FWP Title: Dynamics and Structure of Interfaces and Dislocations **Sandia National Laboratories**
Subtask on Atomic Structure and Function of Internal Interfaces **B&R Code: KC0201010**
FWP Number: SCW604

Program Abstract:
We seek to establish the fundamental principles that underpin the structure and function of internal interfaces in materials. A central goal of our work is to explain how the incompatibilities and discontinuities that arise at an interface—whether these are structural, compositional, or electronic—are accommodated and what the implications of these relaxations are on the behavior and properties of the interface. Our approach closely integrates both experiment and theory. Detailed experimental observations using transmission electron microscopy and atom probe tomography on carefully controlled materials systems are combined with theory and computation encompassing continuum elasticity, interfacial crystallography, atomistic simulations, and *ab initio* electronic structure calculations. We pay particular attention to interfacial defects, such as dislocations, steps, and junctions, since these entities provide a route to extending our understanding of ideal, high-symmetry interfaces to more complex configurations. While in the past we have worked primarily on metallic systems, we are increasingly focused on materials where interfaces more directly control the functional electronic and thermal properties of the material. In particular, we have chosen to concentrate on interfaces in thermoelectric materials because of the important, yet poorly understood, influence of interfaces on the thermal and electronic transport processes that underpin energy conversion efficiency in these materials. By exploring the interplay of interfacial structure, composition, and transport properties, we seek to develop fundamental insights that will enable new materials with higher functionality for energy conversion.

Program Impact:
The overarching goal of this program is to establish, at an atomistic level, how interfacial properties and behavior are controlled by the details of interfacial structure. Our work under this program has advanced the theory of dislocations at interfaces, led to new insights concerning how dislocations interact with interfacial junctions, provided new understanding of the mechanisms that control precipitate morphology, and explored the role of line defects in the dynamics of phase separation and island motion. Our most recent work, emphasizing interfaces in thermoelectric materials, has provided fundamental insights concerning the mechanisms of interface formation and stability in nanostructured thermoelectric materials, and has helped explained how such nanostructured materials can enhance thermoelectric properties, for instance by energy filtering at embedded nanoinclusions. Our program has been able to make progress against such problems by closely integrating experimental microscopic observations of interfaces with detailed theory and modeling.. Our experimental work draws heavily on laboratory investments in instrumentation, particularly in advanced electron microscopy and atom probe tomography. Similarly, our theoretical work profits significantly from laboratory investments in methods development and computational infrastructure. Over the life of our program, this integration of theory and experiment has been enabled by the co-location of PIs sharing a culture of meaningful collaboration, and close interactions with our companion BES programs.

FY 2009 Authorized Budget (New BA): $710K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:
D.L. Medlin (PI, 40%), J.C. Hamilton (PI, 40% - retired end of FY2009), C. Spataru (PI, 20%), Jessica Lensch-Falk (postdoc, 40%), Joshua Sugar (postdoc, 60%), Obioma Uche (postdoc, 100%), Mark Homer (technical support staff, 20%), Michelle Hekmaty (technical support staff, 10%)

Interactions:
Quentin Ramasse, Lawrence Berkeley National Laboratory; Christian Kieslowski, Lawrence Berkeley National Laboratory; G.J. Snyder, California Institute of Technology; Art Voter, Los Alamos National Laboratory

FWP Title: Mechanics of Small Length Scales **Sandia National Laboratories**
(new FY10 title: Nanomechanics and Nanometallurgy of Boundaries) **B&R Code: KC0201020**
FWP Number: SCW 93221

