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

FWP and/or subtask title under FWP:
Structure and Dynamics in Condensed Systems and Dynamics and Energetics of Phase Transitions

FWP Number:
AL-90-501-002

Program Scope:
This effort is focused on (i) self-consistent descriptions of relevant liquid, amorphous, and crystalline phases, and (ii) the fundamental principles of competition and dynamical selection governing phase transitions from alloy melts in weakly and strongly driven systems. Approaches include first principles theoretical predictions, atomistic simulations, continuum modeling, and a broad spectrum of experimental methods for the measurement of structure, chemistry, and thermo/kinetic properties.

Major Program Achievements (over duration of support):

- A new semi-empirical potential for Cu-Zr alloys was developed which accurately reproduces crystal phase properties, melting point data, liquid structure, and the hcp-bcc transition (for pure Zr).
- We have reported that small changes in composition alter the devitrification pathway in Zr-Pt alloys, and finite element analysis (in collaboration with D. Miller, ANL) suggests that these may be MRO effects.
- First-principles MD simulations of Al-Si alloys have shown that the local tetrahedral character and diffusivity (of both Al and Si) are found to increase with Si content.
- X-ray diffraction, *ab initio* molecular dynamics, and reverse Monte Carlo simulation have been used for 3D bond-order analysis, revealing that local structure in amorphous $Zr_{73}Pt_{27}$ is dominated by icosahedral SRO.
- MD simulations (for Al) have shown that that the slow diffusion in a viscous, glassy fluid is similar in character to vacancy diffusion in crystalline solid and fundamentally different from Markovian diffusion in liquids.
- We have developed a reliable DFT method for directly calculation of solid and liquid free energies. For the Cu-Au system, these direct calculations are in very good agreement with experiments and MD simulations.
- We have modeled the thermodynamic properties of the Al-Sm system, addressing the metastable intermetallics and the undercooled liquid. Results have shed light on glass formation and devitrification behavior.
- Phase field modeling of high anisotropy dendrites has shown that once the anisotropy becomes large enough to cause missing orientations at the growth tip, the selection parameter (σ^*) becomes only weakly dependent on anisotropy of interfacial free energy.

Program Impact:
By integrating advanced computational methods with theory-critical experiments involving state-of-the-art techniques, this effort is providing new levels of fundamental understanding regarding the structure and dynamics of materials, enabling control, prediction, and discovery of new materials and dynamical structural pathways.

Interactions:
(Internal) T.A. Lograsso, Rational Growth Project, R.W. McCallum, Multiferroics Project.
(External) X.L. Wang, Spallation Neutron Source, ORNL ; D. Miller, (ANL); S. David, ORNL; R. Hyers, U. Mass.; X-ray Operations and Research Team, APS; J.H. Lee, Changwong National U., Korea; M. Plapp, Ecole Polytechnique, Paris; M. Kaufman, U North Texas; K. Kelton, Washington U.; M. Asta, U. California; G.J. Ackland, U. Edinburgh; M. Feuerbacher, Institut fuer Mikrostrukturforschung, Jeulich.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
R.E. Napolitano, Symposium Organizer *"Critical Issues and Future Directions in Solidification Science,"* (A symposium in honor of Rohit Trivedi) Ames, IA, 2006. Outstanding Young Researcher, College of Engineering, Iowa State U.; **Eren Kalay**, Best Student Poster and Best Photograph, 2006 MPIF Annual Meeting; **I.E. Anderson**, 2006 Iowa Inventor of the Year, 2006 Fellow of American Powder Metallurgy Institute; **C. Z. Wang,** workshop panel member, "Basic Research Needs for Advanced Nuclear Energy Systems", "Computational Research Needs for Alternative and Renewable Energies"

Personnel Commitments for FY2007 to Nearest +/- 10%:
R.E. Napolitano [FWP Leader] (50%), M.J. Kramer (70%), S. Liu (90%), M.I. Mendelev (100%), R.T. Ott (100%), Xueyu Song (10%), D.J. Sordelet (30%), R.K. Trivedi (30%), C.Z. Wang (10%); 8 Assistant Scientist (360%); 6 Postdocs (360%); 10 Graduate Students (320%)

Authorized Budget (BA) for FY05, FY06, FY2007:
FY05 BA ~$1150k **FY06 BA** ~$1012k **FY07 BA** ~$1974k

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

FWP and possible subtask under FWP:
Mechanical Behavior of Materials and Radiation Effects

FWP Number:
AL-90-501-003

Program Scope:
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.

Major Program Achievements (over duration of support):
- Two different mechanisms were identified for the interaction between the screw dislocations and self-interstitial loops (SIA) in bcc iron, with detailed MD simulations, leading to better understanding of screw mobility.
- Combined kinetic Monte Carlo and 3D dislocation dynamics simulations indicated a diminishing effect of dislocation junction configuration owing to solute segregation.
- Developed accurate tight-binding atomistic simulation of diffusion, coalescence, and reconstruction of vacancy defects in graphene, and vacancy self-healing mechanism for junction formation in carbon.
- Single crystal slip line and TEM $\mathbf{g}\cdot\mathbf{b}=0$ analyses revealed that the <100> slip normally seen in B2 crystals is active in the RM intermetallics. However, <111> slip also occurs in the ductile B2 intermetallics; <111> slip is unusual for B2 compounds with high ordering energies. High-resolution TEM study shows that RM B2 dislocation motion is facilitated by planar defects (stacking faults and anti-phase boundaries).
- Using anisotropic dislocation dynamics simulations, we were able to better understand the unusual slip activity involving <100>{110} in RM intermetallic alloys. We also showed that junction formation is much less common in RM intermetallic alloys than that seen in conventional intermetallics such as NiAl and Fe-25Al.

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.

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. Ghooniem (UCLA) dislocation dynamics simulations. S. Hu (PNL) Phase-field modeling.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
K.A. Gschneidner was elected to the National Academy of Engineering in 2007 and awarded the Acta Materialia Gold Medal in 2008. C. Z. Wang served as a panel member for the U. S. Department of Energy workshops on "Basic Research Needs for Advanced Nuclear Energy Systems", Bethesda, MD, July 31 – August 2, 2006, and on "Computational Research Needs for Alternative and Renewable Energies", Rockville, MD, September 19-21, 2007.

Personnel Commitments for FY2007 to Nearest +/- 10%:
S.B. Biner (100%), K.A. Gschneidner, Jr. (10%), A.M. Russell (10%), C.Z. Wang (20%); 6 Assistant Scientists (200%); 2 Postdoc (150%); 4 Graduate Students (130%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA ~$505k **FY06 BA** ~$495k **FY07 BA** ~$690k

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

FWP and possible subtask under FWP:
Extraordinary Responsive Magnetic Rare Earth Materials

FWP Number:
AL-90-501-004

Program Scope:
Integrated experimental and theoretical investigations of responsive systems, where a small change of an extrinsic thermodynamic variable such as temperature, pressure, or magnetic field triggers an intrinsic phase change. Our goal is to uncover the underlying electronic, atomic and microscopic interactions that result in an extraordinarily strong coupling of the magnetic and crystal lattices in some rare earth materials. Development and validation of phenomenological models of transformations that range from magneto-volume to magnetic-martensitic is another prime objective. Model systems include R_5T_4, RCo_2, RNi, $(R_{1-x}R'_x)Al_2$, and $La(Fe,Si)_{13}$ compounds.

Major Program Achievements (over duration of support):
- Developed X-ray powder diffraction with *in situ* low temperature and high magnetic field capabilities to map the field-induced structural transformations, thus linking crystallographic and physical property data.
- Discovered that the displacive, structural-only transformation in Er_5Si_4 can be affected by magnetic fields of 50 kOe or higher with the compound remaining in the true paramagnetic state.
- Discovered and mapped out regions where R_5T_4 compounds exist in phase separated states.
- Demonstrated that a structural change results in anisotropic magnetoresistance of $Gd_5Si_2Ge_2$ due to a significant reduction of electronic velocity in the [100] direction and the anisotropy of the electrical conductivity.
- Discovered a novel magnetic glassy state in Gd_5Ge_4.
- Discovered that Griffiths-like phase region in the paramagnetic state and short range ferromagnetic correlations in antiferromagnetic state of Gd_5Ge_4 are quenched by magnetic fields in excess of 5 kOe.
- Discovered that a structural change in Er_5Si_4 is exceptionally sensitive to pressure ($dT_t/dP = 0.03$K/bar).
- Discovered that low temperature properties of $Er_{0.75}Dy_{0.25}Al_2$ are determined by strong quadrupolar interactions.
- Discovered that spin-dependent hybridization between Ge 4*p* and Gd 5*d* states enables long-range RKKY ferromagnetic interactions between Gd 4*f* moments in adjacent Gd slabs connected by Ge(Si) bonds in $Gd_5Si_2Ge_2$.
- Employed exchange coupling calculations to obtain the effective Heisenberg model parameters of $Gd_5Si_2Ge_2$.
- Computed the free energy of $Gd_5Si_2Ge_2$ as a function of temperature using the mean-field approximation, reproduced a first order magneto-structural phase transition with a large value of $|\partial M/\partial T|$ which is observed experimentally.

Program Impact:
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 and is crucial for guiding the discovery of new materials, thus providing the foundation to future energy-related applications, such as sensors and smart materials, energy conversion, generation and utilization devices.

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

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
K.A. Gschneidner, Jr. – Fellow of the American Physical Society (2002); Excellence in Research Award (MSE Department, ISU, 2006); Elected to the National Academy of Engineering (2007); Acta Materialia Gold Medal (2008); V.K. Pecharsky – Excellence in Research Award (MSE, ISU, 2003); Distinguished Professor, Iowa State University (2006).

Personnel Commitments for FY2007 to Nearest +/- 10%:
K.A. Gschneidner, Jr. [Co-coordinator] (70%), V.K. Pecharsky [Co-coordinator] (30%), L.S. Chumbley (10%), G.J. Miller (10%); 2 Assistant Scientist (190%); 7 Postdocs (340%); 5 Graduate Students (160%)

Authorized Budget (BA) for FY05, FY06, FY2007:
FY05 BA ~$1011k **FY06 BA** ~$993k **FY07 BA** ~$1161k

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

FWP and possible subtask under FWP:
Complex Hydrides — A New Frontier for Future Energy Applications

FWP Number:
AL-04-501-051

Program Scope:
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 tuning processing strategies at the nano-, meso- and microscopic scales.

Major Program Achievements (over duration of support):

- Developed a unique apparatus enabling ball-milling in hydrogen at pressures up to 350 bar H_2 in order to facilitate reversible sorption of hydrogen by materials which were difficult or impossible to hydrogenate to date.
- Designed an SEM environmental attachment enabling transfer of air-sensitive samples from a glove box to the SEM.
- Discovered that mechanochemical transformations of 1:1 (molar) mixtures of $Li(Na)AlH_4$ and $Li(Na)NH_2$ proceed differently compared to those induced by temperature. Amounts of released hydrogen vary from ~4 (systems with sodium) to over 9 per cent by weight (systems with lithium).
- Developed a characterization protocol for nanocrystalline products after ball-milling. This includes solid state NMR, x-ray powder diffraction, residual pressure measurements, SEM and TEM.
- Mapped out mechanisms of solid state transformation between Li(Na) amides and Li(Na) alanates. Intermediates include pure and mixed hexahydroaluminates, and monohydrides of alkali metals. Final products are aluminum nitride and corresponding alkali metal monohydrides.
- Demonstrated feasibility of supporting complex hydrides on mesoporous carbon nanoparticles which have uniform pore seize of ~2.5 nm.
- Guided by a theoretical prediction of stability of Al_nH_m - ($4 \le n \le 8$, $0 \le m \le 10$) clusters, we discovered that AlH_3 may be formed from metallic aluminum and hydrogen in a ball mill at hydrogen pressures below 200 atm.
- Using density functional theory we discovered that vacancies destabilize sodium alanate, and therefore, promote hydrogen desorption much better than substitutions by Ti, thus approaching a better understanding of the role of defects and dopants on hydrogenation and dehydrogenation behavior of complex hydrides.

Program Impact:
This research is being carried out by a multidisciplinary team of scientists from the Materials and Engineering Physics 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.

Interactions:
We interact closely with P. Jena, a Co-PI from Virginia Commonwealth University. 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.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
V.K. Pecharsky – Distinguished Professor, Iowa State University (2006). P. Jena (VCU) - Jefferson Science Fellow at the US Department of State (2007).

Personnel Commitments for FY2007 to Nearest +/- 10%:
V.K. Pecharsky [Coordinator] (20%), L.S. Chumbley (10%), V. Lin (10%), M. Pruski (10%); 1 Postdoc (100%); 3 Graduate Students (130%)

Authorized Budget (BA) for FY05, FY06, FY2007:
FY05 BA ~$545k **FY06 BA** ~$545k **FY07 BA** ~$545k

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

FWP and possible subtask under FWP:
Multiferroic Materials

FWP Number:
AL-06-501-056

Program Scope:
The purpose of this project is to investigate the multiferroism in RMn_2O_5 oxides, where R is a rare earth cation. While there has been a large amount of experimental work on multiferroic materials in the recent past, there is limited understanding of the fundamental origins of the complex properties that are exhibited. Some calculations of the magnetostriction have been performed for non-rare earth systems but, in general, no thorough description of the exchange mediated magnetostriction has been achieved in any realistic materials. This is particularly true for the rare earth based compounds where previous *ab initio* calculations do not include 4f electrons and have not analyzed the exchange coupling on a microscopic basis. We plan to study these technologically promising compounds through definitive experiments supported by detailed theoretical calculations. Polycrystalline and single crystal materials will be prepared for a series of compounds. We will perform a unique combination of complementary diffraction experiments with electron, x-ray, and neutron beams. DOE-sponsored national user facilities will be intensively utilized to carry out the critical diffraction studies.

Major Program Achievements (over duration of support):
- By manipulating the driving force for formation using oxygen partial pressure and exploiting chemical solution processing techniques, phase pure YMn_2O_5, $GdMn_2O_5$, $TbMn_2O_5$, $TbFe_xMn_{2-x}O_5$ can now be prepared.
- Attempts on YMn_2O_5 crystal growth with the molten salt electrolysis technique were successful and resulted in millimeter sized single crystals.
- Completed the acquisition of an inductance-capacitance-resistance meter for dielectric measurements. We are working on combining this apparatus with a Physical Properties Measurement System for measurements under magnetic fields.
- Demonstrated our ability to image nano-domains at cryogenic temperatures with Lorentz microscopy and applied electric field using known materials in the new Tecnai Transmission Electron Microscopy.
- Initial theoretical calculations on the related, but simpler compound, $YMnO_3$, predict an energy gap. The magnetic moment at Mn site was found to be 3.2 μB. We identified that the introduction of certain oxygen defects produces the energy gap in multiferroics. In addition, we identified several stresses which lead to the increase of the energy gap and electric polarization in $YMnO_3$ type of materials. The exchange coupling parameters have been obtained for the first time in those materials.

