Sandia National Laboratories

FY2007
Annual BES/DMS&E
One-Page Summaries

(Includes both NM and CA sites)

Laboratory Name: Sandia National Laboratories
B&R Code: KC020101

FWP and subtask under FWP:
FWP Dynamics and Structure of Interfaces and Dislocations
Subtask: Dynamic Surface Microscopy of Functional Materials

FWP Number: SCW 604

Program Scope:
This project's goal is to quantify the fundamental atomic processes governing the dynamics of surface structure and morphology. We use state-of-the-art microscopy (low-energy electron microscopy and scanning tunneling microscopy) to measure, often in real time, the time evolution of surface structure on nanometer length scales. We use these measurements to write down precise equations of motion to describe the observed time dependence and then relate these equations of motion to atomic processes. We use this general approach to answer important questions about a variety of the functional materials used in energy technologies. This work has often revealed unanticipated mechanisms of surface evolution. We currently emphasize five focus areas: 1) film wetting and de-wetting, 2) mass exchange between the bulk and surface, 3) surface self-assembly, 4) oxide surfaces and metal oxidation, and (5) surface alloying. The goal of future work is to apply our approach to increasingly complicated material systems (such as ice and graphene) and further develop the conceptual framework needed to account for our observations. The ultimate goal is to provide the groundwork for quantitative predictions needed to engineer surface properties.

Major Program Achievements (over duration of support):
Key accomplishments include: determining the atomic-scale dynamics governing self-assembly of nanoscale patterns on surfaces; real-time observations and atomistic interpretation of the evolution of thin-film microstructure (e.g., twin-boundary motion); quantitative measurements of dislocation dynamics in thin films and their relationships to surface morphology; discovery of new surface growth modes due to surface alloying; measurement of the thermodynamic stability of supported oxide nanostructures; discovery of new fundamental atomic mechanisms for the dynamics of surface morphology. In particular, we have determined the quantitative link between bulk vacancy formation and transport to surface smoothing and the role of substrate atomic steps in the de-wetting of thin films.

Program Impact:
By a combination of experiment and theory, we are among the first to be able to account quantitatively for the kinetic processes that determine the nanoscale surface structure. There is considerable recent interest in the materials science of nanoscale features on surfaces because of their possible applications in the development of new energy technologies. For example, understanding bulk-surface exchange is important for the development of hydrogen storage materials, and metal-oxide surfaces are important industrial catalysts.

Interactions:
J. de la Figuera (Instituto de Química-Física "Rocasolano"); J. I. Cerda (Instituto de Ciencia de Materiales); M. Bode (ANL); P. A. Thiel (Ames Lab); P. Hou, Andreas Schmid (LBNL); C. B. Carter (Univ. Connecticut); S. Chiang (UC Davis); J. B. Hannon (IBM Research); G. L. Kellogg, P. J Feibelman, B. S. Swartzentruber, R. Q. Hwang (SNL/NM); F. Besenbacher (Aarhus).

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
31 Publications (2005-2007), including two articles in Science, 11 articles in Physical Review Letters, and one article in Nanoletters. 2001 MRS Medal (Bartelt); 2001 Nottingham Prize (Thayer). Editorial boards of Physical Review Letters and Surface Science (Bartelt) and Materials & Engineering Reports (McCarty).

Personnel Commitments for FY2007 to Nearest +/- 10%:
N. C. Bartelt (100%), K. F. McCarty (80%), K. Thuermer (100%), J. C. Hamilton (20%), J. P. Pierce (post-doc) (100%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $1150K **FY06 BA** $1034K **FY07 BA** $1034K

Laboratory Name: Sandia National Laboratories
B&R Code: KC020101

FWP and possible subtask under FWP:
FWP Dynamics and Structure of Interfaces and Dislocations
Subtask on: Atomic Structure and Function of Internal Interfaces

FWP Number: SCW 604

Program Scope:
This sub-task seeks to establish the basic principles that control the structure and function of internal interfaces. Over the course of this project, we have advanced from an initial emphasis on grain boundaries in simple metals to more complex, planar and three-dimensional heterophase interfaces. An area that is of growing interest is the exploration of the structure and behavior of interfaces in thermoelectric alloys. A central aspect of much of our work is to determine the nature of interfacial defects. Just as bulk crystal behavior is dominated by the properties of lattice defects, interfacial processes are similarly controlled by the point defects (e.g., vacancies and impurities) and extended defects (steps, dislocations, and junctions) present on the interface. It is also critical to understand how interfaces are controlled by composition. To address such questions, we combine detailed experimental observations using atomic resolution microscopies with comprehensive theory and modeling, encompassing electronic structure, atomistic, and continuum simulations. Throughout, our approach is to employ both experimental and theoretical tools to obtain a basic scientific understanding of the structural elements, interactions, and excitations that govern interfacial behavior. Ultimately, a comprehensive picture of how these structural elements work in concert will improve our ability to predict and control a diverse range of interface-mediated materials processes.