Program Abstract: One of the tenets of nanotechnology is that the electrical/optical/chemical/biological properties of a material may be changed profoundly when the material is reduced to sufficiently small dimensions – and we can exploit these new properties to achieve novel or greatly improved material's performance. However, there may be mechanical or thermodynamic driving forces that hinder the synthesis of the structure, impair the stability of the structure, or reduce the intended performance of the structure. Examples of these phenomena include de-wetting of films due to high surface tension, thermally-driven instability of nano-grain structure, and defect-related internal dissipation. If we have fundamental knowledge of the mechanical processes at small length scales, we can exploit these new properties to achieve robust nanodevices. ***To state it simply, the goal of this program is the fundamental understanding of the mechanical properties of materials at small length scales.*** The research embodied by this program lies at the heart of modern materials science with a guiding focus on *structure-property relationships*. We have divided this program into three Tasks, which are summarized below: (*(1) Mechanics of Nanostructured Materials (PI Blythe Clark)*. This task aims to develop a fundamental understanding of the mechanical properties and thermal stability of nanostructured metals, and of the relationship between nano/microstructure and bulk mechanical behavior through a combination of special materials synthesis methods, nanoindentation coupled with finite-element modeling, detailed electron microscopic characterization, and in-situ transmission electron microscopy experiments. (*(2) Theory of Microstructures and Ensemble Controlled Deformation (PI Elizabeth A. Holm)*. The goal of this Task is to combine experiment, modeling, and simulation to construct, analyze, and utilize three-dimensional (3D) polycrystalline nanostructures. These full 3D models are critical for elucidating the complete structural geometry, topology, and arrangements that control experimentally-observed phenomena, such as abnormal grain growth, grain rotation, and internal dissipation measured in nanocrystalline metal. (*(3) Mechanics and Dynamics of Nanostructured and Nanoscale Materials (PI John P. Sullivan)*. The objective of this Task is to develop atomic-scale understanding of dynamic processes including internal dissipation in nanoscale and nanostructured metals, and phonon transport and boundary scattering in nanoscale structures via internal friction measurements.

Program Impact: The three tasks create a complete program that is aimed at understanding mechanical processes in small scale materials ranging across several regimes: elastic to plastic, static to dynamic, thermally stable to unstable, and self-assembly to directed-assembly. The program benefits from extensive knowledge sharing and collaborative interaction amongst the investigators. For example, the modeling work of Liz Holm in Task 2 is directly being applied to the experimental work of Blythe Clark et al. in Task 1 on abnormal grain growth in nanocrystalline Ni. Furthermore, the modeling of grain boundary motion by Liz Holm et al. in Task 2 provides critical insight for experiments by John Sullivan et al. in Task 3 on grain boundary sliding internal friction studies of nanocrystalline Ni. The theory work of Normand Modine on single atomic defect relaxation for internal dissipation in Task 3 is complementary to the work of Liz Holm et al. in Task 2: Modine's simulations begin with ab initio (density functional theory) calculations of the precise structure of an atomic defect and progress to molecular dynamics simulations involving thousands of atoms using classical potentials, and Holm's simulations begin with molecular dynamics simulations involving tens of thousands of atoms and progress up to true continuum models. These investigators routinely share their expertise in microstructure synthesis and characterization, which is critical for the realization of complex micromechanical structures.

The Mechanics of Small Length Scales program has fostered important external collaborations in the field of nanomechanics. Most notable is the collaboration between Sandia and UIUC which has led to the hiring of two new staff members (B.G. Clark and K.M. Hattar) from I Robertson's group at UIUC. The program also collaborates with the BES-funded nanolaminates effort at Los Alamos (A. Misra, R.G. Hoagland).

FY 2009 Authorized Budget: $736K

Program Personnel Supported in FY2009 (PI unless otherwise noted): B.G. Clark (20%), G. Gulley (graduate student intern, 100%), C.T. Harris (graduate student intern, 50%), K.M. Hattar (10%), S.J. Hearne (10%), E.A. Holm (20%), J.A. Knapp (20%), T.K. Lemp (co-investigator, 40%), D. Olmsted (postdoc, 40%), R. Stumpf (co-investigator, 10%), A. Subramanian (postdoc, 100%), J.P. Sullivan (10%).
Interactions: M. Miodownik (Kings College, London), A.D. Rollett (Carnegie Mellon), K. Marthinsend and E. Fjeldberg (NTNU, Norway), M.A. Lusk (Colorado School of Mines), R.G. Hoagland and A. Misra (Los Alamos), I.M. Robertson and M. Briceno (Univ. Illinois at Urbana-Champaign), Z. Shan (Xi'an Jiaotong Univ.), E.A. Stach (Purdue Univ.), D. Hurley (INL), M. Yamaguchi (RPI)

