukuba U., Japan; National Research Institute for Metals, Japan; CENG Grenoble; U. of Naples, Italy; Inst. of Mat. Sci.-CSIC, Barcelona; U. Complutense, Madrid; Ecole Polytechnique, France; U. of Bordeaux; ISSP, Chernogolovka, Russia; Landau Inst., Russia; U. of Novgorod; U. of Cologne; U. of Twente; Mat. Sci. Centre, Groningen; Stockholm U.; Forschungszentrum Karlsruhe; Pohang U., Korea; Chinese Academy of Science, Beijing; U. of Izmir, Turkey; U. of Tuebingen, Germany and with industrial programs at SuperPower, Schenectady, NY; American Superconductor Corp, Devens, MA.

FWP Title: Emerging Materials **Argonne National Laboratory**
FWP Number: 58916 **B&R Code: KC020202**

Program Abstract: Our research program emphasizes two science themes: *competing interactions and frustration* and *electronic systems driven far from equilibrium.* To explore these themes, we tailor materials composition, structure, or architecture to strategically control spin, orbital, or charge states. Examples include: extremely narrow phase fields in doped manganites; frustrated magnets beyond pyrochlores and spinels; and the impact of anisotropy on long- and short-range magnetic order. Guiding these activities is our vision that *discovery synthesis*, for example at high pressure, accelerates the pace of scientific innovation; this vision underpins the newly minted Argonne strategy in Materials and Molecular Design and Discovery. Many of our activities are based solely locally, but our resources are maximally leveraged through a network of collaborators who share our samples and scientific drivers.

Program Impact: Our impact derives from a strong synthetic effort embedded in a condensed-matter science environment. Its emphasis is on foundational discovery using a broad range of targeted measurements on well-characterized, pedigreed samples. In many cases, these measurement efforts occurring wholly within the FWP provide essential feedback to synthesis. The complexity of problems we address – strong correlated electron systems with multiple competing ground states, electronic systems driven far from equilibrium–demand comprehensive and integrated solutions. The broad range of capabilities and expertise within Argonne advantages our program for timely, impactful research results. Several examples from the past year illustrate the impact of this concerted approach:

- *Definitive Phase Diagram of Layered Manganites*: A comprehensive integrated study of the charge, spin, and orbital states of the layered manganites on highly homogeneous crystals grown in our program. Our results supersede a decade of neutron studies on inhomogeneous crystals.
- *Colossal Electroconductance*: Joined by APS collaborators, we discovered a strongly non-equilibrium, current-driven phase transition in layered manganites. This is a completely new electronic state whose discovery would have been impossible without our detailed exploration of the phase diagram.
- *Patent on Compact THz Source*: Crystal growth, device fabrication, and measurement expertise in our FWP coupled to ANL theory and external collaboration. This device has potential significance in the areas counterterrorism, airport screening and medical imaging.
- *Strongly-driven High T_c Mesas*: Separate fabrication of exotic materials and patterned mesas together with tunneling expertise and unique tunneling apparatus were all necessary components available within the group and by collaboration with local university.

Publications: 18 (including 4 PRL, 6 PRB, 1 JACS, 2 APL) Three *Physical Review* papers selected as either cover images or Editor's Suggestions
Citations (2006-2009): 73 publications with 486 citations = average ~7 cites/article
Invited Talks: 8 (4 international conferences, 4 institutional seminars/colloquia)

FY 2009 Authorized Budget (New BA): $1,345 K

Program Personnel Supported in FY2009: Kenneth E. Gray (PI, 70%), John F. Mitchell (PI, 90%), Hong Zheng (Technical Support Staff, 100%), Qing'an Li (Visitor, 100%), Dave Hinks (STA, 30 %), Tamas Varga (PD, 50%)

Interactions: Our program has initiated dramatic breakthrough science at Argonne and worldwide:

Internal Interactions: To predict, create and understand the new multiferroic $FeTiO_3$ required interactions among MSD, CNM and APS scientists; neutron measurements (Rosenkranz) of phonons in our layered manganite crystals support the contention that polarons derive from short-lived charge ordered fluctuations; an unforeseen modulation of magnetic scattering in perovskite cobaltites discovered by the ANL neutron scattering group (Rosenkranz) are connected to models of intrinsic chemical phase segregation; XMCD studies at the APS (Haskel) reveal a pressure-dependent switching from ferromagnet to antiferromagnetic ground state in $(La,Ca)MnO_3$, explained structurally by an orbital ordering transition. To understand the origin of recently discovered colossal electroconductance, required interactions with various scattering scientists/facilities: bulk diffraction Rosenkranz, Osborn; surface magnetism to test for a spin-Hall effect, Freeland (APS); surface diffraction (in progress), Stuart Wilkins (BNL)). Data taken in our facility identified the magnetic origin of loss mechanisms in SC RF cavities (Zasadzinski (IIT) & Proslier). We aid in performance improvements (as with the initial development) of compact THz sources (Koshelev & Welp).

