2012 ARO IN REVIEW

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ARO IN REVIEW 2012

A summary of the U.S. Army Research Office (ARO) research programs for fiscal year 2012 (FY12), including program goals, management strategies, funding information, and accomplishments

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ARO IN REVIEW 2012

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CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY

This report is intended to be a single-source document describing the research programs of the U.S. Army Research Office (ARO) for fiscal year 2012 (FY12; 1 Oct 2011 through 30 Sep 2012). This report provides:

- A brief review of the strategy employed to guide ARO research investments and noteworthy issues affecting the implementation of that strategy
- Statistics regarding basic research funding (*i.e.*, "6.1" funding) and program proposal activity
- Research trends and accomplishments of the individual ARO scientific divisions

I. ARO MISSION

The mission of ARO, as part of the U.S. Army Research Laboratory (ARL), is to execute the Army's extramural basic research program in these disciplines: chemical sciences, computing sciences, electronics, environmental sciences, materials science, mathematical sciences, mechanical sciences, network sciences, life sciences, social sciences, and physics. The goal of this basic research is to drive scientific discoveries that will provide the Army with significant advances in operational capabilities through high-risk, high pay-off research opportunities, primarily with universities, but also with industry and government laboratories. ARO also ensures that the results of these efforts are made available to the Army research and development community for the pursuit of long-term technological advances for the Army.

II. ARO INVESTMENT STRATEGY

ARO emphasizes a general two-pronged investment strategy to meet its mission: *requirements pull* and *technology push*.

A. Requirements Pull

The requirements pull strategy promotes research in response to a wide variety of published requirements and needs, including the DoD Quadrennial Defense Review (QDR), the DoD Strategic Basic Research Plan, the Assistant Secretary of Defense for Research and Engineering [ASD(R&E)] S&T Priorities, the Army Science and Technology (S&T) Master Plan, the Army S&T Challenge Areas, the Training and Doctrine Command (TRADOC) Warfighter Outcomes, the Assistant Secretary of the Army for Acquisition, Logistics, and Technology [ASA(ALT)] Special Focus Areas, and the ASA(ALT) Triennial Basic Research Review. This strategy can also be referred to as needs-driven research, which emphasizes long-term efforts to improve existing capabilities or overcoming identified technology barriers.

B. Technology Push

ARO also invests heavily in discovery research targeted at extraordinarily novel and innovative science that promises tremendous value across many technologies and applications, some of which may be fundamentally new. This technology push strategy emphasizes opportunity-driven research aimed at developing and exploiting scientific breakthroughs to produce revolutionary new capabilities.

The scope of ARO research investment strategy is broad and decidedly long range, with system applications often 10–15 years away, or more. The long-range focus of ARO's investment strategy is designed to maintain the Army's overwhelming capability in the expanding range of present and future operational capabilities. However, there have also been many research programs throughout ARO's history that transitioned to system applications in much shorter times, and these are actively pursued to ensure that extramural basic research is optimally contributing to the advancement of the current Warfighter's capabilities.

C. Specific Strategies

More specifically, ARO employs the following strategies to fulfill its mission:

- Execute an integrated, balanced extramural basic research program
- Create and guide the discovery and application of novel scientific phenomena leading to leap-ahead technologies for the Army
- Drive the application of science to generate new or improved solutions to existing needs
- Accelerate research results transition to applications in all stages of the research and development cycle
- Strengthen the research infrastructures of academic, industrial, and nonprofit laboratories that support the Army
- Focus on research topics that support technologies vital to the Army's future force, combating terrorism and new emerging threats
- Leverage the science and technology (S&T) of other defense and government laboratories, academia and industry, and organizations of our allies
- Foster training for scientists and engineers in the scientific disciplines critical to Army needs
- Actively seek creative approaches to enhance the diversity and capabilities of future U.S. research programs by enhancing education and research programs at historically black colleges and universities, and minority-serving institutions

III. IMPLEMENTING ARO INVESTMENT STRATEGY

As described in the previous section, ARO employs multiple strategies to fulfill its mission. A snapshot of the ARO research programs is provided in this section, and each program is described further in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

A. Program Snapshot

The research programs managed by ARO range from single investigator research to multidisciplinary/multi-investigator initiatives. A typical basic research grant within a program may provide funding for a few years, while in other programs, such as research centers affiliated with particular universities, a group of investigators may receive funding for many years to pursue novel research concepts. The programs for the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) are aimed at providing infrastructure and incentives to improve the diversity of U.S. basic research programs (see CHAPTER 2-IX). The National Defense Science and Engineering Graduate (NDSEG) fellowship program is one mechanism through which ARO fosters the training of a highly-educated workforce skilled in DoD and Army-relevant research, which is critical for the future of the nation (see CHAPTER 2-X). ARO also has extensive programs in outreach to pre-graduate education to encourage and enable the next generation of scientists (see CHAPTER 2-XI). In addition, ARO guides the transition of basic research discoveries and advances to the appropriate applied-research and advanced-development organizations. ARO is actively engaged in speeding the transition of discovery into systems, in part through involvement in the development of topics and the management of projects in the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs (see CHAPTER 2-VIII).