Program Abstract: Our goal is a quantitative, atomic-level understanding of principles that control the mechanical, chemical and thermal stability of surfaces and interfaces. Four major tasks address a suite of increasingly reactive environments from clean surfaces in ultrahigh vacuum, to liquid-solid interfaces, to metallic and oxide nanostructures in electrochemical environments. The *atomistic dynamics of surfaces* task combines low energy electron microscopy (LEEM) and scanning tunneling microscopy (STM) with state-of the art density functional theory (DFT) to determine the basic processes by which atoms and clusters move and interact on surfaces. The *collective phenomena in surface dynamics* task examines surface processes at the next larger length scale, where cooperative phenomena (e.g., pattern formation) often control surface morphology. The *Materials at interfaces: Structural and mechanical properties* task employs the Sandia-developed interfacial force microscope (IFM), along with LEEM, STM and modeling studies, to determine how substrate-film interactions control the behavior of nanometer-thick films. The *nanoscale electrochemistry* task is aimed at a fundamental understanding of the relationship between the structure, chemistry and function of materials critical to electrochemical processes. In all four tasks we focus on materials that both reveal fundamental mechanisms of interest, and are relevant to energy technologies. We also develop new theoretical and experimental methods, including laser-interferometer-based IFM for enhanced measurement flexibility, spectroscopic electrochemical STM to probe changes in electronic properties, electron reflectivity for spatially resolved measurement of adsorbate concentrations, and innovative STM techniques to image insulating films.

Program Impact: Our experimental and theoretical research has led to fundamental insights over a wide range of surface and interface phenomena. We discovered new mechanisms for surface atom transport including exchange-, vacancy-, and other defect-mediated processes and new surface growth modes due to surface alloying. We determined the atomic-scale dynamics governing self-assembly of nanoscale patterns on surfaces and made real-time observations and atomistic interpretation of the evolution of thin-film microstructure (e.g., twin-boundary motion). We revolutionized fundamental research in nanomechanics by inventing the Interfacial Force Microscope (IFM), the world's first scanning probe instrument capable of simultaneously measuring normal and lateral forces throughout the attractive/repulsive interaction regime. Our approach of using engineered defects in controlled oxides to investigate the early stages of pitting has allowed us to address outstanding questions in corrosion science in a controlled manner (e.g., discovered that the nanoscale void and pore formation that occurs prior to aluminum pitting is much more efficient in solutions containing higher proton concentrations.) This program is well suited for a national laboratory because the scope of the proposed research requires (1) a diversity of expertise associated with several academic disciplines and (2) a suite of experimental and computational facilities typically not available at universities. We possess a wide range of experimental and theoretical skills, encompassing physics, chemistry, materials science, and innovation in instrumentation, and we operate in an environment where collaboration is the norm.

FY 2009 Authorized Budget (New BA): $2,531 K (NM-SCW 93219: $1,491 K + CA-SCW 604; $1,040 K)

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE: Staff: G. L. Kellogg 40%, P. J. Feibelman 70%, N. C. Bartelt 90%, N. A. Missert 50%, J. E. Houston 40%, K. F. McCarty 50%, B. S. Swartzentruber 25%, K. R. Zavadil 50%, K. Thuermer 100%, W. L. Smith 50%, P. Kotula 10%; Post-docs: N. W. Moore 60%, S. Nie 100%, E. Loginova 100%, E. Bussmann 20%, I. Ermanoski 50%; Technologists: R. G. Copeland 40%, M. A. Martinez 20%.

Interactions:
M. Salmeron (LBNL); T. Michely (Univ. Cologne); F. Himpsel (Univ. Wisconsin, Madison); J. B. Hannon (IBM); Karsten Pohl (Univ. New Hampshire); R. G. Buchheit (Ohio State); D. A. Fisher (NIST–NSLS); G. S. Frankel (Ohio State); D.P. Krouse (Industrial Research Limited (NZ)); N.J. Laycock (Quest Reliability (NZ)); P. Marcus (CNRS, Paris); T. Suter (Swiss Federal Institutes of Technology – EMPA); J. de la Figuera (Instituto de Química-Física "Rocasolano"); J. I. Cerda (Instituto de Ciencia de Materiales); P. A. Thiel (Ames Lab); P. Hou, A. Schmid (LBNL); S. Kodambaka (UCLA); Oscar Dubon (UC Berkeley).