External Interactions: Collaborators seek out our samples because they are not available elsewhere with known pedigree. In FY09 over 70 samples sent to 20 external collaborators. This is compelling evidence that the Emerging Materials program provides a unique capability and resource in synthesis.

Related Project URL: http://www.msd.anl.gov/groups/em/

FWP Title: Magnetic Films **Argonne National Laboratory**
FWP Number: 58918 **B&R Code: KC020202**

Program Abstract:
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. 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.

Program Impact:
Our comprehensive program - to create, explore and understand nanomagnetic materials and phenomena with goals to define and address grand challenges and lay foundations for emergent technologies - serves as a model for university programs to emulate. Our program is world-class by any metric and is recognized by universities as such, based on the university-based advisory boards we serve. We (i) help set the roadmap for nanomagnetism research in the areas of materials synthesis and neutron and x-ray facilities research via collaborative reports and talks; (ii) helped launch the CNM and its nanomagnetism programs, and coordinated the DOE CSP project on Nanocomposite Magnets for 10 years; and (iii) provide novel samples to a broad user community at DOE synchrotron and neutron sources and electron microscopy centers. Publications coauthored by Bader (h=55) and Grimsditch (h=44) have generated over 16,000 literature citations.

FY 2009 Authorized Budget (New BA): $1,990K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:
S.D. Bader (PI, 20%), A. Hoffmann (PI, 80%), J.S. Jiang (PI, 100%), V. Novosad (PI, 100%), F.Y. Fradin (STA, 60%), M. Grimsditch (STA, 10%), J. Pearson (Technical Support Staff, 90%), G. Mihajlović (PD, 100%), O. Mosendz (PD, 100%).

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

FWP Title: Digital Synthesis: A novel pathway to new collective states in complex oxides **Argonne National Lab**
FWP Number: 58920 **B&R Code: KC020202**

Program Abstract:

In our program, we shall create, characterize, control and understand novel states of condensed matter at interfaces of complex oxides using *digital synthesis* and electric *field-effect doping*. These strategies enable the realization and control of a new generation of interfacial systems whose singular characteristic is that they have no explicit disorder. *Digital synthesis* is a technique where ordered undoped layers are stacked in integer sequences, and all charge transfer or doping takes place at the interfaces. *Field-effect doping* allows for the introduction of charge at an interface capacitively via gate-electric fields, without the introduction of any additional disorder that are associated with chemical doping. When materials with novel strongly-correlated ground states are brought together at highly-ordered atomically-sharp coherent interfaces, intrinsic 'electronic reconstructions' involving states on both sides of the interfaces are allowed to manifest themselves and create new states, with properties that can be radically different from those of their constituents. Our research program will create this new class of materials, and explore their properties using state-of-the-art techniques, leading to an understanding of how these novel systems behave. This program may lead to new materials that may be of societal importance. We shall synthesize such systems using state-of-the-art ozone assisted oxide Molecular Beam Epitaxy at the Center for Nanoscale materials at Argonne and at the University of Illinois at Urbana Champaign, and characterize them using the major DOE facilities for neutron and photon scattering, and the Nanoscale Science and Research Centers.

Program Impact:

The Digital Synthesis research program explores a very promising avenue for discovery of new materials involving interfaces of complex oxides. The complex nature of these materials requires a coherent effort involving multiple PI's with very diverse expertise. Our program addresses the full scope of this opportunity, including synthesis of heterostructures of complex oxides with atomically precise interfaces using oxide-MBE, characterizing these interfaces using state-of-the-art techniques including neutron and x-ray scattering, and atom resolved electron microscopy. We interact closely with leading experts in the world on theory/computation to understand our observations and to better design heterostructures and superlattices where new discoveries may be made.

Our effort has already led to a number of notable successes, including a recent discovery of enhanced magnetic transition temperatures in manganites (published in *Nature Materials* in FY 2010). Our approach is general enough to be extended to try and improve the properties of a broad class of materials in the complex oxides, including multiferroics and high temperature superconductors.