B. Coordination for Program Development and Monitoring

The research programs and initiatives that compose ARO's extramural research program are formulated through an ongoing and active collaboration with a variety of Federal research organizations, including the:

- ARL Directorates:
  - Computational and Information Sciences Directorate (ARL-CISD)
  - Human Research and Engineering Directorate (ARL-HRED)
  - Sensors and Electron Devices Directorate (ARL-SEDD)
  - Survivability/Lethality Analysis Directorate (ARL-SLAD)
  - Vehicle Technology Directorate (ARL-VTD)
  - Weapons and Materials Research Directorate (ARL-WMRD)
- Research, Development, and Engineering Centers (RDECs) within the Research, Development and Engineering Command (RDECOM)
- Army Medical Research and Materiel Command (MRMC)
- Army Corps of Engineers
- Army Research Institute for the Behavioral and Social Sciences
- Army Training and Doctrine Command

While the ARL Directorates and the RDECOM Centers are the primary users of the results of the ARO research program, ARO also supports research of interest to the Army Corps of Engineers, MRMC, other Army Commands, and DoD agencies. Coordination and monitoring of the ARO extramural program by the ARL Directorates, RDECs, and other Army laboratories ensures a highly productive and cost-effective Army research effort. The University Affiliated Research Centers (UARCs) and Multidisciplinary University Research Initiative (MURI) centers benefit from the expertise and guidance provided by the ARL Directorates, RDECs, and other DoD, academic, and industry representatives who serve on evaluation panels for each university center.

The OSD research programs that are managed by ARO include the University Research Initiative (URI) programs, and the Research and Educational Program (REP) for HBCU/MIs. These programs fall under the executive oversight of the Defense Basic Research Advisory Group. Other members of this group include the Assistant Secretary of Defense for Research and Engineering (ASD(R&E)), formerly known as the Director, Defense Research and Engineering (DDR&E), and representatives from the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR) and the Defense Advanced Research Projects Agency (DARPA).

IV. REVIEW AND EVALUATION

ARO Directorates, Divisions, and Programs are evaluated by a wide range of internal (Army) and external (Academic, other Government) reviews. Examples include the triennial Army Basic Research Review and the biennial ARO Division Reviews. For additional information regarding these review processes, readers are encouraged to refer to the corresponding presentations and reports from each review (not included here).

V. ARO ORGANIZATIONAL STRUCTURE

The organizational structure of ARO mirrors the departmental structure found in many research universities. ARO's scientific divisions are aligned to a specific scientific discipline (*e.g.*, chemical sciences), and supported by a variety of divisions in the Operations Directorate (see FIGURE 1).