Major Program Achievements (over duration of support):
Key accomplishments include: Discovery of hexagonal-close-packed grain boundary phase in gold. Explanation of size dependence for shape distributions in embedded metallic precipitates. Quantitative analysis of size effects on grain boundary structure. Discovery of grain boundary interactions through extended stacking fault formation. Analysis of defaceting grain boundary transition and discovery of new faceting mechanism. Discovery of mechanism for heterophase misfit accommodation through an interfacial reconstruction at the Ag(111)/Ru(0001) interface. Development of a quantitative theory for planar offsets at heterophase interfaces. Development of continuum models to study the influence of dislocations on phase separation in binary alloys.

Program Impact: By coupling simulation and microscopy of grain boundaries and heterophase interfaces, we have developed quantitative models that explain a wide range of complex experimental observations. We are increasingly applying this approach to functional materials for energy systems, investigating, for example, the role of interfaces in thermoelectric materials.

Interactions:
Uli Dahmen, NCEM/LBL; C.B. Carter, University of Minnesota; Y. Mishin, George Mason University; A. Voter, LANL; S.M. Foiles, SNL/NM; R.C. Pond, Univ. of Liverpool, UK; E. Johnson, University of Copenhagen, Denmark; E. Marquis, Oxford University; C. Hetherington, Oxford University; M. Haataja, Princeton University.

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
D.L. Medlin: Chair 2006 Gordon Research Conference on Physical Metallurgy.
J.C. Hamilton: Organizer of symposium at the Fall 2005 Meeting of the MRS.
F. Léonard: invited speaker and panelist at Nanocommerce conference; member of advisory committee for joint chemical/semiconductor industry research for National Nanotechnology Initiative.

Personnel Commitments for FY2007 to Nearest +/- 10%:
D. Medlin (60%), J.C. Hamilton (40%), F. Léonard (30%), O. Uche (post-doc) (100%), J. Sugar (post-doc) (100%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA: $701k **FY06 BA:** 660K **FY07 BA:** 683K

Note: In FY07 the tasks under FWP SCW604 on "Metallic Interfaces and Dislocations" and "Alloying at Surfaces and Interfaces" were combined to form the present single task. The amounts shown for FY05 and FY06, which predate their combining, are for BOTH tasks.

Laboratory Name: Sandia National Labs
B&R Code: KC020102

FWP: Mechanics of Small Length Scales

FWP Number: SCW 93221

Program Scope: This program investigates the basic principles of the mechanical response of materials down to the nanoscale. Experiments and theory are used to obtain atom-level control and understanding of properties. These include the elastic and plastic deformation of bulk and nanostructured materials, the thermal evolution of a material's micro- and nanostructure, anelastic relaxation and mechanical coupling in micro- and nanostructures, strain-driven growth and morphology evolution, and nanostructure synthesis.

Major Program Achievements (over duration of support): Collectively, this work spans length scales ranging from single atomic defect mechanical relaxation up to microscale morphological evolution. We have brought new understanding to such diverse mechanical phenomena as plastic deformation in nano-structured materials, mechanisms of abnormal grain growth in polycrystalline materials, strain-controlled self-assembly of ordered nanostructures, and atomic-scale defect relaxation in nanoresonators. Specific program highlights include:

<u>Nanostructured Materials</u>: **Direct *in situ* TEM evidence for grain-boundary processes, large lattice strains and simultaneous dislocation propagation during deformation of nano-grained Ni. **Nanocrystalline Ni found thermally unstable to abnormal grain growth with nanoscale defects (relates to Theory of Microstructures). **Strengthening of metals by dense nano-precipitates understood quantitatively for He bubbles. **Developed new understandings of origin of tensile stress in metal films due to island coalescence.

<u>Theory of Microstructures</u>: **First physically-based model for nucleation of recrystallization from deformation substructure. **New MD method for computing mobility of flat grain boundaries with/without solute. **First comprehensive data set for the energy and mobility of nearly 400 high-angle grain boundaries. **First proof that genetic algorithms exceed simulated annealing for structure optimization. **New scaling theory for 2D/3D grain boundary networks proving R-curve behavior is intrinsic to polycrystals.