FY 2009 Authorized Budget (New BA): $720K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:

A. Bhattacharya (PI, 75%), Steve May (replaced by Brittany Nelson-Cheeseman in July 09) (PD, 100%), S. D. Bader (co-PI, 10%).
Subcontract: J. N. Eckstein, co-PI (University of Illinois at Urbana-Champaign); supports student Brian Mulcahy (100%) and provides 0.5 mo summer salary for Prof. Eckstein
Subcontract: J.-M. Zuo, co-PI (University of Illinois at Urbana-Champaign), supports student Amish Shah (100%).

Interactions:

<u>*Collaborators*</u>:

Oxide-MBE: Tiffany Santos (Distinguished CNM Postdoctoral fellow), Argonne National Laboratory.
Neutron Scattering: Lee Robertson, Oak Ridge National Laboratory; Brian Kirby, NIST Gaithersburg; Suzanne te Velthuis, Argonne National Laboratory; Michael Fitzsimmons, Los Alamos National Laboratory.
X-ray Scattering: Philip A. Ryan, J.-W. Kim, John Freeland, Argonne National Laboratory; Peter Abbamonte, University of Illinois at Urbana-Champaign.
Scanning Tunneling Microscopy: Matthias Bode, Nathan Guisinger (Argonne National Laboratory).

<u>*Interactions*</u>:

Theory/Computation: Sashi Satpathy, University of Missouri; Elbio Dagotto, University of Tennessee/Oak Ridge National Laboratory; Andrew Millis, Columbia University.

FWP Title: Smart, Self-Healing High Temperature Superconductors **Argonne National Laboratory**
FWP Number: 59027 **B&R Code: KC020202**

Program Abstract:

This program explores novel strategies for controlling vortex dynamics at the nanoscale to tailor the electromagnetic behavior of type II superconductors. The program addresses the grand challenges outlined in the BES report on *Basic Research Needs for Superconductivity*. We propose research focused on mitigating giant vortex avalanches, thermo-magnetic runaways and vortex liquid flow in high temperature superconductors including cuprates and pnictides by developing active, adaptive and smart pinscapes. Our project will lead to the development of *active* vortex-flow retardation strategies to minimize and dampen dissipative vortex motion and the associated catastrophic quenches from the superconducting to normal state. These new pinning strategies could have far reaching impact on transforming the future electric grid with superconductivity. Smart pinscapes will be fabricated through the incorporation of hybrid metal/superconductor and semiconductor/superconductor interfaces that could actively trigger vortex flow retardation through eddy current nucleation at the interface. This approach has been shown to be very effective against vortex channel flow, which is one of the dominant depinning mechanisms. Furthermore, pinning sites with tailored temperature and field dependencies will be developed with designer magnetic nanostructures that could serve as a vortex core-pinning site at low temperatures and convert to a 'temperature independent' magnetic pinning site at high temperatures. We plan to tailor such *smart* vortex pinning sites through anisotropic magnetization and shaped magnetic nanoparticles to control the temperature and field profile of the pinning energy near the superconducting transition temperature T_c. From a more microscopic approach, we will investigate the *pinning efficiency* of magnetic impurities and theoretically explore collective spin effects within a vortex core. Furthermore, we will combine these hybrid 'pinscape' strategies with concepts borrowed from the physics of granular matter, such as *jamming and non-Newtonian rheology*, to design methodologies to arrest vortex liquid flow and to collapse giant avalanches into micro-avalanches. Vortex flow retardation in the liquid state will enable ancillary cooling systems to assist the healing of vortex matter, thereby enabling *smart, self-healing* superconductors.

Program Impact:

This new program synergistically combines synthesis, characterization, theory and simulation to solve the grand challenge to achieve the complete prediction and control of the macroscopic electromagnetic behavior of superconductors from their microscopic vortex and pinning behavior, a key advance for transforming the future U.S. electric grid with superconductivity. We manage this program by bringing together a team of accomplished experimentalists and theorists from the areas of superconductivity and granular matter to apply crosscutting concepts to seek new ways to pursue the grand challenge of pinning a vortex fluid under high drive. One of the unique strengths of this program is that it will bring concepts derived from soft condensed matter physics such as jamming and non-Newtonian rheology to the physics of vortex matter under high drive to mitigate giant avalanches. Furthermore, the program will combine experimental and theoretical considerations for magnetic pinning to increase the critical current and develop 3D numerical simulations of thermo-magnetic vortex dynamics. These cross-cutting approaches are only made possible through the synergism of the various expertise and characterization facilities brought to bear on the problem. The program will utilize DOE major facilities such as e-beam lithography, focused ion beam machining and nanofabrication techniques provided by the CNM. It will also rely on the Electron Microscopy Center (EMC) for SEM and TEM studies of the designed SC/FM interfaces and nano-pinscape structures.