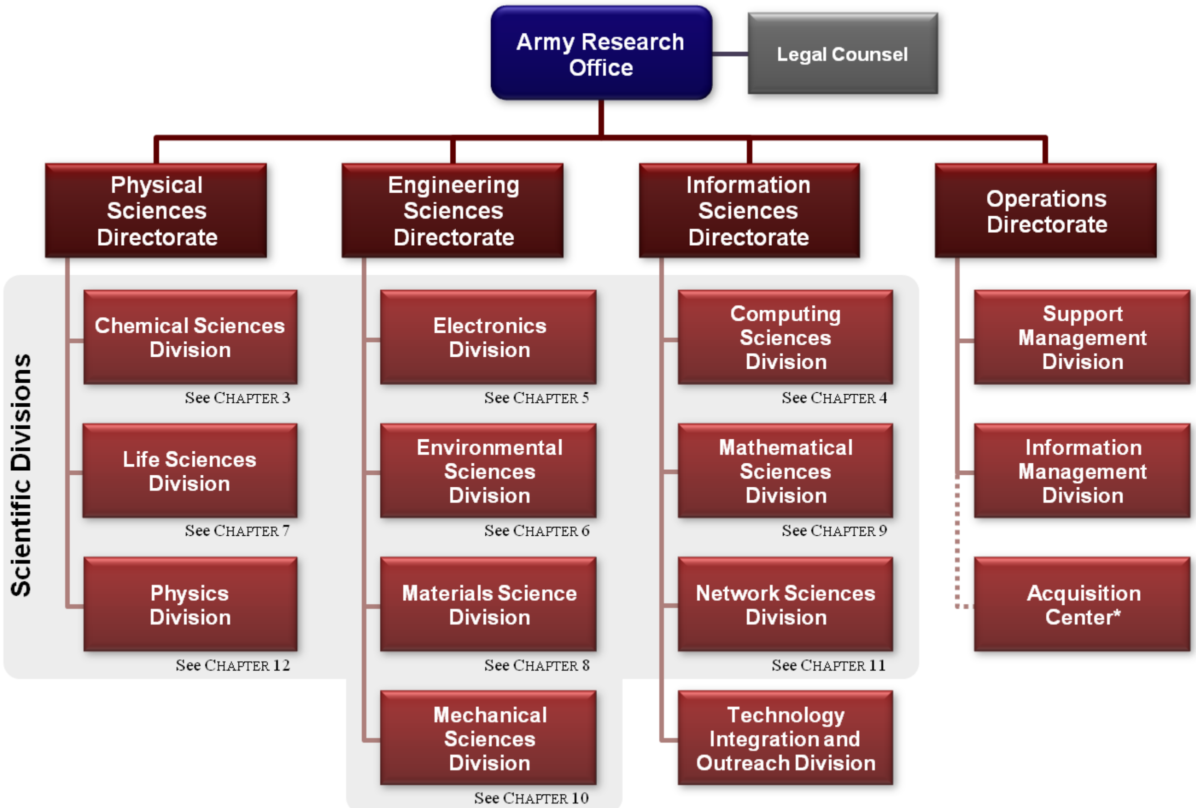

FIGURE 1

ARO Organizational Structure. ARO's scientific divisions fall under the Physical Sciences, Engineering Sciences, and Information Sciences Directorates. Each scientific division has its own vision and research objectives, as described further in CHAPTERS 3-12. *The RDECOM Acquisition Center executes the contracting needs for ARO-funded research; however, as part of the Army Contracting Command, it also provides contracting activities for RDECOM.

CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES

As described in the previous chapter, ARO pursues a variety of investment strategies to meet its mission as the Army's lead extramural basic research agency in these disciplines: chemical sciences, computing sciences, electronics, environmental sciences, materials science, mathematical sciences, mechanical sciences, network sciences, life sciences, and physics. ARO implements these investment strategies through research programs and initiatives that have unique objectives, eligibility requirements, and receive funding from a variety of DoD sources. This chapter describes the visions, objectives, and funding sources of these programs, which compose the overall ARO extramural research program.

The selection of research topics, proposal evaluation, and project monitoring are organized within ARO Divisions according to scientific discipline (refer to the organizational chart presented in CHAPTER 1). ARO's Divisions are aligned with these disciplines, each with its own vision and research objectives, as detailed in CHAPTERS 3-12. Each Division identifies topics that are included in the broad agency announcement (BAA). Researchers are encouraged to submit white papers and proposals in areas that support the Division's objectives.

I. OVERVIEW OF PROGRAM FUNDING SOURCES

ARO oversees and participates in the topic generation, proposal solicitation, evaluation, and grant-monitoring activities of programs funded through a variety of DoD agencies, as discussed in the following subsections. A summary of the funding sources and allotments for ARO managed or co-managed programs is provided at the end of this chapter.

A. Army Funding

The majority of the extramural basic research programs managed by ARO are funded by the Army. These programs are indicated below and are described in more detail later in this chapter.

- The Core (BH57) Research Program, funded through basic research "BH57" funds (see Section II).
- The University Research Initiative (URI), which includes these component programs:
  - Multidisciplinary University Research Initiative (MURI) program (see Section III)
  - Presidential Early Career Awards for Scientists and Engineers (PECASE; see Section IV)
  - Defense University Research Instrumentation Program (DURIP; see Section V)
- Two University Affiliated Research Centers (UARCs; see Section VI)

In addition, ARO manages The Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs for the Army (see Section VIII).

ARO coordinates with the Office of the Secretary of Defense (OSD) in the management of Army-funded URI programs (MURI, PECASE, and DURIP).

B. Office of the Secretary of Defense (OSD) Funding

The funds for a variety of programs managed or supported by ARO are provided by OSD. The objectives for these programs are described in later sections of this chapter.

- Research and Educational Program (REP) for Historically Black Colleges and Universities and Minority Institutions (HBCU/MI; see Section IX)
- National Defense Science and Engineering Graduate (NDSEG) Fellowships (see Section X)
- Youth Science Activities (see Section XI)

These activities are mandated by DoD's Chief Technology Office, the Assistant Secretary of Defense for Research and Engineering [ASD(R&E)], formerly known as the Director, Defense Research and Engineering (DDR&E). Each of these OSD-funded programs has a different focus and/or different target audience. ARO has been designated by ASD(R&E) as the lead agency for the implementation of REP for HBCU/MI activities on behalf of the three Services. OSD oversees ARO management of the Army-funded URI and its component programs (MURI, PECASE, and DURIP).

In FY10, the Defense Experimental Program to Stimulate Competitive Research (DEPSCoR) program officially ended, as DoD no longer included this effort in fund requests for FY10 and future year budgets.

C. Other Funding Sources

In addition to the Army- and OSD-funded programs described earlier in this section, ARO leverages funds from other DoD sources (*e.g.*, Defense Advanced Research Projects Agency [DARPA] and Defense Threat Reduction Agency [DTRA]) to support a variety of external programs with specific research focuses. These joint programs have research objectives in line with the investment strategies of both an ARO Division and the strategies of the funding source or partner agency. Due to the unique nature of these cooperative efforts and their alignment with a specific scientific discipline, each externally-funded effort is discussed within the chapter of the scientific Division with which they align (see CHAPTERS 3-12).

II. ARO CORE (BH57) RESEARCH PROGRAM

ARO's Core Research Program is funded with Army basic research "BH57" funds and represents the primary basic research funding provided to ARO by the Army. Within this program and its ongoing BAA, research proposals are sought from educational institutions, nonprofit organizations, and commercial organizations for basic research in electronics, physics, and the chemical, computing, environmental, life, materials, mathematical, mechanical, and network sciences. The goal of this program is to utilize world-class and worldwide academic expertise to discover and exploit novel scientific opportunities, primarily at universities, to provide the current and future force with critical new or enhanced capabilities.