<u>Advanced Growth</u>: **Developed novel real-time diagnostics for thin film growth: energy dispersive x-ray reflectivity/multibeam optical stress sensor/light scattering spectroscopy. **Quantitative understanding of morphological evolution of heteroepitaxial SiGe quantum dot arrays. **Kinetically-controlled heteroepitaxial self-assembly to produce ordered functional nanostructures. **Identified fracture energetics and slip processes in strained III-nitride heterostructures. **Identified complete epitaxial relationship for ZnO nanorods grown on Ag.

<u>Dissipation and Coupled Systems</u>: **Developed new capability for measuring defect-related anelastic relaxation in micro- and nanoresonators in flexure and shear. **First measurements of defect distributions in amorphous carbon and diamond resonators. **Developed MD method for identifying atomistics of anelastic relaxation for the split-interstitial defect in silicon. **Demonstrated mechanical mode coupling in 1-D and 2-D microresonator arrays as a probe of heterogeneity.

Program impact: Obtained new understanding of the mechanisms of strengthening materials via nanostructuring and developed new computational methods to predict the evolution of micro and nanostructure. This enables the design and performance prediction of new high performance materials. The novel real-time growth diagnostics permit new understanding of the energetics and kinetics of heteroepitaxial self-assembly, leading to the controlled synthesis of nanostructures for mechanical, optical, and electronic applications. Anelastic relaxation studies in thin films are used to identify mechanical defects that are active in materials deformation and thermal evolution.

Interactions: On-going collaborations with 24 institutions including government and universities.

Recognitions, Honors and Awards: Floro: MRS BoD 02-04, MRS Public Outreach Chr, MRS Mtg Chr 01 **Follstaedt**: R&D100 04. **Holm**: NMAB 04-10, TMS BoD 04-07, 08-10 THERMEC 06 & 09 Intl Sci Comm, PRICM5 org 04, NWU John Dorn Lecturer 05. **Hsu**: AAAS Fellow, APS Fellow. MRS BoD 05-07, Treasurer 06-07, Mtg Chr 04. APS DMP EC, 04-07. SSC editorial board since 05. **Sullivan**: Editorial BoD IJNST 07
Invited presentations since 1995: 126 Archival publications since 1995: 128

Personnel Commitments for FY2006 to Nearest +/- 10%: Follstaedt 30%, Friedmann 20%, Hearne 10%, Holm 30%, Hsu 10%, Knapp 20%, Modine 10%, Sullivan 30%, Wendt 10%

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA: $1,030K **FY06 BA:** 1,030K **FY07 BA:** 1,030K

Laboratory Name: Sandia National Labs
B&R Code: KC020103

FWP: Atomic Scale Surface Phenomena

FWP Number: SCW 93219

Program Scope: Our goal is to develop an atomic-scale understanding of physical and chemical processes at surfaces and interfaces in three major thrust areas: (1) adhesion and wetting, (2) localized corrosion, and (3) surface nanostructure formation. Our approach is to combine state-of-the-art experimental probes with modern theoretical techniques to produce the scientific understanding necessary to predict and control macroscopic materials properties.

Major Program Achievements (over duration of support): (1) We revolutionized fundamental research in surface nanomechanics by inventing the Interfacial Force Microscope (IFM), the world's first (and only) scanning probe instrument that can simultaneously measure normal and lateral forces throughout the attractive/repulsive interaction regime. We used the IFM to understand two-stage plasticity in nanoscale contacts, interphase mechanical properties in nanocomposite materials, the origins of friction in alkanethiol monolayers, and how liquids behave at solid surfaces (including studies to answer the 147-year controversy as to why ice is so slippery). (2) We discovered that when aluminum is exposed to water, nanoscale open pores develop at the oxide surface and these pores are linked to aluminum pitting in the presence of aggressive species. We showed that these pores initiate as voids at the oxide/metal interface and grow towards the surface, with the highest concentrations developing at high-curvature surfaces. We found the first evidence of locally induced oxidation of the copper surface in naturally aerated acidic media. (3) We discovered important new mechanisms for dynamic surface processes including a step-overgrowth process during surface alloy formation, a remarkable self-assembly process for Pb atoms on Cu surfaces, spontaneous stripe formation on Si, and exchange- and vacancy-mediated surface diffusion. We developed new surface probes including atom-tracking scanning tunneling microscopy and spatially resolved LEED-IV analysis.

Program Impact: (1) The IFM is finding broad application in the international research community. A completely new concept using our patented Laser-Interferometer, Force-Feedback configuration promises significant gains in user-friendly operation, sensitivity and speed. (2) Our approach of using engineered defects in controlled oxides to investigate the early stages of pitting allows us to address outstanding questions in corrosion science in a controlled manner. The recent Cu oxidation work clearly shows the importance of near-surface pH changes that can drive corrosion processes. (3) Surface nanostructure research is providing new insights on the microscopic origins of thin-film growth and surface self-assembly processes. Over the years, our research has been highlighted in *Science*, *Nature*, *Physics Today*, *Popular Science*, *Popular Mechanics*, *Wall Street Journal, MRS Bulletin, etc*.