Program Impact:
From a fundamental point of view, the nature of the exchange interactions and ferroelectricity are qualitatively understood, but the microscopic mechanism for their existence and coupling in specific material systems is still open to debate. Also, the factors influencing the strength of the magnetoelectric coupling and possibly defining a theoretical maximum coupling are essentially unknown in realistic systems. A quantitative study of the electronic structure, magnetic interactions and the way these interactions are directly or indirectly affected by applied electric field is required to fully understand these materials and produce a recipe to obtain the optimal balance of the competing interactions to define a maximum of the multiferroic effects.

Interactions:
- Internal: A. Goldman, J. Zarestky; R. Prozorov
- External: M. Schilfgaarde (ASU)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Xiaoli Tan, Young Engineering Faculty Research Award, College of Engineering, ISU.
V. Antropov served on program committee of MMM conference.

Personnel Commitments for FY2007 to Nearest +/- 10%:
Xiaoli Tan [FWP Leader] (10%), R.W. McCallum (30%), 1 Postdoc (30%); 1 Graduate Students (50%)

Authorized Budget (BA) for FY07 (new project in FY07):
FY07 BA ~$239k

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

FWP and possible subtask under FWP:
Rational Growth, Control and Modification of Novel Materials

FWP Number:
AL-06-501-057

Program Scope: 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, Basic Energy Sciences' mission. In support of this mission, this effort will advance Ames Laboratory's capabilities to synthesize and characterize high purity, high quality materials, primarily in single crystal form, spanning a range of sizes. This will involve research focused on quantifying and controlling the processing-structure-property relationship of specific responsive materials, explore promising phase spaces that we identify as compelling based upon advances in synthesis and / or control of novel materials and to modify synthesis methods as needed to obtain these materials in high purity, high quality single crystalline form.

Major Program Achievements (over duration of support):
- Synthesize bulk single crystals over a large range of composition in solid solution Fe-X alloys (X=Al, Ga, Ge, Co) by Bridgman methods.
- General magnetostrictive behavior found to be closely related to structural phase distributions. Single phase regions general show positive compositional dependencies. Two phase behavior in Fe-Ge consistent with a rule of mixture relationship.
- Discovered a sign reversal in magnetoelastic coupling energies for chemically disordered and ordered phases in Fe-Ge alloys.
- Magnetoelastic coupling energies have been calculated and compared to Fe-Ga alloys.
- Anomalous positive temperature dependencies are observed for alloys within two phase regions.
- The intrinsic magnetic behavior in Ni-Mn-Sn alloy Heusler alloys have been determined from highly homogeneous samples. Following full structural and chemical homogenization, the nature and sequence of the transitions were found to be: 1) austenite paramagnetic to ferromagnetic transition and 2) coupled ferromagnetic austenite to paramagnetic martensite crystallographic transition; and paramagnetic to ferromagnetic martensite transition with Curie-Weiss behavior on heating above its Curie temperature.
- The use of phase purity (crystal structure) was found to be an insufficient descriptor for determining homogeneity.

Program impact: The impact of this program is tremendous. The growth protocols and materials synthesized under this program are used by many other scientific groups throughout the world. Further because the synthesis and characterization are closely coupled in this effort clear distinctions can be drawn from intrinsic and extrinsic behavior in responsive materials. Another achievement has been the sharing of single crystals for collaborative research. Through such collaborations our crystals form the basis on which critical experiments are conducted.

Interactions:
ORNL, BNL, LBL, MIT, 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

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
- Best Poster Award, MRS, Fall Meeting, 2003
- Best Student Paper, SPIE Smart Structures and Materials International Technical Group, 2003
- 2006 Adaptive Structures and Material Systems *Best Paper Award* in Mechanics and Material Systems, ASME Aerospace Division.
- Over 75 refereed publications in this topic area since 2005.

Personnel Commitments for FY2007 to Nearest +/- 10%:
T.A. Lograsso [FWP Leader] (30%), Canfield (10%), McCallum (40%); 7 Assistant Scientist (240%); 3 Postdocs (170%)

Authorized Budget (BA) for FY07 (new project in FY07):
FY07 BA ~$1105k

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

FWP and possible subtask under FWP:
Materials Preparation Center

FWP Number:
AL-90-501-006

Program Scope:
The Materials Preparation Center (MPC) is a provider of rare earth metals and compounds, metallic alloys, complex intermetallics and inorganic compounds in both single crystalline and polycrystalline form to academic, national laboratory and industrial requesters worldwide. The unique materials synthesis and processing capabilities, which have been largely developed with Department of Energy (DOE) support of this national scientific center, are made available on a fee for service basis. The MPC thus enables fundamental research and development of materials-dependent technologies by providing commercially unavailable materials, synthesis, and processing services. Key capabilities of the MPC include the synthesis of crystals of complex alloys, the processing of high-purity rare earth metals and alloys, and the synthesis of high purity metallic powders. Importantly, the MPC critically supports the Basic Energy Science (BES)-sponsored research projects within the Materials and Engineering Physics (MEP) Program at the Ames Laboratory.

Major Program Achievements (over duration of support):
- Synthesized La-Ni-Sn cryocooler alloy for the ESA/NASA Planck mission vehicle. The hydrogen storage bed materials will be used for the space-based observation vehicle, scheduled for launch in 2008.
- Prepared over 150 lbs of amorphous Al-Y-Ni-Co alloy powder for a DARPA funded Phase II program led by Pratt & Whitney on Structural Amorphous Materials (SAM).
- Sublimation purification of manganese has been instituted and this high purity Mn is now available for polycrystalline and single crystal synthesis. The availability has led to identification of and elimination of key defects in Ni-Mn-Ga ferromagnetic shape memory alloys which inhibit the fundamental mechanism of shape change, twin boundary reorientation.
- Single crystals of Ti-Nb shape memory alloys have been synthesized for the first time. Ti-Nb based alloys are being considered as alternative to Ni-Ti alloys for bio-medical applications due to their better processability, better biocompatibility, better corrosion resistance and lower modulus near the elastic modulus of human bone.
- Large single crystals of alpha-Fe-Cr-Ni alloys have been synthesized for Sandia National Laboratory researchers. These single crystals will be used to determine the mechanical properties and deformation behavior of the alpha phase in support of a larger program on welding of stainless steels.

Program impact:
The MPC is a source and developer of unique capabilities in the synthesis, purification, processing and preparation of metals and alloys for advanced energy and technology research. In particular, the MPC enables scientific excellence by preparing research samples of significant quality and size. In support of this mission, the materials synthesis effort at Ames Laboratory combines the Rational Growth, Control, and Manipulation of Novel Materials effort and the Materials Preparation Center (MPC), a specialized research center managed through the BES Synthesis & Processing core research area (CRA). The MPC staff contributes to the scientific training of students and postdoctoral researchers in the areas of materials processing and synthesis. All MPC work is non-competitive to commercial entities.

Interactions:
- 99 individual researchers requests for materials and services were completed in FY07, generating $533K.
- 71 Ames Laboratory researchers requested services during FY07 generating $425K of support for the MPC.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
I.E. Anderson, 2006 Iowa Inventor of the Year, 2006 Fellow of American Powder Metallurgy Institute.

Personnel Commitments for FY2007 to Nearest +/- 10%:
L.L. Jones (50%), T.A. Lograsso (10%), I.E. Anderson (5%), D.J. Sordelet (5%); 15 Assistant Scientists (210%)

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

FY05 BA ~$**802k **FY06 BA ~$854k **FY07 BA ~**$527k

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

FWP and possible subtask under FWP: Solid State Physics, X-ray and Neutron Scattering
Neutron scattering from correlated electron materials

FWP Number: AL-90-540-001

Program Scope: Neutron scattering techniques are used to study structure, dynamics, and magnetism in hard and soft matter. Investigations explore phase transitions, lattice dynamics, magnetic structures and excitations in exotic materials; such as magnetostrictive and shape memory materials, organic films, correlated electron systems, magnetic molecules and complex magnetic materials synthesized primarily at Ames Lab, but also elsewhere.

Major Program Achievements (over duration of support):
Inelastic studies of the multiferroic Li*M*PO_4 (*M* = Ni, Fe and Co) revealed unusual spin-wave anomalies in $LiNiPO_4$ that can be correlated to the unusual magnetic incommensurate structures found in this system. Magnetic excitation spectra under applied magnetic fields of the magnetic molecules $\{Cr_8\}$ and $\{Fe_{30}\}$ were determined by inelastic scattering techniques and compared with theoretical predictions of the local theory group. Triple-axis neutron scattering experiments were performed to measure and study the spin dynamics of two compositions in a series of giant magnetostrictive Fe-Ga solid solution alloys. Lattice dynamical analysis of the phonon dispersion curve data on these alloys as well as Fe-Be alloys has also begun. The program to study spin dynamics near metal-insulator transitions has been accelerated and has revealed many interesting effects related to the competition of ferromagnetic and antiferromagnetic interactions in mixed valent ferrites, Fe_3O_4, (La,Sr)FeO_3, and $YBaFe_2O_5$. These discoveries have been enabled by growing expertise in powder and single-crystal sample preparation capabilities within the group, and the development of parallel algorithms for calculating neutron scattering cross-sections of spin waves (and phonons) in complex magnetic lattices. Using the liquid surface diffractometer at the APS, a novel spectroscopy method was developed to determine ion distributions at biomimetic membranes. The recently reinstalled and upgraded HB1A Ames Laboratory triple-axis spectrometer at the HFIR has become part of the user program at that facility. We also continue our active participation in the IDT's for the HYSPEC, SEQUOIA, and ARCS spectrometers for the newly commissioned Spallation Neutron Source (SNS), as well as in the design of CG-1 cold-neutron triple-axis spectrometer at the HFIR.

Program Impact:
Our neutron scattering findings in correlated electron oxides help understand the complex interplay between magnetism, lattice dynamics and electronic behavior. Neutron spectroscopy of the magnetic molecule of $\{Mo_{72}Fe_{30}\}$ partially confirms theoretical predictions. Phonon and spin wave measurements in magnetoelastic materials provide valuable information needed for the microscopic understanding of the interaction of magnetic and elastic energy in these systems. Structural and magnetic studies of Li-phosphates ionic conductors help understand the effects of substitutions/vacancies on ionic conductivity, and elucidate the magneto-electric effect. The Ames Laboratory liquid surfaces diffractometer at the Advanced Photon Source has been in used by scientists with diverse interests in materials science, biophysics, and physical chemistry. HB1A is the one of the most reliable and heavily used instruments at the HFIR and has productivity rivaling major international triple-axis instruments.

Interactions: Internal— Materials Preparation Center, numerous Ames Lab groups dealing with magnetic materials (Johnston, Canfield, Kögerler, Gschneidner, Goldman Lograsso, Schlagel, Pecharsky, Bud'ko,)
External— ORNL, BNL, LANL, NIST, PSI (Switzerland), ISIS (UK) Universities: California Irvine, Missouri, Tennessee, Texas, CalTech, Purdue, Oslo (Norway), PSI (Switzerland), Bilboa (Spain), Osaka & CRIEPI (Japan).

Recognitions, Honors and Awards (at least in some part attributable to support under this program)
D. Vaknin – Executive Committee, SHUG, Neutron Biology Task Force, PRP APS.
J. L. Zarestky- Executive Committee SNS/SEQUOIA IDT, HYSPEC IDT member.
R. J. McQueeney – Executive Committee SNS/ARCS and HYSPEC. SEQUOIA IDT member.

Personnel Commitments for FY2007 to Nearest +/- 10%:
D. Vaknin (100%), J. Zarestky (90%), R. McQueeney (PI-17%). Postdocs: Chang (100%), Li (100%), Wei (50%), Yan (100%). Graduate students: Ma (100%), Bu (70%), Du (30%), Pratt (100%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $921k **FY06 BA $**954k **FY07 BA $**950k

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

FWP and possible subtask under FWP: Solid State Physics, X-ray and Neutron Scattering, X-ray Physics

FWP Number: AL-90-540-001

Program Scope:
This project involves investigations of the structural characterization of materials and the investigation of structural changes associated with, or leading to, novel behavior of materials. The emphasis has been on the development of techniques, such as magnetic x-ray scattering, and more recently, studies of liquid structure using a novel electrostatic levitation furnace in the MUCAT sector at the APS.

Major Program Achievements (over duration of support):
The group continues to work in close collaboration with B.N. Harmon's theory group, Paul Canfield's materials group, and the Ames Laboratory neutron scattering group on topics ranging from the physics of the x-ray resonant magnetic scattering and x-ray circular magnetic dichroism in rare earth compounds to fundamental studies of magnetic refrigeration and multiferroic compounds, to magnetic scattering technique development. Most recently they have:

- Demonstrated that investigations of ferromagnetism in rare earth compounds are possible using linearly polarized resonant magnetic scattering in the absence of an applied magnetic field. This will have an important impact upon studies of weak ferromagnetism and ferromagnets with weak anisotropy.
- Clarified the nature of Ho^{3+} ordering in the magnetoelectric multiferroic $HoMnO_3$ compound under applied electric fields and in the absence of an applied field.
- Elucidated the microscopic details of the spin-reorientation transition in Gd_5Ge_4, a parent compound of the $Gd_5(Ge,Si)_4$ magneticaloric (refrigeration) materials.

Program Impact:
On average one student per year, trained in x-ray scattering techniques, graduates from the group. The magnetic scattering program is arguably one of the most productive efforts in the world, particularly in the areas of new magnetic scattering techniques, the elucidation of the origin of the resonant magnetic scattering amplitudes, and the use of magnetic scattering for *ab-initio* magnetic structure determination. Together with groups from Washington University, the University of Massachusetts (Amherst) and NASA's Marshall Space Flight Center, the x-ray scattering group has had a strong impact on investigations of liquid structures using an electrostatic levitation furnace to achieve deep undercooling of liquid metals, intermetallic compounds and semiconductors.

Interactions:
Internal –Materials Chemistry and Materials and Engineering Physics
External – XOR (Argonne), Washington University, NASA MSFC, University of Massachusetts, Brookhaven National Laboratory, TU Dresden, FZ Jülich, x-ray and neutron scattering groups in Grenoble, POSTECH, South Korea

Recognitions, Honors and Awards (in some part attributable to support under this program):
Goldman is a Fellow of the American Physical Society (1999) and was named a Distinguished Professor of Liberal Arts and Sciences at Iowa State University (2007).