ARO Core Research Program activities fall under five categories, discussed in the following subsections: (a) Single Investigator awards, (b) Short Term Innovative Research efforts, (c) Young Investigator Program, (d) support for conferences, workshops, and symposia, and (e) special programs. A summary of the FY11 Core (BH57) Research Program budget is presented in Section XIII-B.

A. Single Investigator (SI) Program

The goal of the SI program is to pursue some of the most innovative, high-risk, and high-payoff ideas in basic research. Research proposals within the SI Program are received throughout the year in a continually-open BAA solicitation. All states are eligible to receive funding within this program, which focuses on basic research efforts by one or two faculty members along with supporting graduate students and/or postdoctoral researchers.

B. Short Term Innovative Research (STIR) Program

The objective of the STIR Program is to explore high-risk, initial proof-of-concept ideas, typically within a nine-month timeframe. Research proposals are sought from educational institutions, nonprofit organizations, or private industry. If a STIR effort's results are promising, the investigator may be encouraged to submit a proposal to be evaluated for potential longer-term funding options, such as an SI award.

C. Young Investigator Program (YIP)

The objective of the YIP is to attract outstanding young university faculty members to Army research, to support their research, and to encourage their teaching and research careers. Young investigators meeting eligibility requirements may submit a YIP proposal. Outstanding YIP projects may be considered for the prestigious PECASE award (see Section IV).

D. Conferences, Workshops, and Symposia Support Program

The ARO Core Program also provides funding for organizing and facilitating scientific and technical conferences, workshops, and symposia. This program provides a method for conducting scientific and technical conferences that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army and help define research needs, thrusts, opportunities, and innovation.

E. Special Programs

Although the ARO SI, STIR, YIP, and conference-support programs constitute the primary use of BH57 funds, the ARO Core Research Program also supports a variety of special programs. These special programs include matching funds applied to the ARO Core-funded HBCU/MI program, and also the Army-supported High School Apprenticeship Program (HSAP) and Undergraduate Research Apprenticeship Program (URAP), which are part of the Youth Science Activities (see Section XI)..

III. MULTIDISCIPLINARY UNIVERSITY RESEARCH INITIATIVE (MURI)

As described in Section I: *Overview of Program Funding Sources*, the MURI Program is part of the University Research Initiative (URI) and supports research teams whose research efforts intersect more than one traditional science and engineering discipline. A multidisciplinary team effort can accelerate research progress in areas particularly suited to this approach by cross-fertilization of ideas, can hasten the transition of basic research findings to practical applications, and can help to train students in science and/or engineering in areas of importance to DoD.

In contrast with ARO Core program SI research projects, MURI projects support centers whose efforts intersect more than one traditional research specialty, and are typically funded at $1.25 million per year for five years. These "critical mass" efforts are expected to enable more rapid research and development (R&D) breakthroughs and to promote eventual transition to Army applications.

Management oversight of the MURI program comes from the Basic Research Office of ASD(R&E) to the Service Research Offices (OXRs), where OXR program managers manage the MURI projects. The OXRs include ARO, the Air force Office of Scientific Research (AFOSR), and the Office of Naval Research (ONR). OXR program managers have significant flexibility and discretion in how the individual projects are monitored and managed, while ASD(R&E) defends the program to higher levels in OSD and has responsibility for overall program direction and oversight. Selection of Army research topics and the eventual awards are reviewed and approved by ASD(R&E) under a formal acquisition process.

Eight MURI projects were selected for funding and began in FY12. These projects are based on proposals submitted to the FY12 MURI topic BAA, which was released in late FY11. The new-start projects, the lead investigator, and the lead performing organization are listed below. The corresponding MURI topic, topic authors / program managers, and the ARO Division responsible for monitoring the projects are listed in parentheses. A description of each of these projects can be found in the corresponding Division's chapter.

- *High-Resolution Quantum Control of Chemical Reactions*; Professor David DeMille, Yale University

  (Topic: *Quantized Chemical Reactions of Ultracold Molecules*; Dr. James Parker, Chemical Sciences and Dr. Paul Baker, Physics)

- *The Physics of Surface States with Interactions mediated by Bulk Properties, Defects and Surface Chemistry*; Professor Robert Cava, Princeton University

  (Topic: *3D Topological Insulators with Interactions*; Dr. Marc Ulrich, Physics and Dr. Pani Varanasi, Materials Science)

- *Translating Biochemical Pathways to Non-Cellular Environments*; Professor Hao Yan, Arizona State University

  (Topic: *Translating Biochemical Pathways to Non-Cellular Environments*; Dr. Stephanie McElhinny, Life Sciences and Dr. John Prater, Materials Science)

- *Multivariate Heavy Tail Phenomena: Modeling, Diagnostics, and Applications in Tactical Operations*; Professor Sidney Resnick, Cornell University

  (Topic: *Multivariate Heavy-Tailed Statistics: Foundations and Modeling*; Dr. Harry Chang and Dr. John Lavery, Mathematical Sciences)

- *Imaging How a Neuron Computes;* Professor Rafael Yuste, Columbia University
  (Topic: *Simultaneous Multi-synaptic Imaging of the Interneuron;* Dr. Elmar Schmeisser, Life Sciences and Dr. Dwight Woolard, Electronics)

