

Laboratory Name: Ames
B&R Code: KC-02-01-02

FWP and possible subtask title under FWP: Mechanical Behavior and Defects in Solids

FWP Number: AL-90-501-003

Program Abstract:

This program focuses on understanding and modeling the mechanical behavior of solids by elucidating the evolution, mutual interactions and collective behavior of crystalline defects from the atomistic to the continuum scale. Ab initio calculations, combined with tight-binding and embedded atom model potentials, are employed to examine lattice stability and the nature and energy of elastic properties, phonon modes and structures of defects. Three-dimensional, fully anisotropic dislocation dynamics simulations and homogenization theories are being developed and used to describe the collective behavior of dislocations over the full range of length scales. The fundamental advancements achieved from these atomistic and simulation studies are being applied to understand the electronic, physical, mechanical, and chemical factors leading to the extraordinarily high room-temperature ductility (>20% elongation) in a class of rare-earth B2 (CsCl-type) intermetallic alloys that were discovered at the Ames Laboratory. The critical mechanical testing experiments and subsequent optical metallographic, SEM and TEM studies on these new RM compounds (where R = rare earth and M = a late transition or main group metal) also serve as a source for the guidance and validation of our modeling and simulation approaches. Late in the year a new task, focused on studying the origins of strengthening in small-sized metallic samples, was introduced.

Program impact:

The work in this project provides important insights into dislocation reactions in highly anisotropic solids, strain-induced phase transformations, twinning-assisted slip, and grain-boundary dislocation sources, as well as their effects on the deformation behavior of polycrystalline solids, with a focus on understanding the anomalously high ductility of the RM B2 intermetallics and, in the long term. Recent simulations have provided important insights in the mechanisms of plasticity in small-scale samples.

FY 2009 Authorized Budget (New BA):

\$690K

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

S.B. Biner (PI, 100%), Kai-Ming Ho (PI, 10%), R. LeSar (FWP Leader, 10%), A.M. Russell (PI, 10%), C.Z. Wang (PI, 20%); 2 Assistant Scientists (60%); 2 Postdoc (200%); 3 Graduate Students (120%)

Interactions:

S. Agnew (Univ. Virginia) twinning; A. Bastawros (ISU) nanoindentation; E. George (ORNL) embrittlement; Y. Grin (Max Planck Inst.) electron localization function calculations. J. R. Morris ORNL. J. Li (OSU) and S. Yip (MIT) calculations and modeling of dislocation structures; Gun-Do Lee (Seoul National University, South Korea) vacancy defects in graphene. N. Ghoniem (UCLA) dislocation dynamics simulations. S. Hu (PNL) Phase-field modeling.

Related Project URL:

(Optional)

Laboratory Name: Ames
B&R Code: KC-02-01-03

FWP and/or subtask title under FWP: Extraordinary Responsive Magnetic Rare Earth Materials

FWP Number: AL-00-501-034

Program Abstract:

Integrated experimental and theoretical investigations of complex metallic systems where, as a result of a small change of an external stimulus, such as temperature, pressure, or magnetic field, the material responds with an intrinsic phase change. This leads to a drastic variation of the majority, if not, all of the physical properties of a material. Model systems under study include intermetallic compounds containing rare earth metals (R) such as Gd, Tb, Dy, etc., main group elements (T) such as Si, Ge, Ga, etc., and transition metals such as Fe, Co, and Ni. We focus on a wide range of stoichiometries, including R_5T_4 , RCO_2 , RNi , $(R_{1-x}R'_x)Al_2$, and $La(Fe_{1-x}Si_x)_{13}$ compounds. Common to different model systems are potent changes of the electronic transport behavior (e.g., electrical resistance), shape (e.g. temperature or magnetic field induced strain), and thermodynamic properties (e.g., strong thermal effects), thus highlighting commonalities related to strong coupling of crystallographic and electronic degrees of freedom that span across different families of materials. Our main goal is to uncover the underlying electronic, atomic and microscopic interactions that result in an extraordinarily strong coupling of the electronic (magnetic) and crystal lattices, and therefore, in extensive changes of their atomic and electronic structures, and all derivative properties in these rare earth-based materials. In order to achieve predictive power (and in the future to facilitate the creation of functional materials by design rather than by serendipity) we are developing and validating phenomenological models of transformations that range from magneto-volume to magnetic-martensitic, which is another prime objective of this research.

Program Impact:

Most functional materials are multicomponent systems with electronic, structural and magnetic properties that become more interesting, and potentially, more relevant for future applications as the materials become more and more complex, which is usually achieved by chemical modifications and/or processing. To date, there is sufficient experimental evidence of phase separation, phase-coexistence, and metastability that exist in a variety of materials ranging from metals to insulators. Knowledge of the mechanisms of a phase change driven by a minor stimulus, followed by a major perturbation of properties is of interest for understanding nonlinear relationships in the free energy has both a fundamental and a technological significance, and is crucial for guiding the discovery of new materials, thus providing the foundation to future energy-related applications. Fundamental in nature, this project holds a promise to improve the performance of many functional materials, by developing innovative approaches to the manipulation of properties of materials that may lead to future technological advancements in energy generation, conversion, utilization and efficiency. A few examples illustrating the impacts include:

- smart sensors that require minimum or no standby power using spontaneously generated voltage;
- materials that self-adapt to changing environments using recoverable shape change;
- materials for harvesting thermal or magnetic energy using various thermodynamic effects;
- magneto-electronic switches using drastic changes in the magnetic and electronic transport properties,

all of which occur when a responsive material is driven through a phase transition by either or all temperature, pressure or magnetic field.

FY 2009 Authorized Budget (New BA):

\$1,161K

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

L.S. Chumbley (PI, 10%), K.A. Gschneidner, Jr. (PI, 60%), G.J. Miller (PI, 10%), V.K. Pecharsky (FWP Leader, 20%); 3 Assistant Scientist (220%); 1 Research Technician (100%); 3 Postdocs (200%); 2 Graduate Students (40%)

Interactions:

Collaboration with scientists at the US DOE Argonne National Laboratory; UCLA; National High Magnetic Field Laboratory, Tallahassee, FL; Rutgers University; McGill University, Quebec, Canada.; University of Campinas and Rio de Janeiro, Brazil; University of Zaragoza, Spain; Centre for Advanced Technology, Indore, India; Imperial College, London, UK; and Institute of Physics of Czech Academy of Sciences, Prague, Czech Republic.