Interactions: Princeton U., U. Houston, U. Minnesota, Carnegie Mellon, U. Wisconsin at Madison, South Dakota School of Mining and Tech., U. Texas at Austin, Arizona State University, U. Western Ontario, Ohio State, North Carolina State, Rutgers U., U. of Twente (Netherlands), RWTH (Aachen), U. Texas at El Paso, New Mexico State, U. New Mexico, U. New Hampshire, Brookhaven Nat. Lab, Los Alamos Nat. Lab, IBM Yorktown Heights,

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Five BES/MS Awards (Houston, Kellogg (2), Feibelman (2), Swartzentruber); 1996 AVS Welch Award (Feibelman); 1997 AVS Peter Mark Award (Swartzentruber); DOE OER's Young Scientist Award (Swartzentruber); 2001 Materials Research Society Medal (Bartelt); Fellows of the AAAS (Houston), APS (Houston, Feibelman, Kellogg, Bartelt), AVS (Houston, Feibelman, Kellogg, Swartzentruber), numerous editorial boards (PRL, JVST, Prog. in Surf Sci.), conference and symposium organizers, national and international scientific committee positions, and invited talks (>20 in 2005-07).

Personnel Commitments for FY2007 to Nearest +/-10%: (Staff) G. L. Kellogg 40%, J. E. Houston 50%, B. S. Swartzentruber 40%, P. J. Feibelman 70%, W. L. Smith 50%, N. Missert 50%, K. R. Zavadil 50%, P. Kotula 10%; N. W. Moore (post-doc) 60%, E. Bussmann (post-doc) 50%, N. Vasiljevic (post-doc) 70%, R. G. Copeland (technologist) 20%, M. A. Martinez (technologist) 30%.

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA: $1,571K **FY06 BA:** $1,591K **FY07 BA:** $1,491K

Note: The FY05 amount includes 20K in "glue" funding. FY06 amount includes 100K converted from capital to operating.

Laboratory Name: Sandia National Labs
B&R Code: KC 020103

FWP and subtasks under FWP: Novel Electronic Materials
FWP Number: SCW 93222

Program Scope: We seek the fundamental understanding that links atomic structure & nanostructure to the interrelated electrical, optoelectronic, ferroelectric, magnetic, & mechanical properties of advanced materials; using this understanding, we further seek to develop nanoscale manipulations for property enhancement. Subtasks 1 (*Luminescence, Structure, & Growth of Wide-Bandgap Semiconductors*) & 2 (*Atomic Processes & Defects in Wide-Bandgap Semiconductors)* analyze defects, nanostructure, & microstructure in GaN & InGaN alloys that alter carrier transport, recombination, & luminescence. This work is enabled by the continuing development of a unique range of capabilities encompassing growth, experimental characterization, density-functional theory, & modeling. Subtask 3 (*Field-Structured Anisotropic Composites*) explores self-assembly in triaxial fields to produce tailored composites with superior magnetic, transport, & mechanical properties. Subtask 4 (*Complex & Cooperative Phenomena in Disordered Ferroelectrics & Dielectrics)* elucidates cooperative phenomena in disordered quantum ferroelectrics. The coordinated application of experiment, first-principles theory, & modeling is a central theme throughout.

Major Program Achievements (over duration of support):

- Subtask 1: We pioneered use of capacitance-voltage methods to investigate piezoelectric fields and the quantum-confined Stark effect in InGaN/GaN quantum wells (QWs) thereby illuminating the carrier behavior underlying luminescence in III-nitride heterostructures. This led to a new model involving hole-localization that accounts for anomalous Stark shifts observed in these highly strained structures. More recently, we used special heterostructure designs & advanced materials-characterization techniques to study the enhanced (~10X) internal quantum efficiency produced in InGaN QWs when grown on dilute-InGaN heterolayers. The results refute a prominent, but incorrect, carrier-recombination theoretical model based on screening of dislocations by v-defects.
- Subtask 2: An integrated effort including experiments, density-functional theory, & modeling yielded quantitative new understanding of the N vacancy (V_N) & N interstitial (N_I) in GaN. This understanding encompasses structure, diffusion, reactions with H & Mg dopants, & their technologically important consequences for p-type doping. Recent achievements include the prediction & experimental detection of the bound complex $MgHN_I$; measurement & prediction of the temperature-dependent diffusivity of N_I; and a predictive model of the device-performance-limiting interplay of dopants, H, & V_N during growth & annealing of p-type GaN.
- Subtask 3: We discovered that time-varying, triaxial magnetic fields enable synthesis of a variety of new particle composites with exceptional properties that facilitate chemical, pressure, & thermal sensing with extraordinary response. These studies include new theoretical models describing the field-influenced dynamics of mixing & structuring, as well as the actuation of composites in magnetic fields. In response to 2007 BES-Program-Review feedback, we have resubmitted our subtask on *Field-Structured Anisotropic Composites* as a separate FWP.
- Subtask 4: In studies of compositionally disordered ABO_3 ferroelectrics, we discovered & elucidated a crossover to a relaxor state with only short-range order, confirmed by the interplay of pressure (favoring the relaxor) & a biasing electric field (promoting long-range order). Because of the loss of key personnel (Samara & Venturini), this task will be redirected in FY08 towards investigating the electronic properities and growth of graphene.