Personnel Commitments for FY2007 to Nearest +/- 10%:
A. I. Goldman (PI-25%), Andreas Kreyssig (P16-50%), Students: Lizhi Tan (50%), Shibabrata Nandi (50%), Technician: Marc McGinn (25%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $268k **FY06 BA $**300k **FY07 BA $**301k

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

FWP and possible subtask under FWP: Condensed Matter Physics, Experiment.
Optical Properties and Photoemission Spectroscopy of Solids and Surfaces

FWP Number: AL-90-540-002

Program Scope:
Angle-resolved photoelectron spectroscopy is used to elucidate the electronic structure and interactions in solids. Materials studied are systems in which electron correlations are very important. This program is developed on two parallel, but not disconnected tracks—unconventional superconductivity and heavy Fermion systems. The most pressing issues in unconventional superconductivity include mechanism of high temperature superconductivity (investigation of the role of collective excitations, inhomogeneities, the pseudogap, the role of dimensionality and the relation between results from various experimental techniques), and the relation between superconductivity and magnetism in a number of systems (symmetry of the order parameter, role of Fermi surface nesting and electron-phonon coupling). The study of heavy Fermion compounds concentrates on rare earth intermetallic compounds. The new approach in this effort is to systematically study the electronic structure of families of compounds where some members display heavy fermion behavior. Current samples include RSb, RSb_2, $RNi2B_2C$, $RAgSb_2$ (R=Y, La-Nd, Sm), $Tl_2Ba_2CuO_6$, $YBa_2Cu_4O_8$. Future instrumentation work includes developing a laboratory-based tunable low photon energy source for bulk sensitive ARPES measurements crucial for studies of 3D materials.

Major Program Achievements (over duration of support):
Major achievements include both advances in methodology of the technique and understanding of electronic properties of specific systems. First observation (Olson, Lynch) of the superconducting gap in any cuprate by photoelectron spectroscopy (or any technique). Early band mapping of two cuprates. Establishment of a Fermi Surface in the cuprates. First demonstration of dispersion, hence band-like states, in a quasicrystal. Showed value of using changes in energy-dependent matrix elements and cross-sections to isolate details of the electronic structure. Development of new technique – AutoCorrelated (AC) ARPES to bridge the results from ARPES, STM and INS. First practical demonstration of ARPES microscopy with direct measurement of layer specific electronic structure. Discovery of superconducting gap and strong renormalization effects in the quasi one-dimensional chains of $YBa_2Cu_4O_8$. Discovery of coexistence of 1D and 2D electron gases in $YBa_2Cu_4O_8$. Establishing pseudogap and superconducting gap are two separate energy scales.

Program impact:
Discovery of two energy scales in cuprates represents a major change in direction aimed at improving their properties. Characterization of electronic states, often including band mapping, leads to a better understanding of correlation in Ce-based systems. Convinced others of importance of dipole matrix elements. Early band mapping of cuprates and observation of superconducting gap attracted wide interest. Contribution to methodology of ARPES data interpretation.

Interactions:
Internal: P. C. Canfield, T. Lograsso, V. Antropov, B. N. Harmon, Jörg Schmalian, Ruslan Prozorov, David Johnston
External: J. J. Joyce (LANL), J.-S. Kang (Catholic University of Korea), Juan Carlos Campuzano (University of Illinois at Chicago), Mike Norman (Argonne National Laboratory) and Mohit Randeria (Ohio State University), Janusz Karpinski (ETH Zurich), Joel Mesot (ETH/PSI Zurich)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Eighty-two invited talks since the inception of the photoelectron spectroscopy program. Olson and Lynch are both Fellows of the American Physical Society. Kaminski was co-organizer of workshop "Frontiers in Soft X-ray, VUV and Infrared Research" and a chairman of 38th SRC Users Meeting.

Personnel Commitments for FY2007 to Nearest +/- 10%:
D. W. Lynch (Emeritus), C. G. Olson (80%), Adam Kaminski (PI, 17%), Takeshi Kondo, Post Doc (100%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $386k **FY06 BA** $378k **FY07 BA** $410k

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

FWP and possible subtask under FWP: Solid State Physics, Experiment
Structural characterization of self-organization on surfaces

FWP Number: AL-90-540-002

Program scope:
The main goal in Nanotechnology is the growth of structures with controllable small dimensions. The scope of our program is to understand the microscopic processes (diffusion, nucleation, island decay, coarsening, etc.) that control nanostructure evolution and stability, and find ways to select structures with uniform dimensions. Two complementary techniques, Scanning Tunneling Microscopy (STM) and High Resolution SPA-LEED, are used. We have developed extensive collaborations with theoretical groups worldwide to understand our experimental results.

Major Program Achievements (over duration of support):
We have focused on the understanding of the unusual kinetics of the wetting layer in Pb/Si(111) that controls the uniform 7-layer height islands in addition to Quantum Size Effects (QSE). In 2007 we began a collaboration with Altman (Hong Kong) using his LEEM machine and confirmed in real time the unusual mobility of the wetting layer. This revealed an extraordinary mechanism of broad interest for mass transport at low temperatures. These experimental studies are complemented by theory collaborators, who have modeled different aspects of the QSE-driven growth. Theory groups from CMSN (DOE supported theory network) include Wang, Ho, Evans (Ames Lab) and Liu (Utah). This work has shown that the controlling kinetic barriers (for diffusion, island decay, etc.) depend on whether an island is stable or unstable. With our long time collaborator Chvoj (Prague) we constructed a non-classical potential energy surface (PES) and performed Monte Carlo simulations to reproduce the ring-like morphology observed in second layer nucleation of the Pb islands. In 2006 we collaborated with an Ames lab theory group (Ho, Wang) to understand the competition between adatom Pb interactions and the charge density wave on the Si(111)-In(4x1) in the sub-monolayer coverage regime. With M. Zaluska_Kotur (Polish Academy of Sciences) and Z. Gortel (Alberta), we collaborated to understand surface diffusion in systems with long range interactions as in the Pb/Si(111) "Devil's Staircase" phases.

Also, we started systematically to study the growth of Indium on Si(111) and graphene layers grown on SiC. We discovered a very interesting crystallographic transition, where fcc islands form first at lower temperatures or coverage followed by In(110) in the normal bulk crystal phase.

Program Impact: We published a *Physics Today* feature article in April 2007 about our work on uniform height Pb islands. This well recognized work motivated 7 other groups worldwide to work on QSE-driven growth. Tringides was an invited speaker to NanoChina 2007, a conference in Beijing attended by 1400 scientists. Our work on surface diffusion has been recognized with an invited chapter in the classic book *"Diffusion in Condensed Matter"* editors: J. Karger, P. Heitjans, and R. Haberlandt.

Interactions: Locally: C. Z.Wang , K.-M. Ho, J. W. Evans, J. Schmalian,, D. W. Lynch, A. Kaminski
Outside with published/submitted papers: Ed Conrad (Georgia Tech), P, Miceli (Missouri), Z. Chvoj (Academy of Sciences, Czech Republic), E. Bauer (Arizona), M.Jalochowski (Lublin Poland), M. Altman (Hong Kong), M. Zaluska Kotur (Warsaw Polish Academy of Science), Gortel (Alberta), Argyrakis (Thessaloniki), F.Liu (Utah),
Other outside collaborators: T. Rahman (Kansas State), Z. Zhang (Oak Ridge), J. Wendelken (Oak Ridge), M. Henzler (Hannover, Germany), M. Hon-von-Hoegen (Essen Germany), K. Roos (Bradley).

Recognition:
- 3 *Physical Review Letters* and 1 *Rapid Communications* in 2006-07
- 15 papers published and 1 submitted within 2006-07
- 15 invited talks at international meetings and institutions in 2006-7, co-organizer of the International Workshop on Physics and Technology of Thin Films, Prague 2006 (IWTF2) Prague June 2006. APS Fellow (2003)

Personnel Commitments for FY2007 to Nearest +/-10%:
M. C. Tringides (PI, 25%), M. Hupalo (100%), PhD students: J. Chen (50%), S. Binz (25%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $290k **FY06 BA** $318 **FY07 BA** $320k

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

FWP and possible subtask under FWP: Solid State Physics – Experiment
New materials; Physical property investigations of new materials and phases

FWP Number: AL-90-540-002

Program Scope: Synthesis and study of new and improved oxide and other materials with potentially novel electronic, magnetic and/or thermal properties. Characterization of these materials using x-ray diffraction, magnetization, magnetic susceptibility, specific heat, electronic transport, thermal analysis, and NMR and NQR measurements, to understand, e.g., the electronic structure and magnetic properties of new superconductors and strongly correlated insulators and metals. Provision of high-quality single crystal and polycrystalline samples to other groups for measurements of additional properties.

Major Program Achievements (over duration of support): 1) Completed a study of the ^{7}Li nuclear spin-lattice relaxation rates in three heavy fermion LiV_2O_4 powder samples versus temperature, magnetic defect concentration and magnetic field. Formulated a model that successfully explains the data. Remarkably, the heavy fermion character is not destroyed by the magnetic defects. 2) Found evidence for two phase transitions below 15 K in the spin chain compound $Sr_4Cr_3O_9$. 3) Completed a ^{51}V NMR study at 4.2 K of the antiferromagnetic spin structure in the antiferromagnetically ordered state of the zig-zag spin $S = 1$ chain compound CaV_2O_4. The data indicate a noncollinear spin structure that consists of two antiferromagnetic substructures with the easy axes of the two substructures separated by 19 degrees. 4) Discovered the spin $S = 1/2$ zig-zag spin chain compound In_2VO_5 has a spin glass ground state. 5) Completed extensive measurements on polycrystalline-layered OsB_2 suggesting the possibility of multi-band superconductivity below $T_c = 2.1$ K. ^{11}B NMR measurements indicate the B *p* contribution to the density-of-states at the Fermi level is important to superconductivity in both OsB_2 and RuB_2.

Program impact: Characterized and modeled the influence of magnetic defects on the physical properties of the unique heavy fermion compound LiV_2O_4 for the first time, which helped us maintain our lead in the area of *d*-electron heavy fermion physics. Our results suggest that at least some observations of non-Fermi liquid behaviors in other compounds reported in the literature may be in error, due to other effects masking the heavy fermion characteristics. CaV_2O_4 single crystals were grown for the first time, allowing the first observation of the antiferromagnetic transition. The discovery of the long-range antiferromagnetic transition in CaV_2O_4 is important to understand the magnetic properties of geometrically frustrated magnetic insulators. Our work on layered OsB_2 suggests the possibility of multiband superconductivity is highly topical.

Interactions: Internal – Ames Lab (Bud'ko, Canfield, Kaminski, Kreyssig, Schmalian, Yan)-CMP, (Kramer, Lograsso)-MEP; External – U. Hamburg, U. Pavia, Catholic U. Korea, Queen's U. (Canada), Hahn Meitner Inst. (Germany), Tech. U. Braunschweig (Germany).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Fellow of the American Physical Society, 1988; Japanese Government Research Award for Foreign Specialists, 1991; Chair, Gordon Research Conference on Superconductivity, 1993; Annual Award for Outstanding Scientific Accomplishment in Solid State Physics (with 10 other Ames Lab scientists), U.S. Department of Energy, 1995; Award for Outstanding Achievement in Research, Iowa State University, 1997; Distinguished Professor, Iowa State University, 2000; named a "Highly Cited Researcher" by the Institute for Scientific Information, 2004; Editorial Board (Divisional Associate Editor), *Physical Review Letters*, 1995-1998 and 2007-present.

Personnel Commitments for FY2007 to Nearest +/- 10%:
D. C. Johnston (PI 17%); A. Niazi, Y. Singh (100%, postdocs); S. Das, X. Zong (50%, graduate students)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $247k **FY06 BA** $370k **FY07 BA** $410k

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

FWP and possible subtask under FWP: Solid State Physics, Experimental
Photophysics of luminescent organic semiconductors and organic light-emitting diodes (OLEDs)

FWP Number: AL-90-540-002

Program Scope:
Fabrication & studies of π-conjugated thin films and OLEDs. The films are studied by photoluminescence (PL)- and PL- and photoinduced absorption (PA)-detected magnetic resonance (PLDMR and PADMR, respectively). The OLEDs are studied by current- and electroluminescence (EL)-voltage measurements, and by EL- and electrical current-detected magnetic resonance (ELDMR and EDMR, respectively).

Major Program Achievements (over duration of support):
- We have extended our spectrally narrowed OLED edge emission studies. While we do not rule out the possibility of amplified spontaneous emission (ASE), aka mirrorless lasing, we suspect that optical misalignment may result in the apparent optical gain. We are currently exploring both possibilities.
- In collaboration with A. Kadashchuk (Nat. Acad. Sci. Ukraine) and H. Bässler (Univ. Marburg), we completed a thermally stimulated luminescence (TSL) and PLDMR study of *trions*, i.e., bipolarons stabilized by a counterion or counterpolaron, in a high-performance poly(para-phenylene vinylene) (PPV) derivative; we previously identified their ELDMR at the organic/cathode interface of OLEDs. They may be very significant for OLEDs, since they may be responsible for their long-term degradation.
- We extended our PLDMR and double-modulation PLDMR (DM-PLDMR) studies of PPV and polythiophene derivatives. The results contradict the "delayed PL" mechanism previously proposed to explain the PLDMR and PADMR, and its underlying assumption that the yield of singlet excitons (SEs) in polymer OLEDs is >25% and may be as high as 60%. They also confirm that the central spin-dependent interaction in luminescent π-conjugated materials is the annihilation of triplet excitons (TEs) by polarons.
- We are rapidly developing the structurally integrated OLED-based platform we invented for luminescent chemical and biological sensors, and sensor arrays, in which the OLED light source is structurally integrated with the sensor film whose PL is sensitive to the target agent. As a spin off, we obtained a NSF SBIR Phase II award to commercialize a dissolved oxygen sensor based on this new platform.

Program impact:
Our ODMR studies (1) support the conclusion that the maximal internal quantum efficiency of all fluorescent OLEDs is ~25%, (2) have identified two PL and EL quenching mechanisms which strongly impact the EL of OLEDs at high excitation densities, and (3) may have identified the role of trions in the long-term degradation of the OLEDs. Our other studies on OLEDs underpin the science for the development of organic injection lasers, OLEDs for solid-state lighting, low-cost ultrafast pulsed light-sources, and a new platform for chemical and biological sensors and microsensor arrays.

Interactions:
External – Dept of Physics, Korea Univ; Dept of Electrical Engineering, MIT; Chemistry Dept, Princeton Univ; Chemistry Dept, Bowling Green State Univ; Chemistry Dept, UCLA; Appl Phys & Mat Sci Dept, City University, Hong Kong; Nat. Acad. Sci. Ukraine, Kiev; Physics Dept, Univ of Marburg, Germany.
Local – R. Shinar & V. Dalal, Microelectr. Res. Cntr; L. Tabatabai, Biochem., Biophys., & Molec. Bio.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
24 invited talks from Oct 1, 2004 until Sept 30, 2007; 10 papers published, 7 accepted or submitted in FY 07.