FY 2009 Authorized Budget (New BA): $750K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:

W. K. Kwok (PI 40%); G. W. Crabtree (PI 20%); A. E. Koshelev (PI 10%); I. Aronson (PI 10%); V. K. Vlasko-Vlasov (PI 25%); U. Welp (PI 50%,); Jiong Hua (PD 50%).

Interactions:

We have strong interactive relationships with the University of South Carolina (Prof. Milind Kunchur), the Institute of Theoretical Sciences (ITS) at University of Notre Dame (Prof. Boldizsar Janko), Universidad Complutense, Madrid (Prof. Jacobo Santamaria) and the Institute for NanoScience Engineering and Technology (INSET) at Northern Illinois University (Prof. Zhili Xiao) which could also serve as a source for graduate students.

FWP Title: Condensed Matter Theory **Argonne National Laboratory**
FWP Number: 59001 **B&R Code: KC020203**

Program Abstract:

Condensed matter theory research programs in the Materials Science Division are currently carried out in the areas of superconductivity, spectroscopy, magnetism, and nanoscience, with emphasis on synergistic interactions with various experimental programs within MSD and ANL.

Program Impact:

Condensed matter theory research contacts the materials research program at ANL through a variety of theoretical studies, with an emphasis on addressing data from experimental groups in MSD and beyond. These studies involve detailed modeling of complex materials and phenomena for which new theoretical methods and concepts are developed.

FY 2009 Authorized Budget: $1600K

Program Personnel Supported in FY2009:

Michael Norman (PI) – 100%
Konstantin Matveev (PI) – 100%
Alexei Abrikosov (PI) – 50%
Alexei Koshelev (PI) – 50%
Tobias Micklitz (PD) – 100%

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); with DOE programs at Ames Laboratory and Oak Ridge National Laboratory; and with university programs at Northwestern University, University of Illinois at Chicago, Ohio State University, University of Wisconsin, the University of Washington, Yale University, Texas A&M University, and Georgia Tech. In addition, collaborations exist with several foreign institutions, including the CNRS, Grenoble (France), the PSI (Switzerland), the University of Cologne (Germany), Ludwig-Maximillian University (Germany), the University of Rome (Italy), the Technion (Israel), and RIKEN (Japan).

FWP Title: Materials Theory Institute **Argonne National Laboratory**
FWP Number: 59002 **B&R Code: KC020203**

Program Abstract:

This program conducts in-depth theoretical investigations into *quantum dynamics, quantum phase transitions, and effects of disorder in strongly correlated systems*. The program operates by assembling world-experts in specific research areas through a visitor program for extensive collaborations and close interactions with the Argonne staff. Our leveraged approach insures timely and aggressive pursuit of topics at the forefront of condensed matter physics. Present research focuses on the areas outlined as strategic directions for theory development at MSD: (i) Quantum Mesoscopic Materials; (ii) Correlating Nanoscale Disorder and Electronic Excitations; (iii) Quantum Criticality (Chubukov, Maslov, Norman); (iv) Emergent Superconductivity; (v) Hidden Order, Pseuodgaps, and Spin Liquids (vi) High Frequency Devices Based on the Josephson Effect; (vii) Physics of Glasses & Dynamics and Noise in Nanodevices.

Program Impact: Statement should reflect why achievements of this multi-PI program could not be achieved by simply funding separate single investigator University grants (complexity of problem investigated, Lab & personnel resources). Significance as DOE-BES program should also be clear.

The main achievements of the program include discovery and developing of the microscopic theory of the superinsulating state; developing a theory of quantum transport and quantum synchronization in nanopatterned systems, developing a theory of dynamic phase transition and pinning in a vortex liquid state, and creation of the new direction of science, *quantum macrophysics*, utilizing effects of quantum synchronization and quantum coherence on a macroscale together with constructing a novel approach to the physics of highly non-equilibrium state. The defined goals and achievements put the program at the forefront of contemporary materials science as a program creating new materials with the unprecedented properties and performance for emergent 21st Century electronics, and energy storage and transport and as a program creating a revolutionary transformational science. Implementation of this task required attracting to the program the world-best and most active scientists working in the field, both experimentalists and theorists.