Related Project URL:

(Optional)

Laboratory Name: Ames
B&R Code: KC-02-01-03

FWP and/or subtask title under FWP: Complex Hydrides — A New Frontier for Future Energy Applications

FWP Number: AL-04-501-051

Program Abstract:

The purpose of the integrated experimental and modeling effort is to achieve a fundamental understanding of the relationships between the chemical composition, bonding, structure, microstructure, properties and performance of novel hydrogen-rich solids, and as a result, develop predictive tools to enable guided discovery of materials at the atomic scale and controlling processing strategies at the nano-, meso- and microscopic scales. This research is being carried out by a multidisciplinary team of scientists from the Division of Material Science and Engineering Programs and Chemical and Biological Sciences Programs in collaboration with Physics Department at Virginia Commonwealth University. A number of experimental (Ames Laboratory team) and theoretical (Virginia Commonwealth University team) approaches are brought to bear on a variety of complex metal hydrides in order not only to achieve controlled dehydrogenation, but also to accomplish full rehydrogenation and long cycle life of extremely hydrogen rich solids to meet US DOE goals of volumetric and gravimetric hydrogen capacity. We attain this through basic knowledge of transformation mechanisms in complex hydrides-hydrogen systems, thus precipitating discoveries needed for future transition to hydrogen – a renewable, clean, and safe energy carrier.

Program Impact:

Large scale commercial applications of hydrogen are at least 10 to 15 years, and possibly, as far as 25 to 40 years away. Consequently, real progress in solving hydrogen storage problems is required now. While the design of a solid with 25+ wt.% hydrogen appears to be impossible (the four-coordinated carbon holds 25 wt.% H₂ in methane), light metal-based complex hydrides that approach this high gravimetric content of hydrogen do exist. For example, 7.6 wt.% H₂ has been obtained from LiAlH₄ (5.1 wt.% at ambient temperature plus 2.5 wt.% below 150°C), 8.5 wt.% H₂ from Mg(NH₂)₂/LiAlH₄ system below 350°C, and 13.5 wt.% H₂ below 450°C from LiBH₄/SiO₂ system. Some reversibility of Ca(BH₄)₂ and the Li₃AlH₆/Mg(NH₂)₂ system, and direct hydrogenation of AlH₃, so far in low yields but at low P_{H₂}, have been demonstrated.

FY 2009 Authorized Budget (New BA):

\$545K

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

L.S. Chumbley (PI, 10%), V. Lin (PI, 10%), V.K. Pecharsky (FWP Leader, 20%), M. Pruski (PI, 10%);
1 Assistant Scientist (50%); 1 Postdoc (90%); 3 Graduate Students (100%)

Interactions:

We interact closely with P. Jena, a Co-PI from Virginia Commonwealth University and with researches at Sigma Aldrich. We are also aware of activities at the DOE's Center for Excellence in Metal Hydrides at Sandia National Laboratories (we have no formal collaborations with the Center), and those of other researchers throughout the world from their publications.

Related Project URL:

(Optional)

Laboratory Name: Ames
B&R Code: KC-02-01-05

FWP and/or subtask title under FWP: Novel Materials Preparation and Processing Methodologies

FWP Number: AL-06-501-057

Program Abstract:

The growth, control and modification of novel materials, in single crystal and polycrystalline form, represent a national core competency that is essential for scientific advancement. Indeed, many of the major discoveries of condensed matter science during the last fifty years have been made possible by the discovery, growth, control and modification of new materials. The design, synthesis and characterization of new materials that lead to important discoveries, both expected and unexpected, as well as new knowledge and techniques, within and across traditional disciplinary boundaries, are critical components of the DOE-BES mission. Discovery and design of new materials is one of the key, cross-cutting research areas called out in every energy-related basic science materials challenge. In support of this mission, the Novel Materials Preparation and Processing Methodologies project strengthens the materials synthesis mission of Ames Laboratory through:

- Quantifying and controlling processing-structure-property relationships of highly responsive materials (Fe-As based superconductors, magnetostrictive (Fe-X alloys) and ferromagnetic shape memory alloys (Ni-Mn-X alloys)
- Advancing the ability to synthesize and characterize high purity, high quality novel materials, primarily in single crystal form, spanning a range of sizes, through identifying operating limits for growth by defining stable morphological growth regimes;
- Developing unique capabilities and processing knowledge in the preparation, purification, and fabrication of metallic elements and alloys;
- Providing high-purity, high-quality, and well-characterized materials in support of research programs at the Ames Laboratory and throughout the United States (and globally) at other government, academic, and private industrial laboratories.
- Exploring promising phase spaces (either physical or chemical) that we identify as compelling based upon advances in synthesis and / or control of novel materials;

Program Impact: The impact of this program is tremendous. We develop unique, novel synthesis capabilities and processing for the preparation, purification, and fabrication of novel materials in both single and polycrystalline form. These growth protocols and the materials synthesized under this program are used by many other scientific groups throughout the world through the sharing of single crystals for collaborative research. Through these collaborations, we participate in critical experiments where the crystals are vital to the research, often allowing measurements that otherwise would not be possible due to lack of quality or size requirements. Finally, the expertise and processing knowledge generated in this research effort are made available to academic, government and industrial researchers worldwide on a cost recovery basis through the Materials Preparation Center at the Ames Laboratory

FY 2009 Authorized Budget (New BA):

\$1,630K

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

I.E. Anderson (PI, 10%); P.C. Canfield (PI, 10%); L.L. Jones (PI, 50%); T.A. Lograsso (FWP Leader, 30%); R.W. McCallum (PI, 50%); 7 Assistant Scientist (360%); 5 Technical Staff (70%); 2 Postdocs (200%); 1 Graduate Student (20%)

Interactions:

ORNL, BNL, LBL, LANL, Argonne, Naval Surface Warfare Center, U. Maryland, U. Liverpool, U. Debrecen, Inst. High Pressure Physics-Troitsk, INRIM Divisione Elettromagnetismo-Italy, U. Newcastle, INPGrenoble, U. Barcelona, ESRF