Personnel Commitments for FY2007 to Nearest +/- 10%:
J. Shinar, PI, 25%; Postdoctoral Fellows, 0.5 FTE; Graduate students, 4.0 FTE

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $333k **FY06 BA** $318k **FY07 BA** $300k

Laboratory Name: Ames
B&R Code: KC02-02-02

FWP and possible subtask under FWP: Solid State Physics, Experimental
Correlated states in magnetic materials

FWP Number: AL-90-540-002

Program Scope:
Design, discover, grow, and characterize novel materials with exotic / interesting physical properties (generally electronic / magnetic).

Major Program Achievements (over duration of support):
Over the past three fiscal years this program has been studying a wide range of intermetallic systems that manifest magnetic and / or superconducting ground states. Since January 2001 this program has been a world leader in the synthesis and characterization of MgB_2, the binary intermetallic superconductor with Tc~40 K. We have delineated the mechanism of the superconductivity, range of the superconducting state and salient physical length scales, and demonstrated a simple synthetic route to making powders, wires and films. More recently (*PRL* 2004) carbon has been identified as a key dopant for doubling the upper critical magnetic field (from 16 T to 32 T). We also systematically studied the effects of neutron damage (*PRB* 2006). In addition, this program continues to be a world leader in the study of the RNi_2B_2C family of magnetic superconductors, the growth and properties of single grain quasicrystals (including the magnetic RMgZn family), and metamagnetic transitions and spin-glass properties in anisotropic local moment systems. During FY04 we identified YbAgGe (a member of the RAgGe family that we have been studying) as the second known, Yb-based, field induced quantum critical point compound. This discovery has generated great excitement and spawned new collaborations throughout the world (France, England, Canada, Germany, Japan). During FY06 we introduced the RT2Zn20 (T = Transition metal) series as a huge phase space for the study of correlated electrons as well as local moment physics.

Program impact:
Ninety-six publications between Jan. 2005 and Nov. 2007 (as well as several patents filed on the processing of MgB_2) 34 *Physical Review* B, 7 *Physical Review Letters*, as well as smaller numbers of papers in journals such as *Nature, Proceedings of the National Academy, Physica C, Physica B, J. Alloys and Comp*., and *Journal of Magnetism and Magnetic Materials*. In addition, a general science review of MgB_2 published in *Scientific American* has now been translated into over a half dozen different languages. This program's work is very highly cited. For example, the work on MgB_2 (less than 6 years old) has been cited over 2000 times.

Interactions: (internal) A. Kaminski, R. Prozorov, V. Antropov, F. Borsa, D. Finnemore, A. Goldman, B. Harmon, V. Kogan, R. McQueeney, J. Schmalian, T. Lograsso, J. Zarestky, J. Corbett, C. Jenks, P. Thiel, M. Kramer, K. Dennis, R. McCallum, G. Miller, S. Malapragada. (external) Risø, Stanford, National High Magnetic Field Lab (LANL and Florida), ESRF (Grenoble), ILL (Grenoble), CEA (Grenoble), CNRS (Grenoble), Brookhaven National Laboratory, Oak Ridge National Lab, ISIS (England), ETH (Zürich), MPI (Dresden), as well as dozens of other labs and universities throughout the world.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Fellow of the American Physical Society (PCC); Divisional Associate Editor for *Phys. Rev. Lett*. (PCC), Distinguished Professor of Physics (PCC). Over 30 invited talks / colloquia, including invitations to write articles for *Physics World, Physics Today, Scientific American* and *Encyclopedia* entries on MgB_2

Personnel Commitments for FY2007 to Nearest +/- 10%:
P. Canfield (PI, 15%), S. L. Bud'ko (95%), G. Samolyuk (10%) post docs: Y. Jennsen (40%), A. Sefat (70%), graduate students: E.D. Mun (100%), S. Jia (100%), M. Tillman (50%), N. Ni (50%), A. Thaler (30%), S. Kim (30%); undergraduate students: Josh Friedrich, Sara Moser, Matt Lampe

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $740k **FY06 BA** $741k **FY07 BA** $760k

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

FWP and possible subtask under FWP: Condensed Matter Physics - Experiment
Correlated states in magnetic materials – magneto-optics

FWP Number: AL-90-540-002

Program Scope:
This project was initially motivated by new capabilities for studying the optical properties of magnetic materials. With David Lynch retiring, experiments covering the low energy range of the optical spectra are made by external collaborators. This project also began with a strong experimental component for the synthesis of new materials. Paul Canfield was hired and his very successful efforts are now funded as a separate group. More recently, magnetic x-ray scattering experiments have become a valuable new tool, and there are a number of collaborative projects involving the x-ray group of Alan Goldman and the group at the Advanced Photon Source at Argonne. The present emphasis on this effort is the development of X-ray magnetic circular dichrosim (XMCD) into a quantitative tool for rare-earth magnetism, and the analysis of XMCD experimental data via first principles electronic structure calculations.

Major Program Achievements (over duration of support):
Measurement of Kerr spectra for over a dozen intermetallic compounds and successful calculations of such spectra. Observation of a metamagnetic (ferro- to antiferromagnetic) transition in $Ce(Fe_{0.9}Co_{0.1})_2$ by magneto-optic spectroscopy and MOKE spectrum in the AF phase. We made the first calculations of MO spectra, employing the LDA+U technique for treatment of correlated electron states (in Gd metal). The calculations were also very successful for magnetite (Fe_3O_4), and for a series of mixed-valent materials (Tm monochalcogenides, SmS, ThB_6, etc.). Spectra were also calculated for x-ray magnetic circular dichroism (XMCD) experiments for $Gd_5Si_2Ge_2$, the complex magnetic refrigeration material being investigated in Ames. We wrote a 500-page book (published by Kluwer), presenting the techniques and results of over 20 publications in the last few years on our MO and XMCD investigations. Last year we analyzed the temperature-dependent changes in the XMCD spectra of Er_2Fe_{17} and showed the previous interpretation was incorrect.

Program impact:
A systematic study of several series of compounds shows rare-earth 4f-states rarely participate directly in MOKE spectra, but their moments polarize other electrons. The off-diagonal component of the dielectric function, proportional to the magnetization, can be calculated rather accurately, as long as the LDA+U technique is used to account for the strong correlations of the 4f electrons. The agreement with experiment is impressive and lends strong support for the LDA+U approach for optical spectral analysis. The success of theory in experiment in this area is excellent and we have written and published a book gathering together a large number of results. The XMCD work on rare earths is widely recognized, highly cited, and nearly unique, in that we perhaps are the only group to use full band structure calculations for XMCD.

Interactions:
Internal: T. Lograsso, P. C. Canfield, A. Goldman; External: J.-Y Rhee (S. Korea), V. Antonov (Kiev)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP):
Lynch and Harmon are Fellows of the APS. Ten invited talks in last three years.
Book: *Electronic Structure and Magneto-Optical Properties of Solids*, (FY05).

Personnel Commitments for FY2007 to Nearest +/- 10%:
D. W. Lynch (Emeritus), B. Harmon (5%), V. Antropov (20%), V. Antonov (visiting scientist, Kiev, 30%), J.Y. Rhee (visiting professor, 10%), Y.B. Lee (postdoc, 30%).

Authorized Budget (BA) for FY05, FY06, FY07
FY05 BA $85k **FY06 BA** $76k **FY07 BA** $77k

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

FWP and possible subtask under FWP: Solid State Physics, Experiment

FWP Number: AL-90-540-002

Program Scope:
Advanced electromagnetic measurements of novel superconducting and magnetic materials. Design and use of unconventional highly precise experimental methods in magnetism and superconductivity, including work at temperatures down to 10 mK and in high magnetic fields.

Major Program Achievements (over duration of support):
Established in the summer of 2005, "The Superconductivity and Magnetism Low-Temperature Laboratory" is now fully operational with several experiments running. In particular, a unique tunnel-diode resonator technique is currently used on ^{3}He, ^{4}He and dilution refrigerators to study ferromagnetic and superconducting materials. This technique measures dynamic magnetic susceptibility with unprecedented sensitivity of few pico-emu (at least four orders of magnitude better than SQUID magnetometers). It is based on a self-resonating LC circuit, where the measured quantity is the shift of the resonant frequency. Another unique technique already established in the lab is magneto-optical visualization of magnetic fields at surfaces. The microscope utilizes Faraday rotation in a special transparent ferrimagnetic Bi-doped iron garnet which is placed in contact with the sample. It is used to image magnetic domains in ferromagnets and flux structures in superconductors. In addition, the lab has extensive conventional experimental capabilities, including Quantum Design MPMS and PPMS systems. Current studies include pattern formation and topological hysteresis in type-I superconductors and ferromagnets, mechanisms of unconventional superconductivity, coexistence of superconductivity and magnetism, dynamic magnetic susceptibility in local and itinerant ferromagnets as well as studies of multiferroics. In close collaboration with other groups, we study critical scaling in ferromagnets (Canfield, Schmalian), magnetic defects (Johnston), magnetic molecules (Luban and Kögerler), superconducting gap structure (Kaminski), domain structure in ferromagnets (Goldman, Kreyssig), theoretical aspects of superconductivity (Kogan, Clem), magnetic nanoparticles (bio-inspired materials program at Ames Lab).

Program impact:
Current techniques have been successfully used to study several important topics and novel materials grown by other groups. The laboratory has become an integral part of the CMP program and, as planned, provides advanced measurement capabilities to study novel effects in novel materials. With the dilution refrigerator installed, building an extensive range of experimental techniques capable of operating at mK temperatures will be a priority for several years. Current capabilities include tunnel-diode resonator, measurements under pressure and angle-resolved transport. It is planned to add AC and DC magnetometry, specific heat, dilatometry, thermal conductivity, directional tunneling. This will greatly enhance the experimental capabilities of the CMP program. In 2007 the lab produced 15 papers, including 2 *PRL*s.

Interactions: (internal) V. Antropov, S. Bud'ko, P. Canfield, J. Clem, D. Finnemore, A. Goldman, D. Johnston, A. Kaminski, V. Kogan, P. Kögerler, A. Kreyssig, M. Luban, J. Schmalian, (external) U of Illinois, U of Maryland, HMFL, Louisiana State U, U of Sherbrook, U of Tokyo (Japan), U of Bristol, ETH (Zurich).

Recognitions, Honors and Awards (at least partly attributable to support under this subtask):
Sloan Research Fellowship (2006-2008). Best graduate student presentation at MMM 2008 conference.

Personnel Commitments for FY2007 to nearest +/- 10%:
Ruslan Prozorov (PI-17%). Postdocs: A. Dobrynin (30%), C. Martin (30%); 5 students: (100%); Technician: M. McGinn (25%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $158k **FY06 BA** $258k **FY07 BA** $300k

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

FWP and possible subtask under FWP: Condensed Matter Physics - Experiment
Magnetic Molecules

FWP Number: AL-90-540-002

Program Scope: Broad-based experimental and theoretical research program, executed in-house and with external collaborators, focused on magnetism at the nano-scale level as manifested in crystalline samples of magnetic molecules. This is a closely coordinated inter-disciplinary effort, coupling skills in synthesis chemistry, experimental, and theoretical condensed matter physics to achieve a comprehensive understanding of the major static and dynamic properties of molecules incorporating a finite number of exchange-coupled transition metal cations. The synthesis effort focuses both on uncoupled and networked magnetic molecules of high symmetry and the controlled modification of parameters (symmetries, spin quantum numbers, and exchange and anisotropy parameters) to allow systematic studies of magnetic behavior. Experimental studies utilize thermodynamic (especially magnetization, down to mK temperatures and magnetic fields up to 60 T), magnetic resonance (NMR, EPR), optical, and neutron scattering methods. Theoretical studies employ analytical and simulational (classical spin dynamics, classical and quantum Monte Carlo) methods to classical and quantum Heisenberg models of magnetic molecules, and first-principles electronic structure calculations for the characterization of specific magnetic molecules.

Major Program Achievements (over duration of support):
Synthesis, and full chemical and physical characterization of over 60 compounds of targeted magnetic molecules comprising 2 to 30 spin centers each, and specialized preparation of compounds for experimental studies. In-house implementation of the quantum Monte Carlo method has provided the detailed characterization (Heisenberg model parameters, magnetization versus temperature and magnetic field) of a variety of large magnetic molecules that are not amenable to matrix diagonalization methods. Development of a quantum model for the low-lying excitations of the giant Keplerate$\{Mo_{72}Fe_{30}\}$ and the intensity of inelastic neutron scattering in good agreement with experimental studies. Synthesis, experimental, and theoretical characterization of $\{Mo_{72}V_{30}\}$ and $\{Mo_{72}Cr_{30}\}$ (spin-1/2 and spin-3/2 versions of $\{Mo_{72}Fe_{30}\}$). Comprehensive theoretical explanation of quantum decoherence and tunneling phenomena in the $\{V_{15}\}$ system. First-principles calculation of exchange constants in polyoxovandate systems using electronic structure methods. Development of a quantitative theory of spin frustration, competing spin phases, and metamagnetic transitions in highly symmetric magnetic molecules, in some cases supporting long-lived metastable spin phases.

Program Impact:
Results of the Ames group have been published in more than 175 scientific articles on magnetic molecules between 1998-2007. This has generated an increased number of collaborations within the U.S., Europe, and Asia.

Interactions:
Internal – Other CMP groups within Ames Laboratory: R. Prozorov and D. Vaknin.
External - *Chemical synthesis*: University of Bielefeld (Germany), University of Manchester, University of Glasgow, and University of Edinburgh (UK); *ESR and high magnetic field methods*: Tohoku University (Japan); *Optical methods*: University of Tennessee; *NMR methods*: University of Pavia (Italy), Hokkaido University (Japan), Catholic University of Korea; *Neutron facilities*: Oak Ridge National Laboratory, ISIS (UK), Hahn-Meitner Institute (Germany); *Computational and Theoretical methods*: Oak Ridge National Laboratory, University of Applied Sciences-Bielefeld and University of Osnabrück (Germany), Catholic University of Nijmegen and University of Gronigen (Netherlands).

Recognitions, Honors and Awards (at least partially attributable to support under this FWP):
10-15 invited talks each year since 2001**.** M. Luban – Honorary doctorate (Dr. rer. nat. h.c.), Universität Osnabrück (Germany), 2006.

Personnel Commitments for FY2007 to Nearest +/- 10%
M. Luban (PI-10%); B. Suh, Visiting scientist (60%); V. Dobrovitski (20%); P. Kogerler (60%); X. Fang, Postdoc (70%); J. Fielden, Postdoc (20%); W.Tan (10%); J. Zarestky (10%).