FY 2009 Authorized Budget (New BA): $250K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:
PI: Valerii Vinokour (20%) Visiting scientists (10%): Nikolay Shchelkachev; Tatyana Baturina

Interactions: (limit to current interactions and collaborations)
L. Bulaevskii (LANL); E. Chudnovski (CUNY); Yu. Galperin (Oslo University); T. Baturina (Institute for Physics of Semiconductors; Russia); N. Shchelkachev (Landau Institute, Moscow); D. Maslov (Florida University); F. Hekking (CNRS, Grenoble, France); R. Fazio (Pisa University, Italy); T. Nattermann (Cologne University, Germany); J. Tejada (Barcelona University, Spain); V. Ryzhov (High Pressure Institute, Moscow, Russia); K. Efetov (Ruhr University, Bochum); N. Kopnin (Helsinki Technological University, Finland); M. Vasin (Izhevsk University, Izhevsk, Russia); D. Khomski (Cologne University, Germany), I. Beloborodov (UCSD); A. Burin (Tulane University, New Orleans); C. Chapelier (CNRS, Grenoble, France).

FWP Title: Quantum Mesoscopic Materials **Argonne National Labatory**
FWP Number: 59006 **B&R Code: KC020203**

Program Abstract:

The project **Quantum Mesoscopic Materials** aims at developing the qualitative understanding and quantitative description of electronic properties of mesoscopic quantum materials, i.e. the materials where the quantum interference of one-particle wave functions remains important at lengths substantially exceeding the electronic wavelength. Properties of these materials are governed by the interplay between the electron correlations, quantum and temperature fluctuations and disorder. Transport properties will be given the special attention. We will be focusing transport properties of granular and nano-patterned materials offering a unique laboratory for studying and verifying new theoretical concepts of correlated disordered systems. We intend to establish a theoretical basis for possible practical application of these materials and structures. In particular, we plan to develop further a theory of recently discovered many body localization and its application to a variety of systems, to construct a theory of the far from the equilibrium state in quantum mesoscopic materials, and establish a theory of macroscopic quantum effects in nanopatterned materials. To this end, we will properly take into account strong correlations between the granules due to long-range Coulomb interactions between the electrons and develop the appropriate analytical and computational techniques and methods.

Program Impact:

The main achievements of the program include discovery and developing of the microscopic theory of the superinsulating state and creation of the new direction of science, *quantum macrophysics*, utilizing effects of quantum synchronization and quantum coherence on a macroscale together with constructing a novel approach to the physics of highly non-equilibrium state. The defined goals and achievements put the program at the forefront of contemporary materials science as a program creating new materials with the unprecedented properties and performance for emergent 21st Century electronics, and energy storage and transport and as a program creating a revolutionary transformational science. Implementation of this task required attracting to the program the world-best and most active scientists working in the field, both experimentalists and theorists.

FY 2009 Authorized Budget (New BA): $780K

Program Personnel Supported in FY2009 to Nearest +/- 10%:
PIs: Valerii Vinokur, (80%); Boris Altshuler, 20% and Igor Aleiner, 20% (Columbia University)
Visiting scientists (10%): Nikolay Shchelkachev, Tatyana Baturina, Christoph Strunk, Nikolay Kopnin, Thomas Nattermann.

Interactions:
L. Bulaevskii (LANL); E. Chudnovski (CUNY); Yu. Galperin (Oslo University); T. Baturina (Institute for Physics of Semiconductors; Russia); N. Shchelkachev (Landau Institute, Moscow); D. Maslov (Florida University); F. Hekking (CNRS, Grenoble, France); R. Fazio (Pisa University, Italy); T. Nattermann (Cologne University, Germany); J. Tejada (Barcelona University, Spain); V. Ryzhov (High Pressure Institute, Moscow, Russia); K. Efetov (Ruhr University, Bochum); N. Kopnin (Helsinki Technological University, Finland).

FWP Title: Nanostructured Carbon Materials **Argonne National Laboratory**
FWP Number: 57504 **B&R Code: KC020301**

Program Abstract:

The Nanocarbon Materials 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 other nanocarbon composites involving diamond either at ANL or via collaborations with leading researchers at other national labs, and universities. 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.