Related Project URL:

(Optional)

Laboratory Name: Ames
B&R Code: KC-02-01-05

FWP and/or subtask title under FWP: Structure and Chemistry of Condensed Systems

FWP Number: AL-90-501-002

Program Abstract:

The freezing of liquid metals and alloys provides accessible pathways to a rich and diverse spectrum of materials and structures with a wide range of properties and applicability. Indeed, the phenomenon of morphological selection during the growth of a crystalline phase from its melt is one where nanoscale interfacial mechanisms and microscale morphological effects act in concert with the longer range processes of thermal and chemical diffusion in response to the global forces which drive the overall freezing transformation. Moreover, driving these processes further from equilibrium can lead to new multi-scale structures, along pathways involving highly undercooled metallic liquids, amorphous solids, and metastable crystalline phases. Effective navigation of these far-from-equilibrium dynamical landscapes, however, requires the resolution of several fundamental questions that have been longstanding barriers to advancement in this area. In this project, we seek to understand the most critical unresolved issues, i.e. the structure of liquids and the behavior of interfaces that govern the multi-scale dynamics under these far-from-equilibrium conditions. More specifically, our aims are (i) to quantify atomic-scale structure of metallic liquids and glasses, (ii) identify the atomistic origins of interfacial properties and quantify their role in multi-scale structural dynamics, (iii) incorporate the atomistic structure of liquids and glasses into appropriate solution-based models for the prediction of relative phase stability, and (iv) to predict phase selection and structural dynamics. With potential applications in magnetic, thermoelectric, and various other anisotropic coupled-response materials with diverse functionalities, the goal of this project is to establish the fundamental basis to enable the realization of new materials and new levels of structural control.

Program Impact:

The Ames Laboratory is uniquely positioned for world-leading contribution in this area. By integrating advanced computational methods (Ab initio calculations, density functional theory, molecular dynamics, phase-field modeling, and solution-base thermodynamic modeling) with theory-critical experiments involving state-of-the-art techniques (in situ synchrotron X-ray scattering, high-resolution transmission electron microscopy, atom-probe spectroscopy, levitation melting, and a host of materials processing methods), this effort is *breaking new ground* in the identification and description of short- and medium-range order noncrystalline materials (i.e. liquids and glasses), providing new levels of fundamental understanding regarding the related dynamics, enabling control, prediction, and discovery of new materials through far-from-equilibrium dynamical pathways.

FY 2009 Authorized Budget (New BA):

\$2,198K

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

M.J. Kramer (PI, 80%); M.I. Mendeleev (PI, 100%); R.E. Napolitano (FWP Leader, 50%); R.T. Ott (PI, 100%); Xueyu Song (PI, 10%); D.J. Sordelet (PI, 10%); R.K. Trivedi (PI, 30%); C.Z. Wang (PI, 10%); 5 Assistant Scientist (370%); 4 Postdocs (200%); 7 Graduate Students (230%)

Interactions: (Internal) T.A. Lograsso, Rational Growth Project, R.W. McCallum, Multiferroics Project. (External) X.L. Wang, SNS-ORNL ; D. Miller, ANL; S. David, ORNL; J. Almer, APS-ANL; R. Hyers, U. Mass.; H. Sheng, George Mason U., K. Kelton, Washington U.; M. Asta, U. California; J.J. Hoyt, McMaster U., M. Li, Renmin U. China, Beijing), S. Y. Wang, Fudan U., Shanghai, China), Paul Voyles, U. Wisconsin, G.J. Ackland, U. Edinburgh; A.Karma, Northeastern U.; J. Perepezko, U. Wisconsin; W. Kurz, EPFL-Lausanne; DOE-CMSN.

Related Project URL:

(Optional)

Laboratory Name: Ames
B&R Code: KC-02-02-01

FWP and/or subtask title under FWP: Correlations and Competition between the Lattice, Electrons, and Magnetism

FWP Number: AL-09-510-007

Program Abstract:

The properties of modern novel materials, such as high-temperature superconductivity, multiferroicity, and colossal magnetoresistivity, are all sensitively controlled by correlations and competition among the lattice, electronic, and magnetic degrees of freedom. A complete understanding of the interrelations between these different subsystems and the necessary conditions for enhancing or tailoring desirable physical properties has been identified as a Grand Challenge to the scientific community. Within this FWP, neutron and x-ray scattering are used to directly investigate the structural, electronic, and magnetic aspects of complex ground states, excitations, and phase transitions. The varied expertise of the PIs is employed in a synergistic approach and systems are studied using a wide range of complementary neutron and x-ray techniques. The experimental program is supported by a closely coupled effort in *ab initio* band structure calculations, theoretical modeling, and scattering simulations. Topics investigated include; unconventional superconductivity in iron-arsenide compounds, metal-insulator transitions and multiferroicity in correlated electron oxides, and complex magnetism in rare-earth intermetallic compounds. The program supports the HB1A spectrometer at the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory and the MUCAT sector at the Advanced Photon Source (APS) at Argonne National Laboratory.

Program Impact:

The research program broadens our fundamental understanding of the microscopic interactions that, when properly tuned by chemical doping or other external parameters such as pressure or applied magnetic fields, can lead to novel properties with promising applications in new technology and devices. Joint efforts between this project and the *Complex States* FWP have made a major impact in the study of iron-arsenide superconductors, including measurements of the crystal and magnetic structures as functions of temperature and pressure, magnetic excitations, and phonon excitations. We have identified the microscopic origins of the coupling between both magnetism and superconductivity and structural distortions and how they evolve with chemical composition and applied pressure. This identification provides deep insight into potential mechanisms of superconductivity and will help to guide the discovery of new superconducting materials.

In addition, substantial advancements have been made in our understanding of the origins of multiferroicity, including the role of magnetic incommensurability and frustration in lithium phosphates and the role of rare-earth magnetic ordering in hexagonal manganites. We have also elucidated novel mechanisms of charge ordering and spin polarized conduction in mixed valent magnets with relevance to the area of spintronics.

This FWP continues to be leaders in the development and use of large-scale DOE x-ray and neutron scattering facilities. In particular, this FWP manages and operates HB1A instrument at HFIR and the MUCAT sector at APS which have been reliable and productive instruments that service the Ames Laboratory scattering efforts as well as the general user community.