Authorized Budget (BA) for FY05, FY06, FY07 (project started in FY02):
FY05 BA $550k **FY06 BA** $523k **FY07 BA** $400k

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

FWP and possible subtask under FWP: Solid State Physics, Experiment
Photonic Band Gap (PBG) Materials

FWP Number: AL-90-540-002

Program Scope:
To design, model, and fabricate novel periodic structures resulting in photonic band gap crystals.

Major Program Achievements (over duration of support):
Collaboration with Shawn Lin at Rensselaer Polytechnic Institute on thermal emission from 3D metallic photonic crystals. Economical microtransfer-molding method for fabrication of photonic crystal filaments for tailored energy-efficient thermal emitters. Measurements and simulations of coupling 3D PBG waveguides to resonant cavities at microwave X-band frequencies. Development of tunable infrared emitter with metallo-dielectric photonic crystal for efficient gas sensor devices in collaboration with scientists at Ion Optics. Design of 2D PBGs for waveguides and resonant cavities. Fabrication and detailed characterization of high-quality large-scale face-centered cubic layer-by-layer structures with fundamental stop bands ranging from 1.3 to 1.7 μm using direct laser writing (*Nature Materials*). Directional emission out of a subwavelength aperture in periodically corrugated metallic thin films and PBG waveguides *(PRL).* The surface termination of PCs and the existence of surface waves were accessed. Spontaneous emission rates of dipoles in photonic crystal slabs evaluated.

Program impact:
Our group is one of the pioneers in the field of photonic crystals and continues to play a major international role in leading the development in this field. The work on metallic PBGs with exceedingly high thermal radiation may lead to very energy efficient lighting systems. Our results for emission out of subwavelength apertures hold promise for the integration of PBG waveguides with conventional optical systems.

Interactions:
Hong Kong University of Science and Technology, UC Berkeley, Rensselaer Polytechnic Institute, Canon Development America, Fudan University (China), Hanyang University (Korea), Bilkent University (Turkey), Ion Optics, Research Center of Crete, Sandia National Labs, Agilent Technologies, University of Twente (Netherlands), ETH, Zurich and University Karlsruhe (Germany).

Recognitions, Honors and Awards (attributable to support under this FWP or subtask):
DOE Energy 100 Award and DOE Science 100 Award, U. S. Dept. of Energy, organized three international conferences. 6 US patents have been issued to our group in this area. Soukoulis and Ho are Distinguished Professors, Iowa State Univ. and Fellows of the APS. Soukoulis is also a Fellow of AAAS and OSA, has a Senior Alexander von Humboldt Award, and is editor of the new journal *Photonics and Nanostructures: Fundamentals and Applications* since 2002. Both Ho and Soukoulis receive over 1000 citations/year.

Personnel Commitments for FY2007 to nearest +/- 10%:
Theory: K. M. Ho (15%), C. M. Soukoulis (8%), R. Biswas (50%), Postdocs: Z. Y. Li (10%), T. Koschny 20%), R. Moussa (10%); Students: Anan Fang (20%), Weitao Dai (20%), Lili Peng (20%), M. Kafesaki (unpaid), M. Li (25%).
Experiment: G. Tuttle (15%), K. Constant (9%), W. Leung (60%); postdocs: C. H. Kim (50%); students: Y-S. Kim (50%), J.-H. Lee (50%), J.Muehlmeier (50%), Lei Zhang(25%), Jiangfeng Zhou (25%), Bingnan Wang (25%), H. Kang (50%),

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $658k **FY06 BA** $684k **FY07 BA** $677k

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

FWP and possible subtask under FWP: Solid State Physics, Theory
Optical and Surface Physics

FWP Number: AL-90-540-003

Program Scope: To study the structure, dynamics, and electronic properties of solid surfaces using a combination of first-principles density functional calculations and tight-binding molecular dynamics simulations. Accurate and transferable environment-dependent tight-binding (TB) potentials are developed for accurate description of surface properties as well as genetic-algorithm schemes for efficient atomistic structure optimization on surfaces.

Major Program Achievements (over duration of support):

- We investigated the electronic structure effects of Pb atom adsorption on the quasi-one-dimensional In(4x1)-Si(111) surface. Instead of a period of even multiples of the underlying In lattice spacing a along the In wire, as favored by the low temperature charge-density wave (CDW) modulation, the Pb adatoms are frequently found to occupy the odd adsorption sites separated by a distance 3a or 5a. These observations indicate a strong antiphase interference between the indirect interaction of adsorbed Pb atoms and the intrinsic CDW of the In(4x1)-Si(111) surface. Work done in collaboration with M. Hupalo and M. Tringides. (Chan, Wang, Ho) (see Tringides section)
- Using genetic algorithm structural optimization followed by ab initio density functional calculations, we studied the atomic structure and energetics of H−passivated silicon nanowires that are oriented along the [112] crystallographic direction and have effective diameters of approximately 1 nm and below. Work completed in collaboration with Prof. Ciobanu at the Colorado School of Mines.

Program Impact:
Our theoretical studies interact closely with experimental studies both at Ames Lab and other institutions. The interplay between the theoretical and experimental studies provides a comprehensive picture of the structures and properties of surfaces. Understanding the structures, electronic properties and dynamical behavior of surfaces and interfaces has an important impact on our ability to grow and stabilize various surface-based nanostructures such as quantum dots and quantum wires.

Interactions:
Internal- M. Tringides, M. Hupalo (Ames Lab-CMP), J. Evans (Ames Lab-Chemistry), External: C. Ciobanu (Colorado School of Mines), M. Y. Chou (Geogia Tech, Atlanta). Our group is part of a new DOE-BES Computational Materials Science Network (CMSN) project on "Formation and Stability of Surface-Based Nanostructures."

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Ho is a Fellow of the APS.
Our Tight Binding MD has been previously recognized as a DOE outstanding scientific accomplishment.

Personnel Commitments for FY2007 to Nearest +/- 10%:
C. Z. Wang (10%), K. M. Ho (10)%, B.J. Min, Visiting Scientist (10%); S.G. Hao, Postdoc (10%); J. Min, Postdoc (50%); 2 Students (70%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $123k **FY06 BA** $200k **FY07 BA** $200k

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

FWP and possible subtask under FWP: Condensed Matter Physics - Theory
Superconductivity Theory

FWP Number: AL-90-540-003

Program Scope:
The objective of this program is to develop theoretical understanding of the properties of superconductors in magnetic fields. We have studied the critical fields, critical currents, ac losses, and the structure and dynamics of vortices and vortex lattices. We have focused much of our attention on the effects of strong anisotropy in the high-temperature cuprate superconductors, on two-gap behavior in MgB_2, and on properties of antiferromagnetic superconductors.

Major Program Achievements (over duration of support):
- Introduced concepts of weak-link behavior in granular high-temperature superconductors.
- Developed theory of two-dimensional pancake vortices and interlayer Josephson vortices in layered high-temperature superconductors.
- Developed theory for the combined effects of geometrical barriers and bulk pinning on the field-dependent critical current in type-II superconducting strips.
- Wrote editorials for the *High-T_C Update* newsletter and web site.
- Using nonlocal London equations, developed theory for vortex-lattice transitions in borocarbides.
- Using a two-gap model, developed theories predicting different temperature-dependent anisotropies for the upper critical field and the London penetration depth in MgB_2.
- Developed a theory for the field dependence of the vortex-core size.

Program impact:
- New low-noise 77 K SQUIDs are currently being fabricated worldwide following our theoretical predictions that, in the earth's magnetic field, vortices are not trapped in superconducting lines of width less than ~5 mm.
- The *High-T_C Update* had a major impact on the development of high-temperature superconductivity.
- Small-angle neutron scattering, scanning tunneling microscopy, and decoration experiments in superconducting borocarbides have confirmed our predictions of vortex-lattice transitions.
- Different temperature behaviors of anisotropies of the upper critical field and of the penetration depth of MgB_2 have been confirmed in a number of experiments.

Interactions:
- Internal: P. Canfield, S. Bud'ko, D. Vaknin, and R. Prozorov
- External: Brookhaven National Lab, IBM, Los Alamos National Lab, Naval Research Laboratory, Oak Ridge National Lab, Institute of Solid State Physics (Moscow, Russia), Max Planck Institute (Germany), National Institute of Advanced Industrial Science and Technology (Japan), and these universities: Notre Dame, Stanford, Texas A&M, Isfahan (Iran), Napoli (Italy), Tel Aviv (Israel), and Tübingen (Germany).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
- V.G. Kogan and J.R. Clem are Fellows of the American Physical Society.
- JRC: DOE Annual Award for Sustained Outstanding Research in Solid State Physics, fellow of the Institute of Physics, London, founding editor of AIP and APS's *Virtual Journal of Applications of Superconductivity,* editorial boards of *Physical Review B* and *Superconductor Science and Technology.*
- Invited talks: 302 by JRC since 1969 and 56 by VGK since 1989.

Personnel Commitments for FY2007 to Nearest +/- 10%:
J.R. Clem (25%), V.G. Kogan (100%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $247k **FY06 BA** $267k **FY07 BA** $287k

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

FWP and possible subtask under FWP: Condensed Matter Physics - Theory
Strongly Correlated Systems

FWP Number: AL-90-540-003

Program Scope:
The development and application of modern approaches in many body theory to novel materials, including hard condensed matter systems like unconventional magnets, transition metal oxides, organic conductors, heavy fermion systems, and nearly magnetic systems, as well as soft condensed matter systems like micro-emulsions and physical gels formed of block-copolymers. Emphasis is given to the prediction or description of new physical effects and extreme materials properties caused by strong quantum fluctuations, the competition between interactions and disorder as well as between interactions on different length scales. Energy landscape approaches, concepts of field theory and quantum criticality, and computational techniques are used.

Major Program Achievements (over duration of support):
1) Demonstration that the emergent relativistic symmetry of electrons in graphene near its quantum critical point implies a crucial importance of the Coulomb interaction. Our analysis yields numerous predictions for how the Coulomb interaction will be manifested in experimental observables such as the diamagnetic response and electronic compressibility. 2) Theoretical prediction for the shape and shape variations of cooperatively rearranging regions in glass forming liquids. The theory unifies seemingly contradictory results and predicts a significant change of the shape of regions determining dynamical heterogeneity in glasses from stringy (at higher temperatures) to compact (at lower temperatures). 3) Development of a new theory for universality of liquid-gas Mott transitions at finite temperatures. We explained in a consistent manner the set of seemingly conflicting experiments on the finite temperature Mott critical point. 4) We showed that the spatial dimensionality of the quantum critical point associated with Bose--Einstein condensation of high magnetic field triplets is reduced when the underlying lattice comprises a set of layers coupled by a frustrating interaction. Our theoretical predictions correspond very well with recent measurements in $BaCuSi_2O_6$. 5) Development of a new theory for spin liquid behavior, superconductivity, and valence bond crystal formation in the doped Mott insulator $SrCu_2 (BO_3)_2$.

Program impact:
Our theory for charge Kondo superconductivity initiated new core level photoemission experiments by A. Kaminski and his group in Ames, who demonstrate the existence of two distinct valence states in Tl-doped PbTe. Our prediction for unconventional superconductivity and strong asymmetry between electron and hole doping in doped valence bond solids influenced several efforts to synthesize holde doped systems. Our theory for shape variations of cooperatively rearranging regions in glass-forming liquids attracted experimental as well as theoretical interest, since it allows for a unified view of seemingly contradictory observations.

Interactions:
Internal- CMP (Tringides, Canfield, Johnston, Kogan, Kaminski, Prozorov, Ho, Harmon, Wang), Chem. (Mallapragada, Lamb). External- LANL (Batista, Harris, Pines, Curro); ANL (Norman); UCSD (Wolynes), Columbia Univ. (Millis); Univ. of Wisc. (Chubukov), UIUC (Fradkin, Philipps), UI-Chicago (Morr), Rutgers (Kotliar, Coleman), Univ. of Missouri (T. Vojta), Ohio State (Trivedi), Orsay (Pepin), Cologne (M. Vojta), Stanford (Fisher).

Recognitions, Honors, and Awards (at least partly due to support under this FWP or subtask):
Mid-Career Award for Excellence in Research of Iowa State University's College of Liberal Arts and Sciences (2007); Graduate Teaching Award, Department of Physics and Astronomy, Iowa State University (2007); Fellow, American Physical Society (2006); Early Achievement in Research Award, ISU-Foundation (2003). Research Innovation Award of the Research Corporation (2001), 39 invited talks at major international conferences.

Personnel Commitments for FY2007 to Nearest +/- 10%:
J. Schmalian (17%), Postdoc, D. Sheehy (100%), 2 Students (50%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $145k **FY06 BA** $150k **FY07 BA** $150k

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

FWP and possible subtask under FWP: Condensed Matter Physics, Theory
Magnetic and Electronic Properties – Exploratory Projects

FWP Number: AL-90-540-003

Program Scope: This subtask is the skunkworks for condensed matter theory. It supports projects that are not restricted by specific roadmaps, and as such it has had wonderful success in spawning new initiatives such as a) Phononic Band Gap Materials, b) Magneto-Optics, which expanded to Correlated States, c) Spin Dynamics, d) Mesoscale Ordering, and e) Magnetic Molecules. It was the nurturing place for the Computational Materials Science Network, and has led to funding from the Army for quantum computing simulations. Currently, this subtask supports work in molecular dynamics (from first principles, to tight-binding, to classical). It supports work in disordered systems, and it supports work in bridging length scales in magnetism.

Major Program Achievements (recent):
We developed a jellium-passivated cluster model to study short-range ordering in supercooled liquid and glass systems. The energy difference between icosahedral clusters and FCC embryos in jellium is found to correlate with the glass-forming ability of liquid Al alloys. This model will be useful for studying the short-range order tendency with minor chemical additions in metallic glass formation, without the use of large unit cell calculations.

We developed a dynamical approach for understanding the properties of random lasers, especially above the laser threshold (*PRL*). When the optical gain is inhomogeneously broadened, we discovered the possibility that some lasing modes are coupled through photon hopping or electron absorption and reemission, which can lead to synchronization of their lasing action for weak coupling, and to antiphase mode locking for strong coupling.

We developed a systematic scheme for dynamical multiscale modeling using statistical coarse graining. It allows the short wavelength modes, essential for thermal equilibrium, to be incorporated in models at all length scales. Successful tests of 1D and 2D systems are complete and 3D tests await a new student. A new mean field theory for treating a central spin decohering in a bath of spins (electron in a quantum dot) has been developed to account for correlation (decoherence) effects. The success of this approach has spawned a new task for the control, and diagnostics of electronic and nuclear spins in nanosystems.