Program impact: Subtasks 1& 2 increased the basic-science knowledge base for solid-state lighting, whose potential U.S. energy savings is $ 30 billion per year. Subtask 3 obtained four patents on new field-structured composites impacting sensor & actuator technologies. Subtask 4 produced breakthroughs in the understanding relaxors, a premier topic in ferroelectricity. In the last 3 years, the combined subtasks produced 41 publications.

Interactions: In last 3 years – 17 universities & research institutions; 2 semiconductor companies.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP): In last 3 years – presented 11 invited/plenary papers, reviews, & talks; organized/chaired 5 conferences, symposia, & workshops; editor for 1 scientific journal; 1 best-paper prize; 1 PhD awarded; 1 Distinguished-Staff-Member appointment.

Personnel Commitments for FY2007 to Nearest +/- 10%: (1) Lee 10%, Smith 20%, Moran 10%, Crawford 10%, Banas 10%, Koleske 20%, Thaler 10%, Russell 20%; (2) Myers 20%, Vaandrager 20%, Wright 10%, Wampler 10%, Van Deusen 10%, Armstrong 15%; (3) Martin 30%, Read 85%, Huber 10%; (4) Venturini 50%, Samara 20%.

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA: $1,450 K **FY06 BA:** $1,388 K **FY07 BA:** $1,388 K

Note: The FY05 amount includes 33K in "glue" funding.

Laboratory Name: Sandia National Labs
B&R Code: KC 020105

FWP: Research Assessment and Performance Measures

FWP Number: SCW 8874

Program Scope:
Pursues basic and applied social science research to provide managers with a set of tools to improve the rate of innovation and promote excellent research, including: a conceptual framework, the Research Profiles approach, that identifies key elements in the research environment; evaluation tools, including an in-depth survey, for assessing and improving research environments; performance management systems, including real-time measures of S&T progress, that link specific performance to specific research environments; and a conceptual framework for assessing a nation's production of knowledge and innovation that identifies bottlenecks at organizational, sector, and national levels.

Major Program Achievements (over duration of support):
The Research Profiles approach relates research strategy and outcomes to organizational structures and tasks, which can be used to inform managerial practice. The Research Environment survey has been extended to measure and assess intra-organizational research networks. National and international teams have been assembled that allow for access to new skills and new research sites and a leveraging of the BES funding. Over the last four years we have had BES-sponsored work in five refereed journals, one reprint in a student publication, and one book chapter. In 2007 alone, six papers were accepted for publication. We have been approached by a number of evaluation teams interested in employing our research tools and frameworks.

Program impact:
The approach developed in this FWP has been recognized by the National Science Foundation (NSF) with a significant award through the Science of Science and Innovation Policy (SciSIP) initiative. With NSF support, we will apply our tools and frameworks in six national laboratories to help inform policy discussions on national science and technology investments. Ongoing work with the Center for Satellite Applications and Research (STAR) at NOAA has facilitated the successful implementation of a number of organizational changes, leading to a four-fold increase in scientific productivity.

Interactions:
Internal: Sandia ST&E Strategic Management Unit and Centers, LDRD; MESA Tech Operations Pilot.
External: NSF Grant to U. of Maryland for Science of Science and Innovation Policy (2007-2010); Focus groups and surveys at BNL, PNNL, Ford, STAR in NOAA; U. Mich., USC, GWU; U.S. Federal Agencies and OSTP; Washington Research Evaluation Network, European RTD Network; NRC Canada; Canadian Academy of Health Sciences.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP):
G. Jordan, elected AAAS Fellow 2007
J. Hage, J. Mote, Best Paper Award, Atlanta S&T Policy & Innovation Conference, 2007
G. Jordan, J. Hage, J. Mote, National Science Foundation award ($448K), Science of Science and Innovation Policy