FWP Title: Novel Electronic Materials **Sandia National Laboratories**
FWP Number: SCW 93222 **B&R Code: KC0201030**

Program Abstract: This project has two global objectives: first, to achieve fundamental understanding of the mechanisms whereby atomic-, nano-, and micro-structure influence the electronic, optoelectronic, and mechanical properties of novel and advanced electronic materials; and, second, by using such understanding, to develop methods of nanoscale manipulation in growth and processing for the enhancement of technologically important macroscopic properties. This effort encompasses 1) a wide variety of experiments exploiting Sandia's extensive facilities for materials synthesis, testing, and characterization; 2) *ab-initio* treatment of atomic configurational energies and electronic states using density-functional theory, which Sandia is advancing through development of the new code *SOCORRO*; and 3) a range of modeling activities to quantify the relationships among atomic and nanostructural processes and macroscopic behavior. The program is divided into two Subtasks:

1) Luminescence, Structure, and Growth of Wide-Bandgap Semiconductors (PI Stephen R. Lee). This subtask is currently developing fundamental understanding of the optoelectronic properties of GaN alloyed with InN. The emission of bandgap light from InGaN is exceptionally strong and consequently of great technological interest for such applications as solid state lighting. However, the light emission varies by orders of magnitude with In content for reasons that are not yet understood. This project seeks to elucidate carrier transport and the interplay of radiative and non-radiative pathways for electron-hole recombination. To do so, we are combining optical and electrical measurements with materials characterization by x-ray diffraction, atomic force microscopy, and transmission electron microscopy, using specially grown microstructures and device configurations. Of particular interest are the influences of point and extended defects and other microstructural irregularities, compositional modulation, and interfaces. This research is enhanced by the atomic-scale understanding being developed in Subtask 2.

2) Atomic Processes and Defects in Wide-Bandgap Semiconductors (PI Alan F. Wright). We are elucidating the fundamental properties and reactions of point defects, impurities, and dopants in GaN and its alloys with InN and AlN. Our focus is on the high carrier concentration regimes needed for efficient light-emitting devices. While this class of materials is currently the most promising for light emission at green, blue, and ultraviolet wavelengths, optimally high doping levels, especially p-type, remain elusive. The compensation and complexing of dopants by point defects and impurities are believed to be important contributors to this problem. (Also contributing is the non-radiative carrier recombination of concern in Subtask 1). However, to date understanding of the underlying atomic processes has been very limited. The present effort is addressing this deficiency through 1) experiments where electrical, spectroscopic, and ion-beam analyses reveal the responses to such stimuli as heating, voltage bias, and ion irradiation; 2) the use of density-functional theory to determine formation energies, electronic states, and diffusion and reaction energies for the defects, impurities, and their complexes; and 3) mechanistic modeling of thermodynamics, atomic processes, and device behavior.

Program Impact: *Multi-PI Program Justification*: The BES project on Novel Electronic Materials is made possible by the extensive range of scientific expertise, experimental facilities, and computational resources uniquely co-located at Sandia National Laboratories. For example, the project relies on the recently completed MESA complex, which includes some of the world's most advanced class-10 cleanroom & laboratory facilities now available for compound-semiconductor research. In addition, the project's advanced computational work will soon transition to the newly established Red Sky high-capacity super-computer cluster, which offers a massively parallel, ~217 TeraFLOP, 18544-processor computing capability. *Relevance to DOE/BES Program Missions*: Project results have increased the basic-science knowledge base for solid-state lighting, whose potential U.S. energy savings is ~$30 billion per year, and whose potential reductions in atmospheric carbon emissions are tens of millions of tons per year. In pursuit of this energy-security mission, our project's research further addresses multiple BES themes including the behavior of complex materials, multi-scale and nano-scale phenomena, predictive modeling, and advanced computational methods.

FY 2009 Authorized Budget (New BA): $769 K

Program Personnel Supported in FY2009 (percentage-FTEs based on actual recorded labor charges):
Principal Investigators: S. R. Lee (Subtask 1) 26%, A. F. Wright (Subtask 2) 9%; *Co-Investigators*: A. Armstrong 22%, M. H. Crawford 12%, R. M. Fleming 11%, D. D. Koleske 18%, N. A. Missert 4%, S. M. Myers 11%, J. Wierer 3%; *Post Docs*: G. Thaler 3%; *Students*: R. Snow (UC-Davis) 100%; *Technical Support Staff*: J. M. Campbell 15%, R. G. Copeland 2%, K. C. Cross 2%, K. W. Fulmer 3%, J. M. Kempisty 11%, M. L. Smith 26%, K. Westlake 35%; *Line Managers*: D. L. Barton 5%, R. M. Biefeld 2%, D. E. Peebles 4%

Interactions (during FY09): University of California-Davis, University of Virginia, Rensselaer Polytechnic Institute, Arizona State University, Inlustra.