Program Impact:
Our tight-binding potentials have been adopted by many research groups worldwide for molecular dynamics simulations of various complex systems. The light localization and random laser work has attracted attention of several outside groups and collaborations with several research groups are exploiting the theory for new experiments and possible device designs. The multiscale modeling work is being incorporated into a micromagnetics code developed under the Computational Materials Sciences Network.

Interactions:
Internal- Ames Lab Chemistry (K. Ruedenberg, M. Gordon, M. Schmidt).
External - J. R. Chelikowsky (Minnesota); Seoul National University (Korea): Gun-Do Lee; Mingsheng Tang (China); M. Stocks (ORNL); M. Katsnelson (Nijmegen); E. Economou (Greece).

Recognition:
The TB work was awarded the Materials Science Award for Sustained Outstanding Research in Solid State Physics (before this funding period). Ho, Soukoulis, and Harmon are APS Fellows. (As mentioned in the "scope" above, this subtask is vital for exploratory work, and has been remarkably successful in spawning new directions.)

Personnel Commitments for FY2007 to Nearest +/- 10%:
C. Z. Wang (60%); V. Antonov, Visiting Scientist (10%); Y. Lee, Postdoc (25%), W. Zhang, Postdoc (33%); 4 Students (83%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $230k **FY06 BA** $277k **FY07 BA** $300k

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

FWP and possible subtask under FWP: Condensed Matter Physics, Theory.
Spin Dynamics

FWP Number: AL-90-540-003

Program Scope: Create, develop, and use first principles methods that will allow accurate simulations at the atomistic level of complex realistic magnetic materials. We partner with ORNL scientists in implementing these methods on modern supercomputers to allow treatment of large unit cells so that thermal and other dynamical properties can be simulated. Exact quantum treatment of spin dynamics for relevant model systems is pursued.

Major Program Achievements (over last 3 years):
A new expression for the critical temperature of a magnetic phase transition was obtained in the framework of Green function techniques. Simultaneously, the influence of short-range order on magnetoresistance was found significant above the critical temperature. Conditions for spin wave existence above the critical temperature were formulated. Deviation from the Bloch law was found practically in all magnets, while for rare earth materials a very detailed study with experimentalists was performed and a '5/2' T-dependence was identified. We developed an approach for self-consistent calculations of the many body Green function in transition metals and insulators, and used it for ab-initio studies of 3d-, 4d- and 5d- metallic systems. A new general technique for the calculation of exchange coupling parameters and spin waves was developed and used for the study of numerous magnetic systems. Based on ab-initio spin dynamics simulations, we predicted the existence of large magnetic short range order in itinerant magnets above their Curie temperature. This has the potential to radically change the common view of finite temperature magnetism and could impact many interpretations of experiments related to itinerant magnets. A new classification of magnetic materials, based on this short-range order idea, was proposed and applied to real materials. A theory of spin current in non-collinear systems was proposed and applied for Co-based multilayers. Simulation methods were developed to follow quantum spin oscillations in quantum dots and in magnetic molecules when those systems (qubits) are subjected to decoherence effects caused by a dynamical thermal spin bath of surrounding nuclear spins. An unexpected suppression of decoherence was found and explained for even numbers of qubits. Chaotic spin baths were found to be particularly effective for destroying coherence in qubit systems.

Program Impact:
Our development of first principles spin dynamics (and our treatment of non-collinear magnetism in general) has been widely disseminated; although for large systems, the simulation of the thermal fluctuations in very large unit cells is still very demanding and requires considerable supercomputing resources (ORNL). Our newly proposed technique for the calculation of exchange parameters is very general and is being used for both localized and itinerant magnetic systems. Our newly developed GW code is publicly available. Several experimental groups have expressed interest in pursuing our predictions of short-range magnetic order at high temperatures. The studies on spin bath decoherence are being picked up by NMR experimentalists (at Yale) to analyze recent investigations.

Interactions:
Internal – Ames Laboratory B.McCallum and V. Pecharsky (MEP), R. Prozorov, S.Bud'ko and F. Borsa (CMP).
External – M. van Schilfgaarde (Arizona State), N. Nadgorny (Wayne State), M. Stocks (ORNL), N. Zein (Russia), M. Auslander (Izrael), M. Katsnelson (Nijmegen, the Netherlands), H. De Raedt (Groningen, the Netherlands).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
This project is one of the DOE Science 100 accomplishments (for the first 25 years of DOE). Harmon is a Fellow of American Physical Society and has helped organize focused sessions at three March meetings and the invited symposium at the MMM conference. Both Harmon and Antropov have been on the program committee of the MMM conference. Two invited review articles, 21 invited talks in last 3 years.

Personnel Commitments for FY2007 to Nearest +/-10%:
V.Antropov (PI-70%), B.Harmon (PI-10%), V. Dobrovitski (30%), J. Joseph, postdoc (100%) +ORNL personnel

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $365k **FY06 BA** $456k **FY07 BA** $400k
(Note: Approximately $140k/year is sent to ORNL(Stocks) as a reconciling transfer for work on this project)

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

FWP and possible subtask under FWP: Condensed Matter Physics, Theory
Left –Handed Materials

FWP Number: AL-90-540-003

Program Scope:
Left-handed materials (LHMs) are composite materials with novel and unique electromagnetic (EM) properties, 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 LHMs, and also the investigation of their feasibility for potential applications.

Major Program Achievements (over duration of support):
Another part of our research concerns attempts to move the artificial magnetic response and the LH behavior from the microwaves (as in our initial experiments) to the infrared and optical regime. We succeeded to fabricate and to demonstrate the magnetic response of Split Ring Resonator (SRR) structures operating at 100 THz (*Science* **306**, 1351 (2004)), at 200 THz (*PRL* **95**, 203901 (2005)) and at 780 nm (*Opt. Lett.* **32**, 53 (2007)).

We design, fabricate, and characterize a low-loss silver-based negative-index metamaterial at 1.5 micron and 780 nm. The 1.5 micron structure has the best figure of merit reported for any negative-index photonic metamaterial to date (*Opt. Lett*. **31**, 1800 (2006)). Using the same sample, we were able to measure the phase and the group velocity, and found that both can be negative. These results were published in *Science* (**312**, 892 (2006)) and the negative *n* at optical frequencies (*Science* 315, **47** (2007)) and have generated a lot of publicity.

Our group has been instrumental in designing new structures that give negative n with low losses and finding the limits of the highest frequency of the LHMs. (*APL* **88**, 221103 (2006); *PRL* **95**, 223902 (2005); *PRB* **73**, 041101 (2006)).

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. Our work plays a major role in leading the development of LHMs both in theory and experiment.

Interactions:
External - E. Ozbay, Bilkent University, Turkey; D. R. Smith, Duke; Boeing's Phantom Works, Seattle; Research Center of Crete, FORTH; M. Wegener, Karlsruhe and J. Pendry, Imperial College.

Recognitions, Honors, and Awards (at least partly attributable to support under this subtask):
Soukoulis: Distinguished Professor of Liberal Arts and Sciences, Iowa State University, 2005; shared the **Descartes award** for collaborative research on left-handed materials in 2005; Fellow of **APS**, **AAAS** and **OSA**; Senior Alexander von Humboldt Award, 2002.
Invited Talks: *CLEO Europe*, Munich, Germany, June 2007; *NRC Photonics Meeting of the National Academies,* Washington, DC, January 2007; *PECS-VII* ***(Director)***, Monterey, CA, USA, April 2007. CMS gave also 21 additional invited talks at conferences and 10 seminars at universities in 2006-07.

Personnel Commitments for FY2007 to nearest +/- 10%:
Soukoulis (10%), T. Koschny (20%); 3 students (80%); Collaborators: M. Diem, E. Ozbay, Jiangfeng Zhou, G. Tuttle, E. N. Economou, Peter Markos.

Authorized Budget (BA) for FY05, FY06, FY07: (New program, in FY03)
FY05 BA $197k **FY06 BA** $193k **FY07 BA** $130k

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

FWP and possible subtask under FWP: Condensed Matter Physics, Theory.
Spin Susceptibility in Magnets

FWP Number: AL-06-540-029

Program Scope: The aim is to achieve a fundamental understanding of magnetic excitations, zero-point motion and the influence of temperature-dependent magnetic fluctuations in the systems with arbitrary magnetic ordering. This project is based on a new computational approach developed at Ames Laboratory and in collaboration with the group of Mark van Schilfgaarde at Arizona State University (ASU). Some computational and methodological aspects of this project have been developed previously under DOE support.

Major Program Achievements (over last 3 years):
GW code has been developed using linear muffin tin orbital basis set and applied for many different materials. In general, the biggest improvements over local density approximation (LDA) are found for semiconducting systems and for insulators. We developed a new computational scheme of calculating the dynamic susceptibility in the framework of the many body Green function approach and LDA. This technique combines the advantage of the basis product of the wave functions and an effective inversion procedure. These programs have been tested for 3d metals, many magnetic semiconductors and actinides. For the first time, we compared fully ab-initio calculations of $S(q,\omega)$ for Fe and Ni with the experimental data and explained the character of magnetic excitations at larger q and ω. We found a new mechanism of the spin wave decay, which exists at very low q and ω, and contributes to the temperature-dependence of the magnetization at low temperature. This mechanism is similar to the Stoner mechanism and is related to the bands crossing the Fermi level in magnetic metals. The corresponding theory has been formulated.

Program Impact: Our newly proposed technique of GW method implementation is very general and is being used for both localized and itinerant systems: metals, insulators, and semiconductors. Our newly developed GW full potential code is publicly available now, together with the LDA full potential code. Several theoretical groups are using these codes for electronic structure or susceptibility type of calculations.

Interactions:
Collaboration exist with K. Takao (ASU), N. Zein (Kurchatov Institute, Moscow, Russia) magnetism theory, S. Savrasov (UC Davis) dynamic mean field theory, M. Katsnelson (Nijmegen, The Netherlands) magnetism theory. This work is being performed jointly with the group of M. van Schilfgaarde of ASU.

Recognitions, Honors, and Awards (at least partly attributable to support under this FWP or subtask):
Both van Schilfgaarde and Antropov have been on the program committee of the MMM conference. One invited review article, 6 invited talks last year.

Personnel Commitments for FY2007 to Nearest +/-10%:
V. Antropov (10%), Visiting Scientist (100%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $0k **FY06 BA $**0k (new project) **FY07 BA** $96k

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

FWP and possible subtask under FWP: Condensed Matter Physics, Theory
Modeling, Control, and Diagnostics of Electronic and Nuclear Spins in Nanosystems

FWP Number:
AL-06-540-032

Program Scope:
Development and comprehensive characterization of novel quantum control approaches designed to mitigate the critical problem of decoherence of spins in solid-state nanostructures (electron spins in quantum dots, nuclear spins in solid-state low-dimensional systems). Determination of the optimal combination of deterministic and random protocols aimed at decoupling the system from decohering environments. Provide a detailed assessment, using both analytical and advanced numerical simulations, of performance and robustness of the promising decoupling schemes. Use of quantum control approaches to produce quantum diagnostics of experimentally relevant spin baths.

Major Program Achievements (over duration of support):
Studied the influence of an external magnetic field and nuclear polarization on the decoherence dynamics of an electron spin located in a GaAs quantum dot. Found that the external magnetic field not only suppresses longitudinal relaxation but also induces oscillations in the longitudinal component of the electron spin; provided analytical and numerical description of this effect. Demonstrated that, in order to suppress transversal relaxation, the polarization of the nuclear spins should exceed 99%; established this approach is impractical.

Studied in detail and characterized eight different control protocols (deterministic and random) for extending the coherence time of electron spins in GaAs quantum dots in the case of a small external field. Identified the most promising protocol based on concatenated design. Analyzed the influence of realistic non-idealities (finite pulse width, finite bias field, small rotation errors, small intra-bath coupling). Theoretically demonstrated the possibility of extending the coherence time by 2-3 orders of magnitude. Discovered the phenomenon of decoherence freezing at long times for certain families of control protocols, identified the origin of this effect, and gave simple analytical explanation supported by direct numerical simulations.

Program Impact:
Developed efficient control protocol, based on concatenated design, for extending coherence time of electron spins in GaAs quantum dots by 2-3 orders of magnitude at zero bias field. Possibility of experimental implementation is under discussion with the group of A. Rimberg (Dartmouth College).

Interactions:
The work is performed jointly with the group of L. Viola (Dartmouth College). Collaborate with the experimental NMR group working on control of nuclear spins (C. Ramanathan, D. Cory, MIT, and P. Capellaro, Harvard University). Collaborate with an experimental group focusing on controlling electron spins in semiconductor quantum dots (A. J. Rimberg, Dartmouth College). Simulations partially performed at NERSC.

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
V.V. Dobrovitski – 1 invited review article, 5 invited talks during 2007.
L. Viola – 4 invited talks during 2007, Member of Advisory Board of the First Conference on Quantum Error Correction (University of South California, Dec. 17-21, 2007).

Personnel Commitments for FY2007 to Nearest +/- 10%:
V. Dobrovitski (20%); Postdocs - R Hristov (10%), N. Konstaninidis, (20%).

Authorized Budget (BA) for FY05, FY06, FY2007:
FY05 BA $0k (New Project) **FY06 BA $**160k **FY07 BA $**150k

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

FWP and/or possible subtask under FWP:
Materials Chemistry and Biomolecular Materials: 1. Electronic Stabilization in Metal-Rich Solid-State Phases

FWP Number: AL-90-360-001

Program Scope: The program seeks to expand our knowledge and understanding of solid-state chemistry by combining experiment—particularly exploratory synthesis and structure—with theory in order to uncover new families of intermetallic phases and to understand the factors that stabilize both new and known phases. These families include Zintl, cluster, Hume-Rothery, quasicrystalline, and related phases. Experiments encompass high temperature synthesis (arc melting, reactive metal fluxes, sealed metal container) and variable-temperature single crystal and powder diffraction. Theoretical efforts span first-principles to semi-empirical calculations.

Major Program Achievements (over duration of support):
We have explored, developed and organized new polar intermetallics formed between active metals and the triels (Ga, In, Tl) as well as with Mg, Li, Zn, Au, Hg, discovering much unique chemistry beyond the classical Zintl (valence) boundary. We synthesized and characterized new Zintl (valence) and related compounds: K_5InPb_8, a Bergman-type structure in $Na_{11}(Cd,Tl)_{27}$, new hyper-electronic networks ($SrIn_4$, Sr_3In_5, $SrMgI_3$, $BaAu_2In_2$, $BaMg_5In_3$), and numerous tunnel structures in the K–Au–In system.. We identified and interpreted electronic deviations from Zintl concepts in terms of structure, properties, and theory; i.e., the importance of atom size limitations, and the means of structural and electronic tuning via Li, Mg, Zn, etc. substitutions in triel networks,. Important relativistic effects have been defined for substituted triel phases such as $BaAuIn_3$, BaPtIn3, and $BaAu_2In_2$. Several ab-initio studies have demonstrated the absence of the closed shell (Zintl) anions Bi^{-3} and Ge_2^{-6} in certain salts, and the major roles that cations play in the bonding in Na_3AuIn_2, Na_6TlSb_4, KNa_3In_9, $Ba_2Yb_2Sn_6$, and $Eu_3Bi(Sn,Bi)_4$.