FY 2009 Authorized Budget (New BA):

\$1,508K

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

V. Antropov (PI, 60%), A. Goldman (PI, 20%); B. Harmon (PI, 10%); R. McQueeney (FWP Leader, 20%); D. Vaknin (PI, 60%); J. Zarestky (PI, 100%); D. Robinson (PI, 100%); Asst. Scientist (100%); 3 Postdocs (270%); 3 Graduate students (100%)

Interactions: Internal—Complex States FWP, P. Canfield, K. Gschneidner, Jr., A. Kaminski, T. Lograsso, R. McCallum, G. Miller, R. Prozorov. External— ORNL, BNL, ANL, LANL, NIST, NASA MSFC, PSI (Switzerland), ISIS (UK), ILL (France), HMI, TU Dresden, FZ Jülich (Germany), HMI (Berlin). Universities: Missouri, Tennessee, Johns Hopkins, Texas, CalTech, Purdue, Oslo (Norway), Osaka (Japan), Washington University, Massachusetts.

Related Project URL:

(Optional)

Laboratory Name: Ames
B&R Code: KC-02-02-02

FWP and/or subtask title under FWP: Photonic Systems

FWP Number: AL-09-510-008

Program Abstract:

This FWP focuses on the design, fabrication, and properties of photonic crystal structures (PC) and the photophysics of luminescent organic semiconductors and organic light-emitting diodes (OLEDs). In this project we aim to control the flow of light and the conversion of light energy into other forms of energy (and vice versa) through the use of artificially designed and fabricated structures. Two of the most exciting and promising developments in physics and engineering are (i) the endowment of photons with revolutionary propagation and spectral properties, through their interaction with novel artificial structures, and (ii) the emergence of organic semiconductors and organic electronics. In this FWP, we continue and integrate these two thrusts. Our overall strategy is to explore the new physics enabled by photonic structures and organic semiconductor materials and devices both theoretically and experimentally and to examine the impact of photonic structures and organic semiconductor materials and devices in areas supporting the mission of DOE in energy-efficient lighting, efficient solar energy utilization, thermophotovoltaics, and novel sensors. We will investigate the behavior of organic semiconductors and photonic structures incorporated into devices in these areas, in particular organic devices. We will leverage our work with our expertise in simulation, design, and fabrication of photonic structures as well as our experience in OLEDs developed in our previous studies under DOE. Over the last 5 years, we have developed a patented economical in-house soft-lithographic method for fabrication of three-dimensional polymer molds. These molds are then coated or backfilled with metal or dielectric materials to achieve three-dimensional (3D) micro- and nano-structures structures with the desired optical properties. In addition to work within the FWP, we also work with other external groups, worldwide to explore new functionalities enabled by new photonic structures. In the study of luminescent organic semiconductors, π -conjugated thin films are studied by photoluminescence and photoinduced-absorption-detected magnetic resonance and the operation of OLEDs fabricated in our experimental group is studied by electroluminescence- and electrical-current-detected magnetic resonance measurements.

Program Impact: Our group is one of the pioneers in the fields of photonic crystals and p-conjugated materials and OLED photophysics, and continues to play a major international role in leading developments in these fields. In the last 4 years, the Ames Photonics group has published 55 papers in this field. In the same period our BES supported work received ~3800 citations. Advances in photon science have critical impact on the mission of DOE in the areas of efficient energy utilization; in particular, the fabrication and design of new photonic materials have the potential to make solar cells and light emitting systems with much better performance than current designs and architectures. Some examples of recent achievements: We designed and fabricated photonic materials whose emission spectrum can be concentrated into a narrow frequency range. The polarization of thermal emission can also be tailored in such structures. We have also demonstrated structures that improve light absorption in solar cells. We developed a novel economical method for wide-area fabrication of three-dimensional patterned structures using soft-lithography. We have also designed surface structures that stopped the divergence and diffraction of light that emerge from a small hole with dimensions smaller than a wavelength. We also discovered that light emitted from the edge of an OLED have a frequency spectrum much sharper than light emitted from the top

FY 2009 Authorized Budget (New BA):
\$693K

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

R. Biswas (PI, 50%); K. Constant (PI, 10%); K.M. Ho (FWP Leader, 10%); J. Shinar (PI, 10%), C.M. Soukoulis (PI, 10%), G. Tuttle (PI, 10%); 1 Assistant Scientist (60%); 3 Postdocs (200%); 12 Graduate Students (680%)

Interactions:

Hong Kong University of Science and Technology, Rensselaer Polytechnic Institute, Canon USA, Fudan University (China), Korea University (Korea), Bilkent University (Turkey), ICX Photonics, Research Center of Crete, Sandia National Labs, FOM Institute (Netherlands), ETH, Zurich, Southampton Univ. (UK), and University Karlsruhe (Germany).

Related Project URL: (Optional)

Laboratory Name: Ames
B&R Code: KC-02-02-02

FWP and/or subtask title under FWP: Complex States, Emergent Phenomena, and Superconductivity in Intermetallic and Metal-like Compounds

FWP Number: AL-09-510-009

Program Abstract: Humanity's quest for materials with better properties is so integral to the fabric of its history that epochs are named after the materials that define them: stone, bronze, iron, and silicon. Currently humanity is desperately trying to develop materials that will allow for improved generation, transport, and even storage of energy. Among these materials, compounds that exhibit correlated electron states, emergent phenomena and / or superconductivity have great promise, but also great difficulties that need to be overcome: problems associated with our need to reliably find, understand, improve and control these promising ground states. New systems are needed both for better properties and for providing further experimental insight that, in turn, can inform and inspire better theoretical understanding. With such systems and understanding we hope to manipulate and control superconducting, magnetic, thermoelectric, and other properties, so as to address humanities pressing energy needs. To this end, the specific scientific goal of this FWP is, to develop, discover, understand and ultimately control and predictably modify new and extreme examples of complex states, emergent phenomena, and superconductivity.