Personnel Commitments for FY2007 to Nearest +/- 10%:
G. Jordan (30%); Jerald Hage, U. Maryland (10%); Jonathan Mote, U. Maryland (80%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $ 226k **FY06 BA** $ 226k **FY07 BA** $226k

Laboratory Name: Sandia National Labs
B&R Code: KC020105

FWP: Biointegration

FWP Number: SCW 93411

Program Scope: This project involves fundamental materials science studies at the intersection of biology, nanomaterials, and integrated systems. It represents the recent merger of two smaller projects: 1) Active Assembly of Dynamic and Adaptable Materials, which involves learning how to exploit active biomolecules such as motor proteins and microtubules to transport, assemble, and reconfigure nanomaterials, and 2) Artificial Biocompatible Semiconductors for biosystem/material interfaces which involves learning surface functionalization for biocompatibility, processing into micro/nanocavities, and physics of nano-optical transduction for studying biological "soft matter" (biomolecules, pathogens, organelles, and cells) on material surfaces.

Major Program Achievements (FY05-07):
Active Transport of Nanomaterials: Stabilized active proteins (motor proteins and microtubules) were produced for use in artificial systems via both genetic engineering and chemical crosslinking. Genetic engineering was also used to insert an "on-off switch" or "molecular shackle" into kinesin motors for controlling transport. Monolayers containing kinesin motors were used to propel microtubule shuttles plus associated nanoparticle cargo within patterned microfluidic devices. Fundamental nanomechanics studies of cargo loading/unloading were performed. Actin "comets" were explored as a way to use active protein polymerization for cargo transport and propulsion.
Active Nanocomposites: Artificial Microtubule Organizing Centers - central particles have been used to organize polar-oriented arrays of microtubules as scaffolds for directing motor protein-cargo motions. Simulations are directing experiments aimed at using such constructs to move and assemble nanomaterials to duplicate processes such as diatom assembly and the color changing system of the chameleon. Rotating-Ring Nanocomposites – Mechanisms were developed to show how the kinetic energy from kinesin motor transport leads to the formation of unusual rotating-ring nanocomposites containing microtubules and quantum dots.
Biocompatible Semiconductors: A nano-optical transduction method for high-speed, ultra-sensitive spectral analysis of nanoparticles was developed based on nano-squeezing of light within submicron semiconductor laser cavities. The laser cavity uses high ($\sim 10^4$) semiconductor gain to amplify signals from tiny particles, allowing ultrafast detection and identification. Using a newly developed technique called nanolaser spectroscopy, the refractive index of nano-bio particles (mitochondria and other organelles in cells) was determined. Large refractive index changes were measured in genetically engineered bioparticles.

Program Impact: The Active Assembly activity has shown that energy-consuming proteins can assemble and manipulate materials in new ways that are not limited by diffusion and energy minima constraints encountered in the classical nanomaterial self-assembly. The project also highlights a new transport mechanism for microfluidic systems, impacting "on-chip" analyses for Homeland Defense (DARPA). The Biocompatible Semiconductors project discovered Nano-Squeezed Light Spectroscopy that has widespread application, including analysis of genetically manipulated yeast mitochondria for high-efficiency ethanol production, detecting biowarfare agents like anthrax spores, and measuring composition and distribution of synthetic organic and inorganic nanoparticles.

Interactions: Co-investigator H. Hess (U. Florida), R. Haddon (UC Riverside), A. Barhorst (Texas A&M), D. Bear + J. Oliver (U. of New Mexico), A. Parikh (UC Davis), C. Yip (U. Toronto), K. Kurihara (Tohoku Univ., Japan), R. Naviaux (UC San Diego), K. K. Singh (Roswell Park Institute, NY), and M. F. Gourley (NIH).

Recognitions, Honors and Awards (FY05-07):
1) Active Assembly - 2005 Research Prize, German Phillip Morris Foundation (Hess), Symposia Organizers/Chairs 2 MRS Meetings + 2 AAAS Meetings, invited participant "Frontiers in Engineering" (Nat. Acad. Eng.), featured in Popular Science (20 incredible inventions list (06)), best poster (06 Spring MRS), 18 publications (3 invited) + 26 invited talks. 2) Biocompatible Semiconductors - ACS Most Highly Accessed Article in *BioTechnology Progress*. Cover Article (Nanotech. in Biomed. J.), *APS News* March Meeting top ten news article (05). 7 publications, 6 invited talks, & two Conf. Organizer roles (BioMicroNano Symposium, Nanoscale Imaging & Sensing).

Personnel Commitments for FY2007 to Nearest +/- 10%:
Bunker 30%, Gourley 50%, Bachand 30%, Osbourn 50%, Sasaki 45%, Boal 30%, Spoerke 35%, McDonald 60%

Authorized Budget (BA):
FY05 BA: $1,381 K **FY06 BA:** $1,197 K **FY07 BA:** $1,197 K

Note: The FY05 amount includes 160K sent to the Univ. of Washington.