Program Impact:

Statement should reflect why achievements of this multi-PI program could not be achieved by simply funding separate single investigator University grants (complexity of problem investigated, Lab & personnel resources). Significance as DOE-BES program should also be clear.

This program is widely recognized as a leading program in the world on nanostructured carbon materials. The work has lead to numerous invited talks, highly cited papers, and publications including articles in Nature-Materials, Advanced Materials, Langmuir, Physical Review Letters, and several in Applied Physics Letters. This work could not be done without the multidisciplinary teams of synthesis, characterization, and modeling researchers that can be assembled at Argonne National Laboratory. In addition, the achievements are only possible with the state-of-the-art facilities that are located hear including the Advance Photon Source, Leadership Computing Facility, and Electron Microscopy Center.

FY 2009 Authorized Budget (New BA): $825 K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff): L. A. Curtiss (PI, 25%), D. M. Gruen (PI, 80%), P. Zapol (PI, 10%), P. Bruno (PD-Fermi Scholar, 100%)

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 Electron Microscopy Center, the Laboratory Computing Center, and Center for Nanoscale Materials.

Related Project URL: N/A

FWP Title: Nanostructured Biocomposite Materials for Energy Transduction **Argonne National Laboratory**
FWP Number: 57525 **B&R Code: KC020301**

Program Abstract:

The research program has as its overarching goal the design, synthesis, and characterization of a new class of functional nanoscale materials that exploit the native capabilities of biological molecules to store and transduce energy. Two thrust areas comprise the FWP. The first of these areas involves the development of self-assembled, nanostructured soft materials that can stabilize, orient and control the activity of biomolecules, while the second involves combining these materials with "hard" materials to provide improved durability (i.e., use under a range of demanding environmental conditions) and to facilitate connection of the nanoscale functional unit (i.e., the core protein) with traditional device materials/architectures.

Program Impact:

Externally responsive soft nanostructures that have been integrated with hard materials that stabilize active biomolecules have been synthesized, thereby laying the groundwork for the assembly of functional, protein-based materials**.** The work integrates efforts of Chemists (MSD), Biologists (BIO and the University of Chicago), Spectroscopists (Northwestern University) and Physicist (Neutron and X-ray scattering, APS and nanofabrication, CNM).

FY 2009 Authorized Budget (New BA): $650K

Program Personnel Supported in FY2009 to Nearest +/- 10%:

M. Firestone (PI, 80%), P. Zapol (PI, 5%), P. Laible (PI, 20%), M. Wasielewski (ANL/Northwestern University Joint Appointee, 20%), G. Brecht (PD, 100%), M. Sofos (PD, 100%), H. Pandya (STA, 100%)

Interactions:

This project benefits from the Center for Nanoscale Materials at Argonne. In addition, this program reaches out to fundamental work in the Materials Science, Chemistry, and Bioscience Divisions at Argonne, providing the foundation for interdisciplinary work extending well beyond the objectives of this proposal. This research program has lead to extensive collaborations with University of Chicago Medical School and the University of Louisville, Department of Chemical Engineering.

FWP Title: Molecular Materials **Argonne National Laboratory**
FWP Number: 58510 **B&R Code: KC020301**

Program Abstract:

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.

Program Impact:

This synthesis and characterization effort in tailoring the electron and spin transport properties in molecular framework architectures is world-leading with potential for applications in 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. This program is widely recognized as a leading program in the world on molecular materials. The work has lead to numerous invited talks, highly cited papers, and publications including articles. This work could not be done without the multidisciplinary teams of synthesis, characterization, and modeling researchers that can be assembled at Argonne National Laboratory. In addition, the achievements are only possible with the state-of-the-art facilities at Argonne.

FY 2009 Authorized Budget (New BA): $450K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:
J. A. Schlueter (PI, 80%), H. Wang (PI, 20%)

Interactions:
Collaborations with other groups in MSD, as well as other divisions at the Laboratory. Over 50 collaborations with national and international research facilities, such as, Clark University, University of Oxford, Los Alamos National Laboratory, Ioffe Physico-Technical Institute, University of Stuttgart, Claredon Laboratory, Institute for Molecular Physics at the Polish Academy of Science, Eastern Washington University, University of Toulouse, Gothe University in Frankfurt, University of Tennessee, Rutherford Appleton Laboratory, National High Magnetic Field Laboratory, North Carolina State University, University of Dresden, University of Bristol, UCLA, University of California – Riverside, Tokyo Institute of Technology, and Oak Ridge National Laboratory.