- *Associating Growth Conditions with Cellular Composition in Gram-negative Bacteria*; Professor Claus Wilke, University of Texas at Austin

  (Topic: *Revolutionizing High-Dimensional Data Integration for Microbial Forensics*; Dr. Virginia Pasour, Mathematical Sciences and Dr. Wallace Buchholz, Life Sciences)

- *Coherent Effects in Hybrid Nanostructures for Lineshape Engineering of Electromagnetic Media*; Professor Naomi Halas, William Marsh Rice University

  (Topic: *Novel Nanostructures for the Controlled Propagation of Electromagnetic Energy*; Dr. Jennifer Becker, Chemical Sciences and Dr. Richard Hammond, Physics)

- *Evolution of Cultural Norms and Dynamics of Socio-Political Change*; Professor Ali Jadbabaie, University of Pennsylvania

  (Topic: *Predictive Models of Culture and Behavioral Effects on Societal Stability*; Drs. Jeffrey Johnson and Elisa Bienenstock, Life Sciences, Drs. Virginia Pasour and Russell Harmon, Mathematical Sciences, and Dr. Bruce West, Information Sciences Directorate)

The following topics were published in FY12 and constitute the ARO portion of the FY13 MURI BAA. The topic titles, topic author(s), and corresponding ARO Division(s) are listed below.

- *Artificial Cells for Novel Synthetic Biology Chassis;* Dr. Stephanie McElhinny, Life Sciences and Dr. Jennifer Becker, Chemical Sciences
- *Molecular Co-Crystal Design and Synthesis;* Dr. James Parker, Chemical Sciences and Dr. Pani Varanasi, Materials Science
- *Reduced Cyber-system Signature Observability by Intelligent and Stochastic Adaptation;* Dr. Cliff Wang, Computing Sciences
- *Non-equilibrium Many-body Dynamics;* Drs. Paul Baker and Marc Ulrich, Physics.
- *Materials with Spin Mediated Thermal Properties;* Dr. Pani Varanasi, Materials Science and Dr. Mark Spector, Office of Naval Research
- *Transforming Information within Nonequilibrium Nanosystems;* Dr. Samuel Stanton, Mechanical Sciences

- *Controlling Collective Phenomena in Complex Networks;* Dr. Randy Zachery, Information Sciences Directorate and Dr. Samuel Stanton, Mechanical Sciences
- *Physiochemical Determinants of Cognition and Decision Making;* Dr. Elmar Schmeisser, Life Sciences and Dr. Janet Spoonamore, Network Sciences

IV. PRESIDENTIAL EARLY CAREER AWARD FOR SCIENTISTS AND ENGINEERS (PECASE)

The PECASE program, also part of the URI program, attracts outstanding young university faculty members, supporting their research, and encouraging their teaching and research careers. PECASE awards are the highest honor bestowed by the Army to outstanding scientists and engineers beginning their independent research careers. Each award averages $200K/year for five years. PECASE awards are based in part on two important criteria: (i) innovative research at the frontiers of science and technology (S&T) that is relevant to the mission of the sponsoring organization or agency, and (ii) community service demonstrated through scientific leadership, education, and community outreach.

Of the candidates nominated in FY11 by ARO for consideration in the PECASE program, four investigators were selected in FY12 to receive PECASE awards. These awards began as “new start” projects in FY12 and are listed in this section, with the project title followed by the principal investigator (PI), performing organization, ARO PM and corresponding scientific division. Additional details for each of these projects can be found in the corresponding scientific division’s chapter.

1. *Biologically Patterned Amyloid Scaffolds for Multifunctional and Multiscale Materials*
   PI: Dr. Timothy Lu, Massachusetts Institute of Technology,
   ARO PM: Dr. Jennifer Becker, Chemical Sciences
2. *Computing Game-Theoretic Solutions for Security in the Medium Term*
   PI: Dr. Vincent Conitzer, Duke University,
   ARO PM: Purush Iyer, Network Sciences
3. *Strongly Coupled Multiferroic Materials by Design - Hierarchical Organization at the Atomic and Nanoscales*
   PI: Dr. Craig Fennie, Cornell University,
   ARO PM: Dr. John Prater, Materials Science
4. *Attosecond Electronic Dynamics Probed Using an EUV-Pump-EUV-Probe Technique*
   PI: Dr. Wen Li, Wayne State University,
   ARO PM: Dr. James Parker, Chemical Sciences

V. DEFENSE UNIVERSITY RESEARCH INSTRUMENTATION PROGRAM (DURIP)

DURIP, also part of the URI program, supports the purchase of state-of-the-art equipment that augments current university capabilities or develops new university capabilities to perform cutting-edge defense research. DURIP meets a critical need by enabling university researchers to purchase scientific equipment costing $50K or more to conduct DoD-relevant research. In FY12, the Army awarded 61 awards at $10.1 million total, with an average award of $166K.