Program Impact: This program is world renowned as a pioneer in the physics of novel, correlated electron and superconducting materials. It consists of leaders in experimental physics with skills ranging from design and growth to advanced measurements at extremes of temperature, field and resolution (magnetic and spectroscopic) as well as leaders in theoretical physics specializing in superconductivity and many-body ground states with over 50,000 citations to their work between them. Through extensive collaborations within the FWP as well as within the Lab unprecedented, rapid, and accurate advances have been made toward understanding systems such as high- T_c superconductors, RNi_2B_2C magnetic superconductors, heavy fermion and quantum critical systems, MgB_2 and, most recently, in the field of FeAs-based superconductivity. As a result of these efforts scientists throughout the U.S. as well as world have a clearer understanding of how to control and even harness some of these properties (for example use MgB_2 as a wire material for the production of less energy consumptive MRI units).

Between Jan. 2009 and Nov. 2009 this FWP has been produced over 80 refereed publications: 43 *Physical Review B*, 14 *Physical Review Letters*, and 3 *Nature*, *Nature Physics*, *Nature Materials*, as well as 23 papers in journals such as *Physica C*, and *Superconductor Science and Technology*. The members of this FWP have given over 30 invited talks over the same time period. This program's recent work on FeAs superconductivity has been recognized as world leading (growth and characterization of first single crystals, determination of the normal and superconducting state anisotropy as well as superconducting gap anisotropy, discovery of new phases, doping studies, etc.) and had over 1000 citations to its work in 2009, even though many of the papers were less than a single year old.

FY 2009 Authorized Budget (New BA):
\$2,144K

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

S. Budko (100%), P. Canfield (10%) [FWP Leader], J. Clem (20%), D. Johnston(10%), A. Kaminski(20%), V. Kogan (100%), R. Prozorov (10%), J. Schmalian (10%), M. Tanatar (100%); 6 postdocs (575%); 12 graduate students (600%)

Interactions: Internal: This FWP has internal interactions with over 15 other Ames Lab PI's, spanning 7 other FWPs. External: *Other DOE labs:* ANL, BNL, ORNL, LANL; *U. S. Universities and Labs:* National High Magnetic Field Lab, NIST, IBM, Naval Research Lab, UIUC and UIC, Ohio State, Cornell, Harvard, Stanford, Notre Dame, Texas A&M, SDSU, U Maryland, LSU, UCSD, Columbia, U of Wisconsin, Rutgers, Rice, U of Missouri; *International Universities and Labs:* U Hamburg, U Pavia, Catholic U Korea, Queen's U (Canada), Hahn Meitner Inst. (Germany), Tech. U Braunschweig (Germany), Risø, ESRF (Grenoble), ILL (Grenoble), CEA (Grenoble), CNRS (Grenoble), ISIS (England), ETH and PSI (Zürich), MPI (Dresden), U of Sherbrook, U of Tokyo, U of Bristol, Inst. of Solid State Physics (Moscow), Max Planck Inst. (Germany), National Inst. of Advanced Industrial Science and Technology (Japan), U of Napoli, U of Tel Aviv, U of Tübingen, U of Orsay, U of Cologne, CBPF (Brazil).

Related Project URL:
(Optional)

Laboratory Name: Ames
B&R Code: KC-02-02-02

FWP and/or subtask title under FWP: Surface Structures Far-from-Equilibrium

FWP Number: AL-09-510-010

Program Abstract:

Phenomena on the nanoscale can be very different from phenomena in the bulk. Either because of dangling atomic bonds at corners and edges of the nanostructure, or because quantum mechanics becomes more important on the nanoscale, unexpected effects and properties emerge. One of the goals of this FWP is to discover robust ways to grow surface-supported nanostructures with less than ~1000 atoms (nanoislands, nanodots, nanowires etc.) with controllable dimensions (height, size, shape) and morphology (flat-top, wedding cake, stepped etc). This requires a better understanding of the many atomistic processes that determine how atoms diffuse and build and retain these structures. The project partly builds on the fact that metallic islands can be grown of identical “magic” height because quantum mechanics requires the confined electrons to “fit” only certain heights. A different goal is to use these custom-made, controllable nanostructures to enhance the rate of atomistic processes (nucleation, adsorption) and the yield of chemical reactions (that do not occur or have low rates on surfaces of bulk materials). We are currently pursuing molecular hydrogen adsorption on Mg nanostructures (which does not adsorb on bulk Mg crystals) and adsorption of oxygen and hydrocarbons (relevant to ethylene oxidation) on Ag nanostructures.

Program Impact:

The program has been highly visible worldwide in understanding key atomistic process in the predictive growth of nanostructures and in using Quantum Size Effects (QSE, i.e. the dependence of confined electronic levels on structure dimensions) to control growth. The unusual uniformity of heights attainable with QSE has stimulated work with other techniques and other groups worldwide (with photoemission, STM/STS, surface X-ray scattering, LEEM, LEED, in-situ conductivity, etc.) and theory (first principles and kinetic Monte Carlo simulations) to verify the effects and confirm them in other systems. A major recent result of these collaborations has been the realization that a surprisingly efficient kinetic pathway exists at low temperatures. The theory members of the FWP have established a network (Computational Materials Science Network) that interacts very closely with other theorists and experimentalists on problems partially related to the results of the FWP. With the more recent emphasis on how to modify reactivity with island geometry and QSE, we aim for an impact on nanoscale catalysis. Over the last year, the group has published two PRLs, have given 10 invited talks to major international conferences and 7 invited presentations at institutions. Previous work in 2007 included a Physics Today article presenting the QSE results to the entire physics community.

FY 2009 Authorized Budget (New BA):

\$418K

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

K. M. Ho (PI, 10%); P. A. Thiel (PI, 10%); M. C. Tringides (FWP Leader, 20%); C. Z. Wang (PI, 10%); M. Hupalo PI (50%); 2 Postdoc (50%); 5 Graduate Students (100%)

Interactions:

U.S. Natl. Laboratories: M. Salmeron (LBNL), N. Bartelt, K.F. Mcarty (SNL-CA) U.S. Institution: R. Diehl (Penn. State Univ.) E. Conrad (Georgia Tech) P. Miceli (Missouri), T. C. Chiang (Illinois), M.Y. Chou (Georgia Tech), F. Liu (Utah), V. Shenoy (Brown) J.W. Evans and D.J. Liu (Ames Laboratory) and the full CMSN group. Foreign Institutions: Fournée (CNRS Nancy France) Tohoku Univ., Nat. Institute Mater. Sci. (Tsukuba), Lappeenranta Univ. Technol., M. Altman (Hong Kong) M. Jalochowski (Lublin, Poland) Z. Chvoj (Prague), Horn von Hoegen (Essen Germany).