FWP Title: Directed Energy Interactions with Surfaces **Argonne National Laboratory**
FWP Number: 58600 **B&R Code: KC020301**

Program Abstract:
The Directed Energy Interactions with Surfaces program focuses on fundamental studies of the interaction of directed energy sources such as energetic ions, electrons, and photons with materials. The knowledge gained enables us to develop world-class quantitative elemental, isotopic, and molecular analysis instruments for nanoscale multi-dimensional materials characterization, which in turn enables us to answer questions about new or previously unobservable phenomena, and to develop and study new materials for use in extreme environments. This is an integrated fundamental research program focused on three related activities:

A fundamental understanding of energetic ion- and laser-solid interactions: The interaction of energetic ions, electrons, and photons with surfaces provides the basis for modifying, patterning and analyzing 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. It is designed to increase the knowledge base in directed energy-material interactions, and forms the basis of all of our instrument development and analysis work.

The development of world-class trace analysis instrumentation: This activity focuses on creating tools to push the frontiers of surface analysis to ever lower concentrations and ever smaller dimensions, both for practical analytical applications involving increasingly complex materials and material structures, and for enabling more advanced studies of the mechanisms of directed energy interactions with materials.

Radiation tolerant self healing materials: This activity is aimed at developing a new generation of materials for extreme environments such as harsh radiation fields, using the tools and knowledge gained in the first two activities. It builds on considerable expertise in a new synthesis method, Atomic Layer Deposition. Atomic Layer Deposition builds structures atomic layer by atomic layer, allowing for the synthesis of one- and two-dimensional materials with atomic resolution. This method is used to build materials with high radiation resistance and to build unique nanostructured materials for probing fundamental interactions of directed energy with complex materials

Program Impact:
This program is highly multidisciplinary, relying on the in-house design and construction of world-class instrumentation involving lasers, mass spectrometers, electronics and software. The unique strengths of the program are the combination of (1) the complementary strengths that the three PIs and other staff bring to surface chemistry and surface analysis, (2) the ability of the program to attract the finest graduate students, postdoctoral researchers and visiting scientists from around the world to lend their creativity and energy to the program, (3) the outstanding resources available only at Argonne that enable the synthesis, characterization, & simulation of these materials to be performed and integrated in a synergistic manner, and (4) intensive collaborative relationships with other FWPs both within MSD and with other divisions at Argonne, and with external collaborators.

FY 2009 Authorized Budget (New BA): $520K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:
M.J. Pellin (PI, 25%), M. Savina (PI, 50%), I.V. Veryovkin (PI, 50%), C. Tripa (Technical Support Staff, 10%) A. Zinovev (Technical Support Staff, 20%).

Interactions: (limit to current interactions and collaborations)
Andrew Davis, University of Chicago
Thomas Stephan, University of Chicago
Philipp Heck, University of Chicago
Bruce King, University of Newcastle, Newcastle Australia
Ian Hutcheon, Lawrence Livermore National Laboratory
Kim Knight, Lawrence Livermore National Laboratory
Stan Prussin, University of California Berkeley
Henry Frisch, University of Chicago
Don Burnett, California Institute of Technology

Program Abstract:

The nanoscale design of materials and interfaces that radically enhance both the catalytic limits and the stability of electrochemical systems for direct conversion of chemical energy into electrical energy, i.e., a fuel cell, is proposed. The proposed work offers fundamental understanding of metal-electrolyte interfaces and will transform electrocatalysis from a largely phenomenological subject into a discipline that will be able to address many challenges, opportunities and research needs in the areas of basic science of materials for clean and efficient energy conversion. Our intellectual road map is "drawn" based on synergies between the knowledge accumulated during the last grant period and our vision of obtaining a *science based* predictive understanding of the catalytic activity and stability of metal-electrolyte interfaces; this vision will lead to revolutionary advances in material properties responsible for fundamental processes occurring at the nanoscale. We propose an interdisciplinary, atomic/molecular level, fundamental study that will define the landscape for a *science based* approach to the development of nanostructured materials required for an efficient transformation of chemical energy of hydrogen, hydrocarbons and oxygen into electrical energy

Program Impact:

Our research is aimed at providing the most fundamental level of insight needed for the rational design of catalysts for reactions in fuel cell systems. This approach will ultimately form the basis for any predictive ability in tailor-making multimetallic surfaces to have desirable reactivity properties for the transformation of the chemical energy of hydrogen, hydrocarbons and oxygen into electrical energy. We will rely on the many major research facilities at Argonne National Laboratory and a group of unique, state-of-the-art, *ex-situ* and *in-situ* surface-sensitive probes and spectroscopies. The synergy obtained from variety of experimental and computational methods, together with the application of knowledge, concepts, and tools from several fields, from material science to physics and chemistry, will provide building blocks for the rational design and improvement of a new generation of electrochemical materials for efficient and clean energy conversion. Publications coauthored by Markovic (h=48) and Stamenkovic (h=23) have generated over 9,000 literature citations.