VI. UNIVERSITY AFFILIATED RESEARCH CENTERS (UARCS)

The University Affiliated Research Centers (UARCs) are strategic DoD-established research organizations at universities. The UARCs were formally established in May 1996 by DDR&E [currently ASD(R&E)], OSD in order to advance DoD long-term goals by pursuing leading-edge basic research and to maintain core competencies in specific domains unique to each UARC, for the benefit of DoD components and agencies. One DoD Service or Agency is formally designated by ASD(R&E) to be the primary sponsor for each UARC. The primary sponsor ensures DoD UARC management policies and procedures are properly implemented. Collaborations among UARCs and the educational and research resources available at the associated universities can enhance each UARC's ability to meet the long-term goals of DoD.

ARO is the primary sponsor for two UARCs:

- The Institute for Soldier Nanotechnologies (ISN), located at the Massachusetts Institute of Technology (MIT). The ISN is discussed further in CHAPTER 3: CHEMICAL SCIENCES DIVISION.
- The Institute for Collaborative Biotechnologies (ICB) located at the University of California, Santa Barbara, with academic partners at MIT and the California Institute of Technology (Caltech). The ICB is discussed further in CHAPTER 7: LIFE SCIENCES DIVISION.

VII. MINERVA RESEARCH INITIATIVE (MRI)

The Minerva Research Initiative (MRI) is a DoD-sponsored, university-based social science research program initiated by the Secretary of Defense and focuses on areas of strategic importance to U.S. national security policy. It seeks to increase the intellectual capital in the social sciences and improve DoD's ability to address future challenges and build bridges between DoD and the social science community. Minerva brings together universities, research institutions, and individual scholars and supports multidisciplinary and cross-institutional projects addressing specific topic areas determined by DoD.

Minerva projects are funded up to a five-year base period with one five-year renewal option, with awards ranging from small, single investigator grants for 2-3 years to large multidisciplinary projects for $1-2 million per year for 5 years. The program is tri-service managed, with ARO managing 5 year projects dealing with the Baathist regime in Iraq, vulnerability of political and social stability in Africa in the face of environment stressors, and the relation of the growth of science and technology with the defense transformation in China. ARO also provides technical and managerial support to OSD in formulating the overall program and in establishing Minerva research fellowships and chairs at the military universities (NDU, Army War College, Air University, Naval War College, Marine Corps University, USMA, USNA, and USAFA).

The titles of ARO-managed Minerva projects that began in FY12 are listed below, followed by the name of the lead PI, the performing organization, and the award duration.

- *China's Emerging Capabilities in Energy Technology Innovation and Development*; PI: Professor Edward Stein, Massachusetts Institute of Technology, FY12-FY15
- *Brazil as a Major Power: The Impact of its Military-Scientific-Industrial Complex on its Foreign and Defense Policy*; PI: Professor David Mares, University of California - San Diego, FY12-FY15
- *Quantifying Structural Transformation in China*; PI: Professor David Meyer, University of California - San Diego, FY12-FY15
- *A Global Value Chain Analysis of Food Security and Food Staples for Major Energy-Exporting Nations in the Middle East and North Africa*; PI: Professor Lincoln Pratson, Duke University, FY12-FY15
- *Strategic Response to Energy-related Security Threats*; PI: Saleem Ali, University of Vermont, FY12-FY13

VIII. SMALL BUSINESS INNOVATION RESEARCH (SBIR) AND SMALL BUSINESS TECHNOLOGY TRANSFER (STTR) PROGRAMS

Congress established SBIR and STTR programs in 1982 and 1992, respectively, to provide small businesses and research institutions with opportunities to participate in government-sponsored R&D. The DoD SBIR and STTR programs are overseen and broadly administered by the Office of Small Business Programs within the Office of the Under Secretary of Defense for Acquisition, Technology and Logistics. The Army-wide SBIR Program is managed by RDECOM, while the Army-wide STTR Program is managed by ARO.

A. Purpose and Mission

The purpose of the SBIR and STTR programs is to (i) stimulate technological innovation, (ii) use small business to meet Federal R&D needs, (iii) foster and encourage participation by socially and economically disadvantaged small business concerns (SBCs), in technological innovation, and (iv) increase private sector commercialization of innovations derived from Federal R&D, thereby increasing competition, productivity, and economic growth. The STTR program has the additional requirement that small companies must partner with universities, federally funded research and development centers (FFRDCs), or other non-profit research institutions to work collaboratively to develop and transition ideas from the laboratory to the marketplace.

B. Three-phase Process

The SBIR and STTR programs use a three-phase process, reflecting the high degree of technical risk involved in funding research, and developing and commercializing cutting edge technologies. The basic parameters of this three-phase process for both programs within the Army are shown in TABLE 1.

TABLE 1

Three-phase process of the SBIR and STTR programs. Phase I is an assessment of technical merit and feasibility, Phase II is a larger R&D effort often resulting in a deliverable prototype, and Phase III is a project derived from, extending, or logically concluding prior SBIR/STTR work, generally to develop a viable product or service for military or commercial markets.