Related Project URL:

(Optional)

Laboratory Name: Ames
B&R Code: KC-02-02-03

FWP and/or subtask title under FWP: Nanoscale and Ultrafast Correlations and Excitations in Magnetic Materials

FWP Number: AL-09-510-011

Program Abstract:

Magnetism is a traditional subject, yet one with modern branches experiencing great vitality. One new branch features magnetic materials with nano dimensions exhibiting behavior not encountered in bulk samples. In this FWP the emphasis is on using precise and accurate theoretical and experimental techniques to investigate, understand, and control aspects of magnetic materials where nanometer size dimensions are of importance. Such materials include zero-, one- and two-dimensional magnetic systems (i.e. quantum dots or isolated magnetic molecules, 1-D chains, and 2-D layers or islands). We seek to answer fundamental questions such as how do itinerant characteristics and extended excitations emerge with size? How are magnetic interactions and excitations in magnetic molecules, quantum dots and islands, chains, and layers affected by edges, lines, and different surface substrates? Can we dynamically control the magnetic moment, electronic transport, and optical response by optically pumping selected electronic states? A key approach to these questions is the growth of single crystals of the above magnetic systems with various dimensionalities. Using neutron and x-ray scattering measurements, the exact positions of the atoms are determined, and the emergence of complex magnetic behavior is precisely measured. Accurate theoretical models for these systems are developed. Experimental facilities probe spin interactions (often to milliKelvin temperatures) by NMR, fast optics, highly precise magnetic susceptibility, magnetic x-ray and neutron scattering and magnetic STM techniques. A new approach is to grow uniform (a few atoms in height) magnetic islands on non-reactive substrates exploiting electron confinement. This work has implications for quantum dot devices in spintronics, magnetic recording, ultrafast switches, and qubit technology for quantum computing. The overall goal is to identify clean, prototypical nanoscale model systems where the magnetism can be thoroughly understood experimentally and theoretically, and then to transfer that knowledge to improve or foster applications.

Program Impact:

Magnetic molecules and low dimensional magnetic entities may have important applications in spintronics, quantum computing, or even medicine, where strong paramagnetic species enhance MRI images. There is even local ISU research on nano-magnetic devices controlled by external fields to release encapsulated medicines. This FWP has published over ~200 scientific articles dealing with synthesis, characterization, and theoretical interpretation of magnetic molecules (MM). It has pioneered the application of quantum Monte Carlo (QMC) techniques for analysis of magnetic molecule spin response, and with collaborators it has pioneered distributed computing for classical spin dynamics (having on average 250 TeraFLOPS of machines running at any one time). Samples prepared by this FWP have been shared locally and internationally. Of particular experimental note is the development of a unique tunnel-diode resonator operating down to 15 mK with unprecedented sensitivity of a few pico-emu (four orders of magnitude better than SQUID magnetometers). Recently developed quantum theoretical techniques resulted in a productive collaboration with experimental groups at UC Santa Barbara exploring single spin decoherence of nitrogen-vacancy (NV) centers (qubits) in diamond, with two recent papers published in Science (on the cover in 2008). In FY2009, there were 25 papers published and 9 international invited talks presented. The scientists listed below had >600 citations for their papers published in 2007-2009.

FY 2009 Authorized Budget (New BA):

\$1,078K

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

V. Dobrovitski (PI, 60%); B. Harmon (FWP Leader, 10%); M. Hupalo (50%), D. Johnston (PI, 10%); M. Luban (PI, 20%); R. Prozorov (PI, 10%); M. Tringides (PI, 10%); D. Vaknin (PI, 20%); 2 Assistant Scientists (130%); 6 Postdocs (250%); 6 graduate students (140%)

Interactions:

Internal (other Ames Lab FWPs) - P. Canfield, J. Schmalian, R. W. McCallum, A. Goldman, and R. McQueeney. Internal (with ISU Physics Department) – J. Wang (pump/probe, femtosecond optics), Y. Furukawa (NMR to 100mK). External Foreign: MOU with Jülich and numerous collaborations in Germany, Netherlands, France, UK, Italy, Japan, Poland, Greece, and Taiwan. Domestic: HFIR at ORNL, UT (optics), UCSD (heat capacity), UCSB (NV-centers), APS at Argonne, Utah, Georgia Tech, ASU and Notre Dame.

Laboratory Name: Ames
B&R Code: KC-02-02-03

FWP and/or subtask title under FWP: Exploratory Development of Theoretical Methods

FWP Number: AL-09-510-012

Program Abstract:

The scope this FWP is to generate new theories, models, and algorithms that will be beneficial to the research program at Ames Laboratory and to the mission of DOE. The need to make quantitative theoretical predictions and to obtain detailed agreement between theory and experiment are crucial for the design, characterization and control of complex materials. To stay competitive with the rapid development of advanced theoretical and computational tools, there is an urgent need to invest time and effort in the exploratory development of theoretical methods. This FWP will focus on the development of theoretical tools to study a broad range of problems in physics, materials science, and chemical as well as biological systems. The generality of these tools allows the cross-fertilization of ideas from one problem to problems in an entirely different area with the common link only existing in the mathematical formulation of the problem. Such leaps across topic areas and in some cases across disciplines are characteristic of the power of a fundamental physics-based approach, facilitated by the availability of general theoretical tools applicable to very different sets of problems. Maintaining strength in this FWP will also allow the Ames Laboratory program the capability of agile response to new scientific questions. Currently, this FWP supports work in a) Methods for accurate calculation of strongly correlated electron systems which includes the development of Gutzwiller density functional theory and self-consistent all-electron full-potential GW method; b) Methods for computational prediction and design of complex structures and materials which consists of developments of efficient computational algorithms for exploring configuration space (e.g., genetic algorithm) and accurate interatomic potentials for fast energetic evaluation and large scale atomistic simulation (e.g., tight-binding); c) Methods for studying the dynamics of non-equilibrium or nonlinear systems including quantum control of electron and nuclear spins in nanosystems and first-principles calculation of spin dynamics and magnetic fluctuation in solids.