FY 2009 Authorized Budget (New BA): $1,350K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:

Nenad M. Markovic (PI, 60%), Vojislav R. Stamenkovic (PI, 60%), Hoydoo You (PI, 30%), Arvydas P. Paulikas (Technical Support Staff, 60%), Kee-Chul Chang (Technical Support Staff, 50%), Goran Karapetrov (Technical Support Staff, 10%), Peter Zapol (Technical Support Staff, 10%), Dusan Strmcnik (PD, 100%), Chao Wang (PD, 100%).

Interactions:

Internal: Extensive collaborations within MSD, CNM, APS. External: University of Liverpool.

FWP Title: Dynamics of Granular Materials **Argonne National Laboratory**
FWP Number: 58806 **B&R Code: KC020301**

Program Abstract:

This program combines in-depth theoretical and experimental studies of two fundamental problems of soft condensed matter physics: physics of granular materials and suspensions of swimming bacteria with the focus on new, adaptive, dynamic materials. The design of smart, adaptive, self-healing materials is a very formidable challenge. A wide gap exists between man-made hard materials and living tissues: biological materials, unlike steel or plastics, are "alive". Biomaterials consume energy from their surrounding nutrients to self-repair and adapt to their environment. The symbiosis of biology and hard materials is a major focus of our program. We maintain cutting edge programs in both experiment and theory. On the theoretical side we consider the theory and large-scale molecular dynamics simulations of partially fluidized granular flows in application to sand avalanches and geophysical flows and fundamentals of self-assembly of micro- and nano-particles with competing interactions, such as magnetic and electrostatic. Our experimental activity is focused on three major subjects: modeling of dense granular flows, electromagnetic self-assembly and manipulation of micro and nano particles, and collective behavior and physical properties of active biological systems. A new research thrust focuses on the emergent coherent dynamics found in ensembles of active bioparticles (biograins) at high volume fractions, where recent experiments have revealed novel, large-scale coherent structures. Current activities include experimental and theoretical studies of the onset of collective behavior in ensembles of swimming bacterium *Bacillus subtilus* in the confined geometry of thin film samples and the rheology of bacteria-laden fluids. Our future outlook aims at understanding the collective behavior of driven micro particles systems and exploring the new pathways of out-of-equilibrium self-assembly of nano and bio particles.

Program Impact:

This program synergistically combines innovative experiment, theory and simulation to solve the grand challenge to achieve the complete prediction and control of the emergent behavior and self-assembly in complex soft matter and biological systems, a key advance for understanding of smart, bio-inspired materials. We manage this program by bringing together a team of accomplished experimentalists and theorists from the areas of biohyrodynamics, granular matter, and soft condensed matter physics, to apply crosscutting concepts to seek new ways to understand fundamentals of novel bio-inspired materials. The program will utilize DOE major facilities such as nanofabrication techniques provided by the CNM and unique computing facility provided through the Argonne Leadership Computing Facility (ALCF).

FY 2009 Authorized Budget (New BA): $1006K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:

I. Aronson (PI, 90%), A. Snezhko (PI, 100%), Raymond Goldstein, U Cambridge (subcontract)

Interactions:

We have strong interactive relationships with the University of California at San Diego (Dr. Lev Tsimring); CEA Saclay, France (Dr. Hugues Chate).; ESPCI, Paris, France (Prof. Eric Clement, Dr. Falko Ziebert); University of Arizona (Prof. John Kessler), Cambridge University (Prof. Raymond Goldstein), Penn State University (Prof. Leonid Berlyand), Northwestern University, Nonequlibrium Energy Frontier Center (Prof. Bartosz Grzybowski) and Department of Cell Biology (Prof. Vladimir Gelfand), Notre Dame University, Center for the Study of Biocomplexity (Prof. Mark Alber).