	SBIR Contract Limits	STTR Contract Limits
Phase I	• 6 months, $100K max • 4-month option (at Government's discretion), $50K max, to fund interim Phase II efforts	• 12 months, $150K max • No options
Phase II	• 2 years, $1 million max	• 2 years, $1 million max
Phase III	• No time or size limit • No SBIR set-aside funds	• No time or size limit • No STTR set-aside funds

1. Phase I. Phase I of the SBIR and STTR programs involves a feasibility study that determines the scientific, technical, and commercial merit and feasibility of a concept. Each SBIR and STTR solicitation contains topics seeking specific solutions to stated government needs. Phase I proposals must respond to a specific topic in the solicitation, and proposals are competitively judged on the basis of scientific, technical, and commercial merit. The Phase I evaluation and award process marks the entry point to the program and cannot be bypassed.

2. Phase II. Phase II represents a major research and development effort, culminating in a well-defined deliverable prototype (*i.e.*, a technology, product, or service). The Phase II selection process is also highly competitive. Successful Phase I contractors are invited to submit Phase II proposals as there are no separate Phase II solicitations. Typically 50% of Phase II proposals are selected for award. Phase II awards may also be selected to receive additional funds as a fast track (Phase II-FT), Phase II Enhancement, or Commercialization Readiness Program (CRP), formerly called the Commercialization Pilot Program (CPP).

3. Phase III. In Phase III, the small business or research institute is expected to obtain funding from the private sector and/or non-SBIR/STTR government sources to develop products, production, services, R&D, or any combination thereof into a viable product or service for sale in military or private sector markets. Commercialization is the ultimate goal of the SBIR and STTR programs.

C. ARO FY12 SBIR and STTR Topics

The following SBIR and Chemical and Biological Defense SBIR (CBD-SBIR) topics were published in the FY12 SBIR solicitations. The lead topic author and corresponding Division are listed following each topic title.

- *Advanced Purification Technology for the Manufacture of Vaccines, Biologic Drugs, and Enzymes*; Dr. Jennifer Becker, Chemical Sciences
- *Ultra-Sensitive, Room-Temperature, Mechanical-Optical Cavity Detectors for Long-Wavelength Applications*; Dr. William Clark, Electronics
- *Rapid Analysis of Suspicious Powders*; Dr. Wallace Buchholz, Life Sciences
- *Fusing Uncertain and Heterogeneous Information - Making Sense of the Battlefield*; Dr. Janet Spoonamore, Network Sciences
- *Solid Acid Electrolyte Fuel Cell*; Dr. Robert Mantz, Chemical Sciences
- *Dislocation Reduction in LWIR HgCdTe Epitaxial Layers Grown on Alternate Substrates*; Dr. William Clark, Electronics
- *Formulation Development to Enhance Bioavailability and Pharmacokinetic Profile of Protein-based Drugs*; Dr. Jennifer Becker, Chemical Sciences

The following STTR topics were published in FY12 STTR solicitations. The lead topic author and corresponding Division are listed following each topic title.

- *Effective Cyber Situation Awareness (CSA) Assessment and Training*; Dr. Cliff Wang, Computing Sciences
- *On Demand Energy Activated Liquid Decontaminants and Cleaning Solutions*; Dr. Jennifer Becker, Chemical Sciences
- *Virtual Laboratory of Aggregate Behavior (VLAB)*; Dr. Elisa Bienenstock, Life Sciences
- *Compressive Sampling Video Sensor for Change Detection*; Dr. Liyi Dai, Computing Sciences
- *Wide Temperature Range, High-Speed Optical Interconnect Technology*; Dr. Michael Gerhold, Electronics
- *Inferring Social and Psychological Meaning in Social Media*; Dr. Jeffrey Johnson, Life Sciences
- *Development of Low Temperature Ultracapacitor*; Dr. Robert Mantz, Chemical Sciences
- *Nanostructured Electrode Materials for Enhanced Biological Charge Transfer*; Dr. Stephanie McElhinny, Life Sciences
- *Mesh Generation and Control for Moving Boundary Problems*; Dr. Joseph Myers, Mathematical Sciences
- *Nondestructive Concrete Characterization System*; Dr. Dev Palmer, Electronics
- *High Performance Planar Semiconductor Gas Sensors*; Dr. Dev Palmer, Electronics
- *Battlefield Ultrasound with Automated Applications*; Dr. Dev Palmer, Electronics
- *Non-linear Laser Wave Mixing for Trace Detection of Explosives*; Dr. James Parker, Chemical Sciences
- *Strain-Modulated Diamond Nanostructures for Next-Generation, Biocompatible Nanoelectromechanical Systems*; Dr. Samuel Stanton, Mechanical Sciences
- *High Throughput Forensic Palynology*; Dr. Micheline Strand, Life Sciences

- *High Quality AlGaN Epitaxial Films with Reduced Surface Dislocation Density*; Dr. Pani Varanasi, Materials Science
- *Atomic Layer Deposition of Lead Zirconate Titanate Thin Films for Piezo MEMS Applications*; Dr. Pani Varanasi, Materials Science
- *Sub-Wavelength THz-Frequency Spectrometer for Trace Materials Analysis*; Dr. Dwight Woolard, Electronics
- *Micro-machined THz Probes for Electronic Analysis of Integrated Structures*; Dr. Dwight Woolard, Electronics

D. ARO FY12 SBIR and STTR Phase II Awarded Topics

The following SBIR and Chemical and Biological Defense SBIR (CBD-SBIR) topics were selected for a Phase II award in FY12. The lead topic author and corresponding Division are listed following each topic title.