FWP Title: Field Structured Composites **Sandia National Laboratories**
FWP Number: SCW 126815 **B&R Code: KC0201030**

Program Abstract: The goal of this program is to discover useful methods of manipulating particle suspensions with time-dependent, multi-axial magnetic or electric fields, and to develop a scientific understanding of these phenomena and the impact they can have on technology, including sensing, actuation, microfluidic mixing, and heat and mass transfer. This program on manipulation of materials with multi-axial fields has two thrusts: 1) the development of field-structured composite materials and; 2) the stimulation of functional fluid flows.

The composites thrust focuses on using multi-axial fields to create unique particle assemblies that give composites both optimized physical properties and tailorable anisotropy. Physical properties of interest include the magnetic permeability, electric permittivity, and electrical and thermal conductivity. Technological impact is focused on the magnetostrictive actuation of these composites, and their use as chemical and strain sensors. A significant component of this work involves relating the composite properties to structure with a combination of theory and simulations of structural evolution.

The functional fluid flow thrust focuses on developing methods of using multi-axial magnetic fields to initiate vigorous fluid mixing on the microscale, and to stimulate the formation of both advection lattices and chaotic advection in fluid suspensions. The advection lattices are a new and surprising discovery, and much of our current work is concentrated on exploring the formation of the unique flow patterns and free standing fluid structures we have discovered, and quantifying the attendant heat and mass transfer. These flow patterns have symmetries that are distinct from those produced by natural convection, and offer the possibility of cooling in microgravity environments and transferring reactants and nutrients to a chemical or biological process without extracting heat.

Program Impact: This research program is broad in scope and has involved a variety of laboratory personnel having a broad range of skills. These include programmers and physicists responsible for simulations, theory and the characterization of physical properties, as well as chemists responsible for the synthesis of magnetic and luminescent nanoparticles. This program is now developing interactions with mathematicians, molecular dynamics simulators, and computational fluid dynamics experts in a new effort to understand our recent discoveries on functional fluid flows. A national laboratory enables the rapid development of interactions needed for the success of a broad program, and also provides the state-of-the-art computational resources needed for rapid progress in simulation.

This year this program has had impact on a variety of areas of science and technology. We have developed robust, *tunable* sensors for volatile organic chemicals that are being commercialized for environmental monitoring of leaking gasoline tanks. We have developed a new generation of moldable thermal interface materials with exceptional conductivities by using magnetic fields to optimally organize magnetic platelets for heat transfer. These materials have thermal conductivities significantly better than diamond-filled polymers. We have published both theoretical and experimental papers on our discovery of the ability to mix fluids containing magnetic particles by subjecting them to particular multi-axial magnetic fields. We have shown that anisometric particles, such as platelets and nanorods are especially effective, and this technology will enable efficient mixing in microfluidic devices. Finally, our work on functional fluid flows has resulted in discoveries that impact both science and technology, and rival Benard's discovery of convection cells by demonstrating field-controllable functional flows having unique symmetries. This year we have discovered spontaneous flow symmetry breaking, spontaneous chiral symmetry breaking, helical flow, free-standing fluid structures, and chaotic advection. This *Isothermal Magnetic Advection* enables hand's-off, directed transport of heat and mass without gravity or a thermal gradient and can be used where convection fails, such as in microgravity environments or in stable thermal gradients. This work has generated a patent application.

FY 2009 Authorized Budget (New BA): $459K

Program Personnel Supported in FY2009: Staff Member James Martin, 0.5 FTE; Staff Member Lauren Rohwer, 0.1 FTE; PhD student Doug Read 0.7 FTE; PhD student Kyle Solis, 0.5 FTE

Interactions: The PI is currently interacting with Richard Bell, Penn. State and over the last year has worked with Lauren Rohwer and Pat Brady, both at Sandia. He is currently in discussions with Gary Grest, Frank van Swol, Louis Romero and Jeremy Leachman, all at Sandia Labs, to develop a computational effort to understand the isothermal magnetic advection. It is envisioned that this large computational effort will also be supported by the laboratory.