Laboratory Name: Sandia National Laboratories
B&R Code: KC020202

FWP and possible subtask under FWP:
Quantum Electronic Phenomena and Structures

FWP Number: SCW 93220

Program Scope:
Electronic and optical properties in MBE/CVD grown and/or lithographically patterned nanoelectronic structures. Three subtasks: 1) quantum transport in structured semiconductors, including quantum transport, coherence, and Bloch oscillations in 2D quantum dot superlattices and heterostructures, electron-hole bilayers, 1D quantum wires, and theoretical investigations of exciton physics; (2) nanostructure synthesis and growth, and (3) ultra-fast optical studies, with a focus on collective excitation modes in nanostructures.

Major Program Achievements (over duration of support):
Electron-hole Bilayers: We have fabricated the first completely undoped electron-hole bilayers. Coulomb drag measurements show a dramatic increase in magnitude at low temperatures for a bilayer system with a narrow barrier of 20 nm, a signature of exciton formation and possibly also of exciton condensation.
Coulomb drag in double one-dimensional wires: Analysis of tunneling spectroscopy in separately contacted 1D wires shows good agreement with a non-interacting model of electron tunneling. Coulomb drag devices are currently being fabricated and tested. The new design allows a more uniform wire density.
Dense, Aligned Arrays of GaN Nanowires: We demonstrated epitaxial growth of dense, highly aligned GaN nanowires on unpatterned r-plane sapphire substrates, with alignment enhanced by a collision-based mechanism. Optical & electrical properties were shown to be strong functions of impurities, likely carbon.
Ultrafast Optical Measurements: We discovered unusual soliton dynamics in soft glass SF6 photonic crystal fibers. We have also examined device-relevant carrier dynamics in GaN nanowires, revealing carrier transfer into defect states responsible for undesirable yellow luminescence on a time scale of less than 500 fs.
Theoretical Studies of Transport in Low-dimensional Systems: We studied the time-dependent and steady-state current of a periodically modulated quantum wire superlattice in an arbitrary electric field. We also found that a tilted magnetic field modulates the tunnel-coupling between two adjacent quantum wires.
Bloch Oscillations and Quantum Transport in Quantum Dot Superlattices: We observed evidence of Bloch oscillations, and probably a phase transition from quantum Hall (QH) ferromagnetism to QH spin glass.
Fractional Quantum Hall Effect (FQHE): We observed a very complex electronic transport behavior in the second Landau level (SLL). Residual disorder is shown to have an important impact on the energy gap at the even-denominator nu=5/2 FQHE state. Spin polarization of the FQHE in the SLL was also studied.

Program impact:
The research project described in this proposal is a multidisciplinary, multi-institutional collaboration. The focus of this project is the physics of quantum electron transport phenomena in semiconductor nanostructures, as well as the discovery of new electron condensates. This topic is at the frontier of the field of condensed matter physics, integrates well with the expertise and interests of the participating personnel and institutions, and further extends their work in exciting new directions. This is one of the world's leading activities in this area.

Interactions:
Collaborations have been established with Columbia (H. Stormer), Princeton (D. Tsui), Bell Labs (L. Pfeiffer), Caltech (J. Eisenstein), UMD (S. Das Sarma), McGill (G. Gervais), Rice (R. Du), ARL (D. Huang), and the NHMFL. This project has enhanced collaborations between SNL, LANL and UNM.

Recognitions, Honors and Awards:
Chairs of EP2DS-16 (Simmons, Lilly); Guest Eds. for Physica E (Lilly, Pan, Simmons); A. Taylor, AAAS Fellow (2007); V. Klimov, LANL Lab Fellow (2003); J. Simmons, APS Fellow (2002); Invited presentations at: 2005 APS March Mtg (Reno), EPQHS05 (Pan, Lilly), LT24 (Pan); PPHMF5 (Pan), QHSYST06 (Pan); EPQHS07 (Pan), ICSI5 (Pan), QPEQHS (Lilly), ICSCE4 (Lilly); many invited seminars; 1 Ph.D. thesis (Seamons, 2007); > 40 pubs.