Following up on theoretical studies of gamma brass structures in the Pd-Zn and Cu-Zn phases, the atomic distributions in Cu_9Al_4 and "Cu_5Sn" have been examined. In Cu_9Al_4, we can account for the two distinctive 26-atom clusters, one $[Cu_{22}Al_4]$ cluster at unit cell corners and one $[Cu_{14}Al_{12}]$ cluster at the unit cell centers. Theory also predicts the existence of Al-rich phases with a distinctive site preference for these additional Al atoms. We have already experimentally and theoretically characterized the Cu/Zn system near Cu_5Zn_8 for distributions of Cu and Zn atoms. This study revealed $[Cu_4Zn_4]$ kernels for the entire composition range. This arrangement optimizes a combination of site energies and bond energies in the solid. This work suggests a chemical (real space) interpretation for the stability ranges of gamma brasses.

Program Impact:
Our methods and discoveries have impacted or motivated solid-state chemistry concepts and programs around the world and have correspondingly attracted students and visitors from many places. This impact includes groups utilizing a combination of experiment and theory to investigate problems in solid-state chemistry, as well as in thorough characterization of products beyond crystal structure determinations.

Interactions (External):
PNNL, LANL; U.S. Universities at Cornell, Notre Dame, Houston, Northwestern, Utah State, Arizona State. Overseas organizations: Max-Planck Institutes at Stuttgart & Dresden; FJIRSM, Fuzhou, China. Foreign Universities at Barcelona (Spain), Aachen, Cologne, Muenster & Munich (Germany), and Stockholm (Sweden).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Co-organizers, Symp. on The Chemistry of Intermetallics and Zintl Phases at 226th ACS meeting (JDC & GJM '03); National Academy of Sciences (JDC '92); two ACS National Awards in Inorganic Chemistry (JDC '86 & '00); 2 DOE Awards in Materials Chemistry (JDC '87 & '95); F. H. Spedding Award (JDC '05); Visiting Professor, ETH-Zürich (GJM '00); Visiting Scientist, MPI-CPfS Dresden (GJM '06). Total of 15 invited talks and 38 refereed publications in this subtask since 2004.

Personnel Commitments for FY2007 (Actual Effort):
J. Corbett (40%); G. Miller (5%); S. Gupta (100%); A. Palusyuk (100%).

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $265k **FY06 BA** $260k **FY07 BA** $260k

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

FWP and/or subtask Title under FWP:
Materials Chemistry and Biomolecular Materials: 2. Bulk Structure and Structure-Property Relationships in Intermetallics and Metal-Rich Solid-State Inorganic Compounds.

FWP Number: AL-90-360-001

Program Scope: The goal is to elucidate the atomic positions in complex metal-rich solids, and to understand how this structure relates to physical properties, such as thermoelectric or magnetocaloric properties.

Major Program Achievements (over duration of support): (1) Toward quasiperiodicity in one-dimension: Exploration of the $Zn_{1-x}Pd_x$ binary system ($0.15 \leq x \leq 0.25$) identified a series of structures with unit cells showing two sides with common lengths and the third varying greatly, some with distances in excess of 100 Å. We could interpret these structures as intergrowths based on two different icosahedral blocks, and have developed an "algorithmic" method to prepare new structures that may lead to a one-dimensional quasiperiodic system. Four structures were solved using super-space group methods. Electron diffraction studies also show superstructures. These structures are related to the Hume-Rothery gamma-brasses, and similar behavior occurs in $Mn_{1+\delta}Ga_{1-\delta}$. (See also Electronic Stabilization) (2) Itinerant icosahedral magnets: Crystalline CrGa, MnGa, FeGa and $Cr_xFe_{1-x}Ga$ ($0 < x < 1$) were identified, structurally characterized by X-ray and neutron diffraction, and studied for their magnetic properties. This isostructural series is a set of approximants for icosahedral quasicrystals rich in transition metals. There is a change from antiferromagnetic to ferromagnetic behavior along the binary sequence, while Cr and Fe order according to local magnetic exchange seen in MnGa. $Mn_{1+\delta}Ga_{1-\delta}$ shows formation of the cubic gamma-brass type. (3) Defect-driven distortions: Defect Heusler-type intermetallics in the Ti-Ni-Ga system show a new superstructure that creates linked icosahedra, and further establishes the relationship between bcc-type structures and icosahedral quasicrystals. This phase, $Ti_{0.8}Ni_{1.9}Ga_{1.2}$ is also related to the gamma brasses, and provides a splendid "link" between Hume-Rothery phases and polar intermetallic phases studied in Sub-Task #1. Similar phases in the V-Co-Ga and Nb-Rh-Ga systems exist. (4) Complex cubic phases: New cubic phases in the Lu-Ni-In, Ce-Pd-In, and La-Pd-In have emerged that also show relationships to gamma brasses as well as to another complex cubic structure, the alpha-Manganese structure. Studies of Pd/In and Ni/In distributions show partial ordering of these elements throughout the network. Magnetic properties of these phases remain to be studied. (5) Collaborations: We enjoy ongoing collaborations with groups in Condensed Matter Physics (Canfield) and Materials and Engineering Physics (Lograsso): diffraction analysis of structures and composition in the half-Heusler alloys Yb-Pd-Bi and in Ce-Pd-Al phases.

Program impact: This research continues a strong tradition within the Materials Chemistry and Biomolecular Materials Program at the Ames Laboratory of the discovery of new metal-rich phases, the delineation of their structure, as well as their structural variation with temperature and with conditions of formation.

Interactions (External):
APS at Argonne, Los Alamos; Stanford. Overseas organizations: Max-Planck Institute at Dresden; Foreign Universities at Aachen & Munich (Germany), and Stockholm (Sweden).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Visiting Professor, ETH-Zürich (GJM '00); Co-Organizer, Symp. on The Chemistry of Intermetallics and Zintl Phases at 226th ACS meeting in New York City (GJM '03); Visiting Scientist, MPI-CPfS in Dresden (GJM '06); Symp. Co-Organizer, Quasicrystals, MRS Fall Meeting (DJS '03); Conference Co-Organizer, 9th International Conference on Quasicrystals, Ames (DJS '05); Member of International Program Committee for 12th LAM Conference (DJS '04). Total of 30 invited talks & 17 refereed papers in this topic area since 2004.

Personnel Commitments for FY2007 (Actual Effort):
G. Miller (30%); D. Shechtman (20%); M. Besser (20%); X.-F. Guo (100%); H. Ko (25%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $130k **FY06 BA $**140k **FY07 BA $**160k

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

FWP and/or possible subtask under FWP: Materials Chemistry and Biomolecular Materials (MCBMM): 3. Surface Structure and Structure-Property Relationships in Metal-Rich Solid-State Phases

FWP Number: AL-90-360-001

Program Scope: Our research encompasses fundamental issues in surface science that are central to energy-related applications. In keeping with the goal of the MCBMM Program to understand and control the properties of matter, we focus on structure-property relationship at surfaces. Our research specifically examines the fundamental surface characteristics of complex intermetallics. Aspects probed include microscopic and mesoscopic morphology, atomic locations, electronic structure, interfacial growth, friction, and chemical reactivity. Nucleation and growth of solid films, for example, is important to our energy economy as it is key to some solar cell technologies. Friction—a surface phenomenon—is often detrimental to energy efficiency.

Major Program Achievements (over the last 3 years): (1) Atomic Structure and Reactivity: AL scientists recently discovered that Ni–Al with Pt added produces excellent thermal barrier coatings. The mechanisms that drive the improved oxidation resistance arising from Pt addition were not understood. Surface-sensitive techniques, complemented by theoretical simulations, showed Pt segregation to the surface plays a key role. For the surface structure of quasicrystalline materials, we demonstrated that temperature effects play a vital role. A temperature change from 900 to 925 K is sufficient to dramatically alter the quasicrystal terraces; at the lower temperature, a distinctive void-rich termination is common. These results provided new insight into the way that a surface evolves toward a quasicrystalline structure. (2) Thin Film Growth: Studies of Ag film growth on quasicrystals has produced evidence of site-directed growth below 300 K. We elucidated the conditions that favor saturation of these trap sites; such information is useful for further studies of pseudomorphic growth in related systems. Above 300 K, the novel electronic structure of these materials yields quantum size effects resulting in structures with a dominant height. Key variables that affect growth behavior include temperature, flux, and diffusion barrier variation as a function of terrace structure. (3) Friction and Wear: We collaborated with M. Salmeron. D. F. Ogletree and J.-Y. Park at LBNL to examine the fundamental role of periodicity in friction. To clearly delineate the role of aperiodicity, we limited the variables to just periodicity and aperiodicity by working on the twofold surface of decagonal Al–Ni–Co, which has atoms aperiodically-spaced along one direction and periodically along the other. Atomic force microscopy measurements showed an 8-fold anisotropy in the friction force on this surface, the lowest in the aperiodic direction, hence demonstrating that low friction forces are intrinsic to the aperiodic arrangement. This work was published in *Science* in 2005. An offshoot of this work, published in *Science* in 2006, demonstrated that free charge carriers can play a critical role in frictional energy dissipation on semiconductors.

Program Impact: Our work to date has culminated in the acceptance in the field that atomically flat quasicrystalline surfaces can be produced and that these surfaces are laterally bulk terminated; this work has implications for the relative importance of three-dimensional clusters in stabilizing the icosahedral structure. It has also demonstrated that low friction is intrinsic to the aperiodic atomic structure of a clean quasicrystalline surface, laying to rest the possibility that low friction in these materials is due (solely) to hardness or oxide chemistries. In addition, our work has motivated and facilitated many new research projects around the world.

Interactions (External): U.S. Natl. Laboratories: LBNL, SNL-CA. U.S. Institution: Penn. State Univ. Foreign Institutions: CNRS-INPL-UHP, Tohoku Univ., Nat. Institute Mater. Sci. (Tsukuba), Lappeenranta Univ. Technol.

Recognitions, Honors and Awards (at least partly attributable to support under this subtask): Iowa Board of Regents Award for Staff Excellence (CJ ’06); ISU P&S Council CYtation Award (CJ ’06); Co-Organizers, 9th Intl. Conf. on Quasicrystals (CJ & PT ‘05); Dr. Honoris Causa (honorary degree) from the Institut National Polytechnic de Lorraine (PT ’05), Distinguished Professor of ISU (PT ‘02); Fellow of the AVS (PT ‘01); Fellow of the APS (PT ‘01); ISU College of Liberal Arts and Sciences Award for P&S Staff Excellence (CJ ‘99); DOE Award for Outstanding Scientific Accomplishment in Materials Chemistry (CJ & PT ‘98); Total of 13 invited talks and 19 refereed publications, including 2 in *Science* and 3 in *Physical Review Letters* from FY05 – FY07.

Personnel Commitments for FY2007: C.J. Jenks (10%); P.A. Thiel (15%); F. Qin (40%); B. Unal (50%); D. Jing (50%); M. Duncalf (25%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $380k **FY06 BA** $380k **FY07 BA** $385k

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

FWP and/or possible subtask under FWP:
Materials Chemistry and Biomolecular Materials: 4. Solute Effects in Metal-Rich Solid-State Phases

FWP Number: AL-90-360-001

Program Scope: The goal is to combine experiments and theoretical calculations to elucidate the effect of small concentrations of atomic solutes on phase stability, formation pathways, and high-temperature phase transitions in solid-state inorganic materials, particularly binary glass-forming alloys. Control of low levels of solutes can be very difficult, but this is often possible for groups within the Ames Laboratory because of the specialized synthesis expertise and facilities developed here. Moreover, our time-resolved high-energy X-ray scattering techniques are especially critical for determining the dynamic evolution of glass structure and phase selection during heating.

Major Program Achievements (over the duration of support):
Amorphous $Zr_{75}Pt_{25}$ melt spun ribbons containing between 100 and 2500 ppm oxygen have subtle, yet important structural differences, as determined by synchrotron X-ray diffraction at the Advanced Photon Source. Specifically, at low Q values, the S(Q) shows a "pre-peak", which results from medium-range ordering between the first-shell short-range order and the corresponding nearest-neighbor environment. The height of the pre-peak increases as more oxygen is added. In addition, real-space G(r) data show that the first peak also changes as a function of oxygen content. Combining the experimental scattering data with *ab initio* simulations reveals that Zr-Pt correlations increase as more oxygen is added, while Zr-Zr correlations decrease. Since oxygen has a much stronger affinity for Zr than Pt, these results suggest that Zr-Zr bonding is reduced at the expense of emerging Zr-O pairs, leading both to enhanced Pt-Pt medium-range ordering and decreased Zr-Zr bonding. These details are being used to construct more accurate structural models of amorphous binary metallic glasses to understand how small additions of solute atoms modify short- and medium-range order, leading to new metastable structures during crystallization.

Among the Zintl-related polar intermetallics, we have found numerous phases that are stabilized by hydrogen or other small interstitials, especially those of the tetrels (Si–Pb) and triels (Ga–Tl) with alkaline-earth metal counterions. Many examples have Mn_5Si_3-type structures. Recent examples include Sr_5Tl_3, La_3In_{11}, and Yb_5Sn_4, all of which are actually hydrides. Many polyanionic clusters of Ga, In and Tl have been found that also take up transition metal atoms as interstitials in stoichiometric amounts, e.g., $Rb_8Tl_{11}Pd$, whereas small amounts in other clusters alter counts and, therewith, stabilities.

Program Impact:
A common result is the discovery that phases reported previously in the literature were, in fact, solute-stabilized and exist only as such. It is extremely important to correct such mistakes for many reasons, among them the fact that reliable experimental data is necessary to validate high-level theory for complex solid-state systems. This is also true for metastable phases in model binary metallic glasses, which may well lead to a deeper understanding of the role of solute atoms in changing short- and medium-range order of a metallic glass and, as a consequence, the crystallization pathway.

Interactions (External):
Advanced Photon Source at ANL; US Universities at Notre Dame, Houston, Northwestern, Utah State, Arizona State. National Laboratories and Industries Overseas, at CNRS--Nancy (France), Max-Planck Institutes at Stuttgart and Dresden (Germany), LGChem (Korea), FJIRSM, Fuzhou (China). Foreign Universities at Barcelona (Spain), Cologne, Munich, Karlsruhe (Germany).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
F. H. Spedding Award in Rare Earth Research (JDC '05); Symp. Co-Organizer, Quasicrystals, MRS Fall Meeting (DJS '03); Conf. Co-Organizer, 9th Intl. Conf. on Quasicrystals, Ames (DJS '05); Member of Intl. Program Comm. For 12th LAM Conf. and Intl. Adv. Comm. for the Intl. Conf. on Solidification Sci. & Process. (DJS '04). Total of 16 invited talks and 33 refereed papers since 2004.