FWP Title: Quantum Electronic Phenomena and Structures **Sandia National Laboratories**
FWP Number: SCW 93220 **B&R Code: KC0202020**

Program Abstract:
This project contains two topical thrusts that address the issues of what novel types of quantum collective behaviors can emerge from nanostructures and how well this behavior can be controlled and manipulated. The **Quantum transport in structured semiconductors** thrust addresses quantum transport properties in low-dimensional semiconductor systems. We search and examine novel phenomena arising due to strong electron-electron interactions, including novel fractional quantum Hall phases, quantum criticality and quantum phase transitions in the quantum Hall regime, Bose-Eisenstein condensation in electron-hole bilayers, Coulombic interaction in coupled one-dimensional (1D) quantum wires, Bloch oscillations in 2D quantum dot superlattices, and theoretical investigation of exciton energy transfer and diffusion in low dimensional structures. In parallel to the above top-down approach to nanostructures, the focus of **Growth and properties of III-nitride and III-V nanowires** thrust is to synthesize high quality III-nitride and III-V core-shell nanowires that may exhibit unexpected exciting quantum electronic properties, such as Aharonov-Bohm effect. It involves collaborations between device physics, theory, nanocharacterization techniques, and MOCVD synthesis. Time resolved ultra-fast optical measurements are also utilized to examine the collective electron excitation modes and surface states in these nanostructures.

Program Impact:
This project seeks to understand the fundamental physics of novel quantum electronic phenomena in semiconductor nanostructures by quantum transport studies and optical studies. In FY09, we, for the first time, observed a new even-denominator fractional quantum Hall effect (FQHE) state at the Landau level filling $\nu=1/4$. This new addition to the FQHE family may help us to better understand the properties of the non-abelian FQHE states, a novel class of FQHE state which may find application in fault resistant quantum computation. We carried out seminal work on exciton condensation and Coulomb drag in electron-hole bilayers, which generated a great deal of experimental and theoretical interest. Time-domain THz magneto-measurements in the Bloch oscillation regime in 2D quantum dot superlattices and first ultrafast optical spectroscopy measurements on GaN nanowires were performed. We have successfully grown Al(Ga)N/GaN core-shell nanowires showing enhanced conductivities and band-edge emission and developed a self-consistent theoretical model to calculate nanowire core-shell electronic structure. The work resulted in 10 published papers in 2009, with two appearing on the covers of *Advanced Materials* (on NW-templated GaN), and *Physica Status Solidi (b)* (review article on ultrafast dynamics in semiconductor nanowires). 7 invited talks were presented at international conferences and workshops.

The above research topics are at the frontier of the field of condensed matter physics. A vast skill set, ranging from extremely-low temperature measurements, very fine nanoscale device fabrications, ultra-fast optics, to extensive theoretical simulations and controlled nano-wire growth, etc., is needed to successfully implement this project. Sandia National Lab is well suited for such a multidisciplinary program, as it enables the formation of highly collaborative teams of in-house scientists with diverse expertise and interests. Such a dynamic and interdisciplinary program also helps staff members to further extend their work in exciting new directions. Moreover, we emphasize that the whole program has taken advantage of Sandia's state-of-the-art micro- and nano-fabrication capabilities at the recently commissioned, half-billion dollar Microsystems and Engineering Sciences Applications (MESA) facilities, one of the largest and best equipped semiconductor growth and fabrication facilities in the USA, and the Department of Energy's Center for Integrated Nanotechnologies (CINT). Finally, this project synergizes with several other ongoing LDRD-funded activities at Sandia, e.g., projects on quantum information science and technology, and electron physics in high quality epitaxial graphene. Collaborations and interactions with theorists internal and external to Sandia also inevitably play an important role in the success of this project.

FY 2009 Authorized Budget (New BA): $1,190K

Program Personnel Supported in FY2009: Staff: Wei Pan, 0.5 FTE; Mike Lilly, 0.1 FTE; Ken Lyo, 0.3 FTE; John Reno, 0.3 FTE; George T. Wang, 0.3 FTE; Rohit Prasankumar (LANL), 0.1 FTE; Tech support personnel: Jeffrey Figiel, 0.1 FTE; Denise Tibbetts, 0.1 FTE; Post-docs: Qiming Li, 0.4 FTE; Prashanth Upadhya (LANL), 0.5 FTE; two graduate students

Interactions:
Steve Brueck, University of New Mexico; Guillaume Gervais, McGill University; Dan Huang, Air Force Research Lab; Jun Kono, Rice University; Loren Pfeiffer, Princeton University; Sankar Das Sarma, University of Maryland; Daniel Tsui, Princeton University; Nancy M. Haegel, Naval Postgraduate School.