Program Impact:

Our Gutzwiller DFT provides the formalism for further development of computational code that can calculate the properties of strongly correlated electron systems from first-principles. Our work on genetic algorithm provides an efficient computational tool to determine the structures of clusters, nanowires, surfaces, grain boundaries, and crystalline solids. The development of QUAMBO method is useful for large scale electronic structure calculations. Our methods for controlling and manipulating quantum spin systems should have many applications in coherent spintronics and quantum information processing. Our GW method provides an accurate tool to study magnetic order at high temperature. The FDTD code is useful for studying photonics in dispersive media such as plasmonics and metamaterials.

FY 2009 Authorized Budget (New BA):

\$689K

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

V. Antropov (PI, 40%); S. Dobrovitski (PI, 40%); B. Harmon (PI, 10%); K. M. Ho (PI, 10%);
J. Schmalian (PI, 10%); C. Z. Wang (FWP Leader, 60%); Postdoc (250%); grad students (60%)

Interactions: Internal-B. McCallum, V. Pecharsky, R. Prozorov, P. Canfield, R. McQueeney, M. J. Kramer, R. Napolitano, M. Tringides. External—(Domestic) Arizona State, Harvard, Univ. of Pennsylvania, Massachusetts Institute of Technology, Princeton, Univ. of Illinois-Urbana, Univ Texas, Austin; UCSB. (International) Jilin Univ., China; Inst. of Electronic Structure and Laser, Greece; IV Kurchatov Atom Energy Inst., Russia; Technion, Israel; Radboud Univ. Nijmegen, The Netherlands.

Related Project URL:

(Optional)

Laboratory Name: Ames
B&R Code: KC-02-02-03

FWP and/or subtask title under FWP: Metamaterials

FWP Number: AL-09-510-013

Program Abstract:

Metamaterials are composite materials with novel and unique electromagnetic (EM) properties, which are not determined by the fundamental physical properties of their constituents but by the shape and the distribution of specific patterned inclusions. The scope of the program is the theoretical understanding, analysis, development and testing of metamaterials, particularly left-handed materials (LHMs) and also the investigation of their feasibility for potential applications, that will be beneficial to the research program at Ames Laboratory and to the mission of DOE. Maintaining strength in this FWP will also allow this Ames Laboratory program the capability of agile response to new scientific questions.

Program Impact:

Provided the first transfer matrix and FDTD calculations of LHMs. Provided the first retrieval procedure to obtain the effective ϵ and μ of LHMs. Provided chiral designs and fabricated them at GHz and THz frequencies that gave negative n , and strong optical activity. Our designs and fabricated metamaterials provide magnetic response at optical frequencies, which is not possible in natural materials. The recently developed self-consistent FDTD gain code is useful for studying photonic crystals and metamaterials with gain. Our work plays a major role in leading the development of LHMs both in theory and experiments.

FY 2009 Authorized Budget (New BA):

\$367K

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

C. M. Soukoulis (FWP Leader, 20%); G. Tuttle (PI, 10%); 1 Assistant Scientist (50%); 2 Postdoc (80%); 3 graduate students (100%)

Interactions:

Internal - R. Biswas, J. Wang, K. M. Ho, M. Nilsen-Hamilton, Surya Mallapragada. External - E. Ozbay, Bilkent University, Turkey; D. R. Smith, Duke; M. H. Tanielian, Boeing Research & Technology, Seattle; I. Brener, Sandia National Lab, New Mexico; J. Zhou and T. Taylor, Los Alamos National Lab, New Mexico; E. N. Economou and M. Kafesaki, Research Center of Crete, FORTH; M. Wegener, Karlsruhe, N. Zheludev, Southampton and J. B. Pendry, Imperial College.

Related Project URL:

(Optional)

Laboratory Name: Ames
B&R Code: KC-02-03-01

FWP and/or subtask title under FWP: Bioinspired Materials

FWP Number: AL-08-510-001

Program Abstract:

Synthesis and characterization of novel bioinspired hybrid materials that mimic living systems in their abilities to respond to the environment and self-assemble hierarchically. Use of organic templates coupled with mineralization proteins to direct biomineralization processes, and aptamers for achieving specificity of non-covalent binding, to facilitate a bottom-up approach to nanocomposite materials design. Understanding guiding mechanisms of assembly across multiple length scales through combination of experiment and theory. Advanced solid-state NMR techniques for investigating interactions of the organic templates with inorganic components. The specific thrusts include

- ***Development of multiscale self-assembling bioinspired hybrid materials using bottom-up approaches:*** We are designing hierarchically self-assembling templates (synthetic polymers as well as protein and peptide based templates), and using bioinspired methods for room temperature synthesis of several energy-relevant hybrid materials with hierarchical order difficult to synthesize otherwise.
- ***Development of techniques to probe assembly at multiple length scales and properties of these nanocomposites:*** We are using a combination of solid-state nuclear magnetic resonance (NMR), scattering, and electron microscopy techniques to investigate the nanostructure and composition, and other characterization techniques to investigate the magneto-mechanical properties of these hybrid materials. This will result in fundamental insights into the design principles for synthesizing and organizing nanocrystals using bioinspired approaches.
- ***Development of computational methods for understanding general design rules for self-assembled polymer nanocomposites:*** We are developing and implementing molecular simulations using high performance computational approaches as a powerful tool to understand the underlying principles of self-assembly of complex structures, phase transformation between competing phases, as well as the response of a self assembled system to external stimuli.

Program Impact:

The use of bacterial mineralization proteins to create uniform, monodisperse, monodomain nanocrystals of magnetic nanoparticles represents a new paradigm for nanocrystal synthesis and processing using bioinspired methods. The non-covalent linkages and the hierarchical self-assembly processes enable bottom-up approaches for nanocomposite design for materials of energy relevance. We have developed NMR techniques that are being used worldwide by other groups. The general purpose molecular dynamics code developed to run on graphics processing units (GPUs) has resulted in a popular open source software, HOOMD (Highly Optimized Object-oriented Many-particle Dynamics), that is being used by several groups across the country.