Personnel Commitments for FY07 (Actual Effort):
D. Sordelet (50%); J. Corbett (10%); M. Besser (20%)

Authorized Budget (BA) for FY05, FY06 and FY07:
FY05 BA $280k **FY06 BA** $305k **FY07 BA** $305k

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

FWP and/or possible subtask under FWP:
Materials Chemistry and Biomolecular Materials: 5. Macroscopic Growth of Metal-Rich Solid-State Phases

FWP Number: AL-90-360-001

Program Scope: The primary goals of this subtask are to design, discover, grow, and characterize novel materials with exotic and/or interesting physical properties. This subtask focuses on the development of synthesis routes and the characterization of bulk single grains of aperiodic phases and closely related crystalline approximant phases; and understand the differences in phase stability between aperiodic and crystalline materials. Characterization will be performed using advanced transmission electron microscopy and X-ray diffraction techniques. A secondary goal is to stimulate the international scientific community by sharing our high-quality samples in collaborative studies. The size, quality and detailed characterization of our samples allows for the measurement of intrinsic material properties, often circumventing the relationship between growth quality and properties that can lead to spurious results.

Major Program Achievements (over last three years): We have been the only research group to develop synthesis routes leading to large (up to 2.5 cm^3) single grains of these binary phases, specifically the Cd–Yb icosahedral phase ($Cd_{84}Yb_{16}$), its hexagonal approximant ($Cd_{51}Yb_{14}$) and the cubic approximant ($Cd_{86}Yb_{14}$). We were able to study the correlations between local and long-range order in the quasicrystal phase and its corresponding approximant phase. High resolution transmission electron microcopy (HRTEM) and image simulation techniques through focal images revealed a high degree of structural perfection and the remarkable similarity between the local atomic structure of the QC and its approximant phase. This program also made single crystals of icosahedral phase ($Cd_{17}Ca_3$) and cubic approximant phase (Cd_6Ca). The characterization by HRTEM on these compounds is ongoing. In addition, this group is the first one to grow centimeter-sized Zn-Sc single grain approximant phase which are sufficient for neutron scattering studies. Evaluation of candidate low melting pure metal liquids for fluxes for the single crystal growth Ti-based quasicrystals was initiated. While an appropriate solution has yet to be found we have found and are characterizing several new ternary Ti-Zr based compounds. Our continued efforts in synthesis of Al-Cu-Fe and Al-Pd-Mn quasicrystals, utilizing the highly successful synthesis protocols developed previously under this task, continue to yield high quality single crystals that enable new scientific insight into the nature of aperiodic structures their surfaces and interfaces. This very successful collaborative effort seeded by the Materials Chemistry and Biomolecular Materials program has led to a newly initiated effort in the Materials Engineering and Physics (MEP) program, *Rational Growth, Control and Modification of Novel Materials* (led by Lograsso, in close collaboration with Canfield) which will provide a much larger and more focused approach to synthetic growth of intermetallic compounds.

Program Impact: Our efforts have had a significant impact on the understanding on the structure of quasicrystals and quasicrystalline surfaces and of this program have been tremendous. Over 30 labs throughout the world have used the high quality quasicrystals samples synthesized at Ames Laboratory, thus allowing the field to advance at a pace faster than otherwise possible. We continue to share high quality single crystals for collaborative research and have transferred our synthesis protocols to the Materials Preparations Center, allowing for the general scientific community to access high quality single grains of aperiodic materials.

Interactions (External): U.S. National Laboratories: ANL, BNL, LBNL, LANL, SNL; U.S. Universities at Carnegie Mellon, Penn. State, Stanford.; National Laboratories Overseas at CNRS, INPG, ESRF, CEA, ILL, ETH-Zürich, NIMS; Foreign Universities at Bu-Ali Sina, Liverpool, Newcastle.

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
MRS Fall 2003 Best Poster Award (TAL ‘03); DOE Award for Outstanding Scientific Accomplishment in Materials Chemistry (TAL & CJJ ‘98); Total of 35 refereed publications in this topic area since 2004.

Personnel Commitments for FY2007 (Actual Effort):
T. Lograsso (10%), C. Jenks (10%), D. Wu (20%)

Authorized Budget (BA) for FY05, FY06, FY2007:
FY05 BA $165k **FY06 BA** $80k0 **FY07 BA** $60k

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

FWP and/or possible subtask under FWP:
Materials Chemistry and Biomolecular Materials: 6. Bioinspired Polymers: Self-assembling Hydroxyapatite-Polymer Nanocomposites

FWP Number: AL-90-360-001

Program Scope: Synthesis and characterization of novel bioinspired polymeric materials that mimic living systems in their abilities to switch among several states in response to the environment and self-assemble hierarchically. Use of these polymers as templates to direct biomineralization processes, and 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 polymeric materials with inorganic components and biomolecules.

Major Program Achievements (over duration of support): We have designed and synthesized novel multiblock copolymers with various cationic, anionic and zwitterionic blocks that exhibit hierarchical self-assembly from nanoscale micelles to macroscale gels and solids. Different calcium phosphate phases, both hydroxyapatite and brushite, were templated on these polymer micelles in solution. Since the self-assembly process is driven by the relative hydrophobicities of the different polymer blocks, these nanoscale micelles coated with thin inorganic shells exhibited self-assembly into gels and solids, just as in the case of the pure polymer. New advanced solid-state NMR techniques were developed to investigate the hybrid organic-inorganic structures formed by self-assembly. These NMR techniques provide the thickness of the inorganic layer formed (of the order of a few nm) as well as compositional information about the nanoscale inorganic layer at the organic-inorganic interface, which is very difficult to obtain using other established techniques. In addition, small angle X-ray and neutron scattering studies of these hybrid gels and solids at Argonne indicated that the structure of the polymer gels was preserved even in the presence of the inorganic coatings on the micelles and did not significantly alter the self-assembly process of the underlying polymer template. The chemical structure of the polymer template was seen to have a significant role on the mineralization process and the thickness and composition of the calcium phosphate layer formed.

Program Impact:
Self-assembly across multiple length scales is key to the development of a “bottom-up” approach to materials design and our research has generated a new class of hierarchically self-assembled nanocomposites. We have developed NMR techniques that are being used worldwide by other groups.

Interactions:
Argonne National Laboratory; Univ. of Paris, EPFL; Technion, Israel; Koc University, Turkey.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
NSF-CAREER award (SKM, ‘00); MIT's Technology Review’s "Top 100 Young Innovators" list (SKM, ‘02); John H. Dillon Medal of the American Physical Society (KSR-‘01); Fellow of AIMBE (SKM, ’06); Ross Coffin Purdy Award (MAA, ’06); Big 12 Rising Star Award (SKM, 07); ISU Mid-Career Excellence in Research Award (SKM, 07); 33 refereed publications and 20 invited talks since 2004.

Personnel Commitments for FY2007 (Actual Effort):
S.K. Mallapragada (20%); M. Kanapathipillai (50%); B. Zhang (25%); A. Travesset-Casas (10%); J. Anderson (5%); K. Schmidt-Rohr (5%); A. Rawal (5%); M.A. Akinc (10%); X. Wei (50%); Y. Yusufoglu (50%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $245k **FY06 BA** $240k **FY07 BA** $245k

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

FWP and/or subtask Title under FWP:
Materials Chemistry and Biomolecular Materials: 7. Solid-state NMR of polymers and nanocomposites

FWP Number: AL-90-360-001

Program Scope: Development and application of advanced solid-state nuclear magnetic resonance (NMR) methods and scattering simulations for elucidating the nanometer-scale structure and dynamics of heterogeneous polymer-based materials under the following types of conditions: Ionomers as used, for instance, in all-solid H_2/O_2 fuel cells; Biological and biomimetic apatite-polymer nanocomposites; Silica-polymer nanocomposites.

Major Program Achievements (over duration of support):
Structure of Nafion: A definitive new model of the nanometer-scale structure of the Nafion ionomer, used in fuel-cell proton-exchange membranes, has been developed based on NMR and quantitative scattering analysis. High-resolution ^{13}C NMR of fluorinated polymers such as Nafion and PTFE (Teflon) was achieved for the first time and revealed a high degree of conformational order of the Teflon-like backbone of Nafion. The conformationally ordered helices rotate around their axes and pack with limited orientational order. The branch points are relatively immobile, while the anionic sidegroups move significantly in the presence of water. In order to characterize the supramolecular structure, we have developed an algorithm for simulating small-angle scattering data using multidimensional numerical Fourier transformation as familiar from 2D and 3D NMR. On this basis, we can exclude all specific models of Nafion previously proposed; we prove that instead of spherical clusters, bilayers, channel networks, or polymer bundles, the system forms long, parallel water channels (inverted micelle cylinders) of ~ 2.5 nm diameters, which explain the salient transport properties of Nafion.

Structure of Biological and Biomimetic Nanocomposites: The apatite-collagen nanocomposite in bone has been elucidated in terms of the composition of both components and their distances from the organic-inorganic interface. Several new NMR approaches for studying nanocomposites, including HeteronucleAr Recoupling with Dephasing by Strong Homonuclear Interactions of Protons (HARDSHIP), have been introduced. They have revealed the thickness of apatite nanocrystals in bone, the concentration and location of carbonate and hydroxide ions, the presence of bound and viscous water layers at the interface, and the COO^- and CH-OH apatite-binding sites of collagen. These methods have been applied to help guide the synthesis of biomimetic polymer-apatite nanocomposites.

Improved Characterization of Heterogeneous Polymers: New ^1H spin diffusion NMR methods for characterizing heterogeneities in multicomponent polymer materials, on the 0.5 - 50 nm scale, have been introduced. They provide improved contrast through ^{13}C evolution and detection, and improved accuracy by calibration of local spin diffusion coefficients. Sensitivity enhancement (4 - 10-fold) has been achieved in various NMR experiments by indirect ^1H detection, signal refocusing, or multiple alternating depolarization.

Heterogeneous para/ferromagnetic polymer materials. Many polymer-based materials contain para- or ferromagnetic particles. New insights into their effects on the NMR of the polymer matrix have been obtained.

Program Impact:
This work has provided insights into the microscopic origins of macroscopic properties of nanostructured polymer-based systems; hopefully, this will eventually lead to improved materials. The NMR techniques developed by our group have been and will be used worldwide by other NMR groups.

Interactions (External):
University of Southern Mississippi, Hattiesburg.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
John H. Dillon Medal of the Polymer Division of the American Physical Society (KSR '01). Total of 9 invited talks and 13 refereed publications in this topic area since 2004.

Personnel Commitments for FY2007 (Actual Effort):
K. Schmidt-Rohr (50%); A. Rawal (45%); E. Levin (50%); Y. Hu (45%); X. Kong (45%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $250k **FY06 BA** $245k **FY07 BA** $225k

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

FWP and/or possible subtask under FWP:
Materials Chemistry and Biomolecular Materials: 8. Bioinspired Materials: Aptamer-Mediated Templates for Hybrid Elastic Nanostructures

FWP Number: AL-90-360-001

Program Scope: Creation of a new class of biomimetic hybrid materials involving magnetite nanocrystals embedded in hierarchically self-assembling polymers. Controlling nanoscale magnetite synthesis using bacterial mineralization proteins and using DNA/RNA aptamers for achieving specificity of non-covalent binding within the polymer. Investigation of these novel materials and processes using experimental characterization tools as well as theoretical approaches combining modern polymer theory and the theory of micro-magnetism.

Major Program Achievements (over duration of support): A bacterial mineralization protein from magnetotactic bacteria, mms6, was found to facilitate formation of uniform cubo-octahedral nanocrystals of magnetite in solution with sizes of about 40 nm, as seen by transmission electron micrography. It is very difficult to synthesize nanocrystals with similar size and morphology by using other room temperature synthesis techniques. The magnetite nanocrystals obtained exhibited strong superparamagnetic behavior, which is typical for monodomain nanoparticles. In the presence of a self-assembling polymer gel, the formation of these magnetite nanocrystals was found to be much more controlled than in free solution. DNA and RNA aptamers are being developed to bind to mms6 as well as the self-assembling polymers. The approach was also used to synthesize cobalt ferrite nanocrystals in vitro using mms6 as a templating agent, because of their enhanced magnetic properties. Even though mms6 is not involved in the production of cobalt ferrite nanocrystals in Nature, the use of the mineralization protein was found to promote the formation of uniform cobalt ferrite nanocrystals in vitro, making it a truly general bioinspired approach for synthesis of uniform nanocrystals under ambient conditions. A variety of scattering, microscopy and other characterization techniques were utilized to investigate the structure and magneto-mechanical properties of these hybrid materials. The magnetic property measurements were consistent with the morphology studies using transmission electron microscopy studies. The nanocrystals synthesized in the presence of the mineralization proteins exhibited distinct magnetic properties compared to those synthesized in the absence of the proteins.

Program Impact: The use of bacterial mineralization proteins to create uniform, monodisperse, monodomain nanocrystals of magnetite and cobalt ferrite in vitro 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 materials design.

Interactions:
Argonne National Laboratory

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
NSF-CAREER award (SKM, ‘00); MIT's Technology Review’s "Top 100 Young Innovators" list (SKM, ‘02); ISU College of Liberal Arts and Sciences Award for Excellence in Research Creativity (GAK, ’01); ISU University Professor (GAK, ’04); ISU Regents Faculty Excellence Award (GAK, ’04); Federated Laboratories Consortium Distinguished Service Award (GAK, ’05); MIT’s Technology Review “Top 100 Young Innovators” list -TR100 Award (BN, ’03); 3M Faculty Award (BN, ’03); Fellow of the American Physical Society (PCC ‘02); Divisional Associate Editor for Phys. Rev. Lett. (PCC ‘02); Fellow of AIMBE (SKM, ’06); Big 12 Rising Star Award (SKM, 07); ISU Mid-Career Excellence in Research Award (SKM, 07); 8 publications and 12 invited talks since 2004.

Personnel Commitments for FY2007 (Actual Effort):
S.K. Mallapragada (20%); M. Nilsen-Hamilton (20%); P. Palo (25%); J. Banerjee (15%); L. Wang (15%); G.A. Kraus (5%); T.-W. Guo (20%); B. Narasimhan (5%); T. Prozorov (50%); D. Bazylinski (5%); T. Williams (20%); P. Canfield (5%); R. Prozorov (5%)

Authorized Budget (BA) for FY05, FY06, FY07:
FY05 BA $225k **FY06 BA** $395k **FY07 BA** $400k