FWP Title: Molecular Nanocomposites **Sandia National Laboratories**
FWP Number: SCW 93223 **B&R Code: KC0203010**

Program Abstract: The Molecular Nanocomposites project explores the assembly and unique emergent properties of nanocomposite materials created using solution-based processing methods. The project develops fundamental understanding of the principles that govern the formation and function of novel nanocomposite materials. Scientific issues include: 1) synthesis of complex building blocks, 2) self-assembly, 3) programmable nanomaterials, reconfigurable hosts, and nanocomposites that combine both elements, 4) understanding of assembly mechanisms and structure, 5) interfacial phenomena in organic-inorganic nanomaterials, and 6) properties of nano- to microscale self-assembled materials (e.g., transport, electronic and optical behavior, interfacial chemistry, etc.). The project is comprised of three subtasks: ***Adaptive & Reconfigurable Nanocomposites*** which explores the basic science associated with the use of energy consuming, switchable, and/or responsive components to create programmable and/or reconfigurable nanocomposites; ***Complex Nanocomposites*** whose goal is the discovery and understanding of new chemical synthesis and assembly methodologies to construct and integrate complex porous and composite materials exhibiting structure and function on multiple length scales; and ***Interactions of Organics with Inorganic Nanoparticles & Nanocomposites*** which probes how surface functionalization and organic overlayers used in composite assembly influence the physical properties of both the primary particles and assembled composites.

Program Impact: The Molecular Nanocomposites project brings together 13 highly diverse core scientists that are developing wide-ranging fundamental understanding of nanocomposite assembly and function. This highly interdisciplinary team of chemists, material scientists, and physicts are working to develop programmable nanocomposites whose ability to reversibly switch back and forth between distinct nano-architectures will facilitate the programming of the optical, electrical, mechanical, and even microfluidic properties of materials. Such programming can be applied to applications including adaptive optics and camouflage, integrated microsystems and sensors, composites for water treatment and CO_2 sequestration, and biomedical applications (such as artificial muscles). The work on construction of rigid, 3D nanocomposites is focused on designing structures with dimensional scales and interfacial behaviors to allow energy conversion, transduction, or storage and/or enable biotic/abiotic integration with future impact being in the energy arena. Our work in developing *in situ* characterization techniques is enabling the understanding of self- and directed assembly pathways and the probing of collective properties deriving from hierarchical organization. This when coupled with the basic work on organic-inorganic interactions – from the influence of organic surfactants on the properties of nanoparticle building blocks to the fundamental mechanisms of photoexcitation and charge transport across organic-inorganic heterojunctions – will provide unprecedented insight into composite assembly and function at the nanoscale.

Recently, the Molecular Nanocomposites project has made significant science contributions to three winning R&D 100 awards. Its science has been leveraged into numerous applied research efforts across Sandia including, Lockheed Martin Shared Vision projects, an EERE project on Organic Photovoltaics in collaboration with NREL, and the National Institute of Nanoengineering initiative between Sandia, U.S. industry and universities. Ongoing work will impact future program development efforts at Sandia ranging from energy storage and conversion to new sensor structures and smart skin materials – of interest not only to DOE, but other government agencies. Future efforts will leverage the breadth of the core team, the collaborations, and Sandia's extensive fabrication (MESA) and characterization facilities to develop ever more complex, multifunctional nanocomposites.

FY 2009 Authorized Budget (New BA): $1,445K

Program Personnel Supported in FY2009 (PI unless otherwise noted): T. Boyle (10 %), T. Alam (30%), F. Van Swol (20%), H. Fan (10%), C. J. Brinker (20%), J. Shelnutt (20%), J. Voigt (10%), B. Bunker (20%), D. Sasaki (20%), D. Wheeler (20%), D. Huber (30%), J. Hsu (10%), M. Stevens (10%), R. Davis (Post Doc, 50%), J. Lavin (Post Doc, 50%), F. Zendejas (Post Doc, 50%), Y. Tian (Grad. Student, 50%), K. Martin (Student, 100%), P. Klimov (Student, 100%).