Personnel Commitments for FY2007 to Nearest +/- 10%:
Pan 50%; Lilly 30%, Lyo 30%, Reno 30%, Klimov 20%, Taylor 20%, Prasankumar 20%, Brueck 20%, Wang 30%

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $1,190K **FY06 BA** $1,100K **FY07 BA** $1,100K

Laboratory Name: Sandia National Labs
B&R Code: KC020301

FWP and possible subtask under FWP: Molecular Nanocomposites

FWP Number: SCW 93223

Program Scope: 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) evaporation-induced self-assembly and interfacial assembly, 3) programmable nanomaterials, reconfigurable hosts, and nanocomposites that combine both elements, 4) understanding of assembly mechanisms and structure, and 5) properties of nano- to microscale self-assembled materials (e.g., transport, electronic and optical behavior, interfacial chemistry, etc.).

Major Program Achievements (over duration of support): ***Nano-building block synthesis:*** Demonstrated that the structure of precursors used in nanocrystal synthesis controls morphology and phase. Complex nanomaterials and TiO_2 wires synthesized with an aspect ratio > 100. ***Self and Directed Assembly:*** Assembly of 3D gold NC/silica arrays (Fan *et al. Science*, 2004) extended to include semiconductor and magnetic NCs with spherical and cubic shapes. Developed new method to synthesize *fcc* phase FePt nanorods by confining decomposition and reduction reactions within reverse cylindrical micelles. ***Interfacial Assembly:*** Patterned SAMS on self-assembled mesoporous films used to direct liposome fusion and transmembrane protein localization and function. Dendritic metal nano-disks prepared using liposomes and lipid bicelles as molds. Monte Carlo simulations indicate that the metal dendrites rapidly evolve into a novel ripening-resistant holey sheet topology that preserves active high surface area for catalytic metals (eg platinum, palladium). ***Self-assembly:*** Discovered a new approach, cell-directed assembly, in which living cells direct the formation of functional bio/nano interfaces, producing 3D chemical gradients and localization of added inorganic and biological nanocomponents. ***Nano-assembly characterization:*** Developed high-speed ^1H and ^1H-X nucleus NMR correlation method to probe interactions and domain sizes on the nanoscale in self-assembled materials. Used NMR to investigate the phase space and kinetics of magnetically directed self-assembly in CTAB based systems. ***Nano-scale functionality:*** Probed long-range forces between submerged superhydrophobic surfaces using interfacial force microscopy. Showed unprecedented ultra-long range hydrophobic interactions due to cavitation/capillary drying of intervening water. ***Programmable nanomaterials***: Developed self-assembled monolayers that can be reversibly programmed with heat, light, or electric fields to control interfacial interactions or grab specific functional groups. ***Reconfigurable hosts:*** Developed structured lipid bilayer membranes that can form 2D architectures. Elements were introduced into the membranes that spontaneously organize in response to chemical recognition events. ***Programmable nanocomposites:*** Programmable films and lipid bilayers have been used to coat gold nanorods. By mediating interaction potentials, the rods can be organized into either open end-to-end or dense side-to-side networks. ***Conducting polymer/oxide interface:*** Demonstrated that processing and modification of oxide surface affects interfacial polymer morphology.

Program impact: This program has gained worldwide recognition (ISI top 20 paper of decade), and has stimulated new research in nanoscale assembly at soft 3D interfaces, and has attracted new funding from NIH, AFOSR, and ARO. The mixing of programmable elements with reconfigurable hosts should enable complex nanocomposites whose assembly and reconfiguration capabilities rival those of living systems for tasks such as energy transfer, light harvesting, and information storage. Cell directed assembly developed as model system to understand the influence of nanoconfinement on cellular behavior. New internal programs based on nanocluster materials were initiated for radiation detection, photovoltaics, catalysis, and taggants for homeland security. The new fundamental knowledge of super-hydrophobic surfaces will help into explain long-range hydrophobic interactions implicated in protein folding.

Interactions: University: 39 profs./26 universities National Lab: LANL/LANL(LANSCE)/LBNL/LLNL

Recognitions, Honors and Awards: Pubs. in Science, Nature, Nature Materials, Nano Letters, Phys. Rev. Letters, JACS, etc; MRS Grad. Student Gold Award (Baca '05), UNM Research Excellence Award (Brinker '05), Rutgers Distinguished Alumnus Award & UNM Regent's Professorship (Brinker '06), AAAS fellow (Hsu '07), R&D 100 Award (Fan, Brinker '07), MRS symp organizer (Hsu), MRS Board and Treasurer (Hsu), Editorial Boards: *Nanotechnology* (Shelnutt), *Small* (Brinker), *J. Nanomaterials* (Brinker); 3 BES awards

Personnel Commitments for FY2007: Boyle (30%), Alam (40%), VanSwol (30%), Fan (20%), Brinker (20%), Shelnutt (20%), Voigt (10%), Bunker (20%), Sasaki (20%), Wheeler (25%), Huber (30%), Hsu (10%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA: $1,780K **FY06 BA:** 1,525K **FY07 BA:** 1,075K