FY 2009 Authorized Budget (New BA):

\$749K

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

M. Akinc (PI, 10%); G. Kraus (PI, 0%); M. Lamm (PI, 0%); S. Mallapragada (FWP Leader, 10%); B. Narasimhan (PI, 0%); M. Nilsen-Hamilton (PI, 0%); J. Schmalian (PI, 0%); A. Travesset-Casas (PI, 10%); D. Vaknin (PI, 20%); K. Schmidt-Rohr (PI, 0%); 2 Assistant Scientist (160%); 2 Postdocs (90%); 6 Graduate Students (200%)

Interactions:

Argonne National Laboratory; Technion, Israel;

Related Project URL:

(Optional)

Laboratory Name: Ames
B&R Code: KC-02-03-01

FWP and/or subtask title under FWP: Innovative and Complex Metal-Rich Materials

FWP Number: AL-08-510-003

Program Abstract:

This project works (i) to uncover and ultimately design *new families of intermetallic phases* and to understand the factors that stabilize both new and known phases by combining experiment, viz. exploratory synthesis, temperature-dependent structure determinations, and surface characterizations, with electronic structure theory; (ii) to examine the fundamental surface characteristics of complex intermetallics by investigating *fundamental issues in surface science* related to complex metal-rich solids in bulk phases; and (iii) to establishing *structure-property relationships* for complex metal-rich materials in the bulk and at their surfaces as related to both practical as well as fundamental issues, e.g., thermoelectric, magnetocaloric, catalytic, tribological, and structural behavior. Targeted compound classes include, but are not limited to, Zintl-type, cluster-based, Hume-Rothery-type, polar intermetallics, quasicrystalline and approximant phases, as well as complex metallic alloys.

Program Impact:

This research continues a strong tradition at the Ames Laboratory of discovering and characterizing new metal-rich phases in both bulk and surface states. Our methods and discoveries influence and motivate numerous solid-state and surface chemistry activities and programs worldwide and have correspondingly attracted numerous students and international visitors. We are leaders in utilizing a combination of experiment and theory to investigate problems in solid-state and surface chemistry, as well as in thorough chemical and physical characterizations of metal-rich substances, a leadership which is demonstrated by numerous invitations to national and international conferences in solid-state and surface chemistry. Our discovery and analysis of a great variety of new metal-rich (intermetallic) compounds, their chemistries, and structural and electronic properties has brought new light and insights into the poorly explored field of polar intermetallic phases as well as the growing discipline of complex metallic alloys. Substantial recent developments in this effort include (a) increasing structural and bonding insights through variation of counter-cations in polar intermetallics, which are combinations of metallic elements with very different electronegativities; (b) tuning the chemistry of complex intermetallics with hetero-metal substitutions, such as late transition metals, and, especially, the 6th period elements iridium–mercury (with gold showing especially extraordinary behavior); (c) achieving understanding of atomic distributions and vacancy formation in ternary gamma-brass and other quasicrystal approximant structures; and (d) complete structural and electronic characterization of novel ternary quasicrystalline surfaces.

FY 2009 Authorized Budget (New BA):
\$920K

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

J. Corbett (PI, 10%); G. Miller (FWP Leader, 10%); P. A. Thiel (PI, 10%); 2 Assistant Scientists: (150%); 5 postdocs(350%); 3 graduate students (60%)

Interactions (External):

U.S. Natl. Laboratories: LBNL, ORNL, SNL-CA, PNNL, LANL, APS at ANL; U.S. Universities: Cornell, Notre Dame, Houston, Northwestern, Utah State, Arizona State, North Carolina State. Overseas Organizations: CNRS-INPL-UHP and LEM-CNRS (France), MPI-FKF and MPI-CPfS (Germany), Nat. Institute Mater. Sci. (Japan), FJIRSM (China); Foreign Universities: Barcelona (Spain), Aachen, Cologne, Muenster and TU-Munich (Germany), Stockholm (Sweden), Tohoku Univ. (Japan), Univ. Liverpool. (England).

Related Project URL:

(Optional)

Laboratory Name: Ames
B&R Code: KC-02-03-01

FWP and/or subtask title under FWP: Solid-State NMR of Complex Materials

FWP Number: AL-90-360-001

Program Abstract:

Advanced solid-state nuclear magnetic resonance (NMR) methods are developed and applied for elucidating the nanometer-scale structure and dynamics of complex materials under the following types of conditions: Ionomers as used, for instance, in all-solid H₂/O₂ fuel cells; Biological and biomimetic nanocomposites; Complex tellurides for thermoelectric and other applications. For instance, a definitive new model of the nanometer-scale structure of the Nafion ionomer, the benchmark material for fuel-cell proton-exchange membranes, has been established based on high-resolution ¹³C and ¹⁹F NMR and quantitative scattering analysis. ¹H-³¹P/²⁹Si/¹³C NMR methods for proving nanocomposite formation and measuring the thickness of inorganic nanocrystals in an organic matrix, for instance in bone and bone-mimetic materials, have been introduced. Recently, high-resolution magic-angle-spinning ¹²⁵Te NMR was introduced as a new tool for characterizing the composition as well as the charge-carrier concentration and its distribution in high-performance thermoelectrics.

Program Impact:

This program is positioned at the intersection of materials science, physical and analytical chemistry, condensed-matter physics, as well as biosciences. It is closely integrated with the FWP on "Bioinspired Materials". The research has provided insights into the microscopic origins of macroscopic properties of complex materials such as fuel-cell membranes, nanocomposites, and thermoelectrics; it is anticipated that this will eventually lead to the development of improved materials. The NMR techniques introduced by this group have been and will be used worldwide by other NMR researchers.

FY 2009 Authorized Budget (New BA):

\$450K

Personnel Commitments for FY2009 to Nearest +/- 10%:

E. Levin (PI, 60%); K. Schmidt-Rohr (FWP Leader, 20%); 2 Graduate Students (50%)

Interactions (External):

Mercouri G. Kanatzidis (Northwestern University / Argonne National Laboratory).

Robert B. Moore (Virginia Tech)

Joseph P. Heremans (Ohio State University)

Related Project URL:

(Optional)