Interactions: G.Timmins, E. Carnes, Darren R. Dunphy, K. Ward, A. Dayte, C. Medforth, S. Challa, Y-B Jiang, S. Han, D. Petsev, J. Oliver, B. Wilson (U. of New Mexico); I. Orme, P. Dorhout (Colorado State U.); R. Shen, L. Lee (UC- Berkeley); N. Schore (UC-Davis); B. G. Potter, K. Simmons-Potter (U. of Arizona); M Shannon (U. of Illinois); W. Sigmund (U. of Florida); H. Hillhouse (Purdue); T. Kuech (U. of Wisconsin); J. Erskine, R. Ruoff (UT-Austin); C. Ivory (U. of Washington); Y. Lu (Rutgers U.); D. Boye (Davidson College); W. Liu, (Northwestern U.); S. Weinert (Oklahoma State U.); V. Petkov (C. Michigan U.); J. Farrell (Holy Cross); S. Webb (U. Manchester); J. Duhamel (U. of Waterloo); Y. Song (Chinese Acad. of Sci.); A. Cheung (Dartmouth Medical School); S. Singh, T. Luk, E. Spoerke, C. Hayden (SNL); J. Wang, Y. Ren (ANL); R. Kline (NIST); M. Toney (SSRL).

FWP Title: Active Assembly of Dynamic and Adaptable Materials **Sandia National Laboratories**
FWP Number: SCW127021 **B&R Code: KC0203010**

Program Abstract:
The objective of this project is to exploit key strategies used by living systems to develop materials whose transport, reconfiguration, and disassembly can be programmed or "self-directed" in controlled environments. These strategies are based on the exploitation of two classes of energy-consuming proteins: 1) filament-forming proteins such as tubulin that can be programmed to polymerize or depolymerize on command to form structures such as hollow microtubules, and 2) motor proteins such as kinesin that can provide active transport and assembly functions by "walking" along fibers such as microtubules with desired cargo. The overall program consists of two primary components: 1) ***Active Protein Assemblies***, which involves exploring the use of kinesin and tubulin in artificial systems for the transport, assembly, reconfiguration, healing, and disassembly of man-made nanomaterials, and 2) ***Artificial Microtubules***, which is a newly-funded task that involves creating robust artificial analogues to highly-functional energy-consuming proteins such as tubulin as a means of creating programmable nanomaterials.

Work in the Active Protein Assemblies piece has led to many key advances in the deployment of "active" proteins in artificial materials and systems, including: 1) The use of both chemical and genetic engineering methods to create proteins that are robust enough to use in artificial settings, 2) the development of both physical and chemical patterning methods that create transportation "networks" in microfluidic systems to direct the loading, transport, and unloading of nanoparticle "cargo" by motor proteins and/or microtubule shuttles, and 3) the use of microtubules as templates for the creation of inorganic nanowires via biomineralization processes. For example, motor proteins have been used to transport microtubules to desired locations where they are converted into materials that have desired properties for electrical or optical interconnects. Long-term goals involve developing artificial analogues to both intra-cellular and multicellular processes such as replicating the formation of diatom skeletons, the dye reconfigurations in the color changing system of the chameleon, and the directed motion of artificial amoebas. Work in the Artificial Microtubules piece is just underway. However, molecular dynamics simulations are already revealing how design features incorporated into monomeric building blocks lead to the spontaneous formation of different assembled architectures. These design rules have led to our first artificial monomers based on polymeric dendrimers that can reversibly polymerize into chain-like structures.

Program Impact:
Energy consuming proteins are responsible for much of both the assembly and functionality of complex biomaterials. Functions performed by these proteins range from intracellular functions such as organelle transport and cell division to multicellular functions such as diatom skeletal assembly, muscle actuation, and the color changing system of the chameleon. This program involves learning how to harness energy consuming proteins and their artificial analogues to perform complex assembly and reconfiguration functions involving man made materials and systems. The self-assembly, directed assembly, and emergent behavior themes of the project are of central importance to BES's basic research activities in Biomaterials. The research requires the use of a multidisciplinary team of biologists, chemists, physicists, and materials scientists. This team is available at Sandia National Laboratory, in addition to expertise and fabrication capabilities in integrated systems that are unique to Sandia (including our $500M Microsystem Fabrication facility (MESA)).

FY 2009 Authorized Budget (New BA): $1,290K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE: All are PI's unless otherwise indicated. Bruce Bunker (30%), George Bachand (30%), Erik Spoerke (40%), Jim McElhanon (40%), Darryl Sasaki (40%), Mark Stevens (20%), Marlene Bachand (contract employee)(50%).

Interactions:
Dominic McGrath (U. of Arizona), Henry Hess (Columbia), Alan Barhorst (Texas Tech), Robert Haddon (UC Riverside), Viola Vogel (Swiss Institute of Technology), Peter Satir (Albert Einstein College of Medicine), Stephan Diez (Max Planck Institute), Jessica Winter (Ohio State)