- *Multisensory Navigation and Communications System*; Dr. Elmar Schmeisser, Life Sciences
- *Fabrication of High-Strength, Lightweight Metals for Armor and Structural Applications*; Dr. Suveen Mathaudhu, Materials Science
- *Universal Bio-Sample Preparation Module*; Dr. Robert Kokoska, Physical Sciences
- *Plasmonic Nanosensors for Chemical Warfare Agents*; Dr. James Parker, Chemical Sciences
- *Ultrasound for Neuromodulation and Control of Post-Trauma Pain*; Dr. Elmar Schmeisser, Life Sciences
- *UV-enhanced Raman Sensors with High SNR and Spectral Selectivity*; Dr. Michael Gerhold, Electronics
- *Direct Ethanol Fuel Cell*; Dr. Robert Mantz, Chemical Sciences
- *Space Photonics Technology*; Dr. Michael Gerhold, Electronics
- *Nanofluidic Sensor Platforms for THz-Frequency Spectroscopic Fingerprinting of Bio-Molecules*; Dr. Dwight Woolard, Electronics
- *Rapid Detection System for Decontaminated Bacillus Thuringiensis Al Hakam Spore Strips*; Dr. Jennifer Becker, Chemical Sciences
- *Narrowband Perfect Absorber using Metamaterials*; Dr. Dwight Woolard, Electronics
- *Robust and Efficient Anti-Phishing Techniques*; Dr. Cliff Wang, Computing Sciences
- *Preventing Sensitive Information and Malicious Traffic from Leaving Computers*; Dr. Cliff Wang, Computing Sciences
- *Artificial Vaccines Based on DNA Origami*; Dr. Dwight Woolard, Electronics

The following STTR topics were selected for a Phase II award in FY12. The lead topic author and corresponding Division are listed following each topic title.

- *Design Automation Software for DNA-Based Nano-Sensor Architectures*; Dr. Dwight Woolard, Electronics
- *MEMS Based Thermopile Infrared Detector Array for Chemical and Biological Sensing*; Dr. Michael Coyle, Computing Sciences
- *Multi-input Multi-output Synthetic Aperture Radar with Collocated Antennas*; Dr. Liyi Dai, Computing Sciences
- *Coherent Beam Combining of Mid-IR Lasers*; Dr. Michael Gerhold, Electronics
- *Random Number Generation for High Performance Computing*; Dr. Joseph Myers, Mathematical Sciences
- *Interactive Acoustic Simulation in Urban and Complex Environments*; Dr. Michael Coyle, Computing Sciences
- *Compressive Imaging with Dynamically Programmable Processing Capabilities*; Dr. Liyi Dai, Computing Sciences
- *High Speed Room Temperature Single Photon Counters*; Dr. TR Govindan, Physics

- *Compact, Rugged, and Low-Cost Wavelength-Versatile Burst Laser*; Dr. Michael Gerhold, Electronics
- *High Risk Rapid Ethnographic Assessment Tool (HRREAT)*; Dr. Jeffery Johnson, Life Sciences
- *High-capacity and Cost-effective Manufacture of Chloroperoxidase*; Dr. Stephanie McElhinny, Life Sciences
- *A Priori Error-Controlled Simulations of Electromagnetic Phenomena for HPC*; Dr. Joseph Myers, Mathematical Sciences
- *High Performance Complex Oxide Thin Film Materials to Enable Switchable Film Bulk*; Dr. Pani Varanasi, Materials Science
- *Thin-Film Multiferroic Heterostructures for Frequency-Agile RF Electronics*; Dr. Pani Varanasi, Materials Science
- *Rugged Automated Training System*; Dr. Micheline Strand, Life Sciences
- *Artificial Antibodies for Biological Sensing Based on DNA Origami*; Dr. Dwight Woolard, Electronics

E. Contract Evaluation and Funding

The Army receives Phase I and Phase II proposals in response to SBIR, STTR, CBD-SBIR and OSD-SBIR/STTR topics that are published during specific solicitation periods throughout each fiscal year. Proposals are evaluated against published evaluation criteria and selected for contract award. Contract awards in the SBIR and STTR programs are made pending completion of successful negotiations with the small businesses and availability of funds. The total funding for ARO-managed SBIR and STTR contracts awarded in FY12 and funded by the Army, CBD, OSD and other sources with FY12 or FY11 funding is shown in TABLE 2.

TABLE 2

Total Funding for ARO-managed SBIR and STTR contracts awarded in FY12. Total funding (FY12 and FY11) for ARO-managed SBIR and STTR contracts, including Army, CBD, OSD, and other DoD funding sources. Phase III includes contracts deriving from, extending or completing ARO-managed Phase I or Phase II efforts, awarded at ARO and elsewhere within the DoD.

	SBIR Contracts	STTR Contracts
Phase I	$778K	$1698K
Phase II	$6,232K	$10,560K
Phase II Enhancement	$737K	-
CRP	-	-
Phase III	$13,800K	$40,000K
TOTAL	**$21,547K**	**$52,258K**

IX. HISTORICALLY BLACK COLLEGES AND UNIVERSITIES AND MINORITY INSTITUTIONS (HBCU/MI) PROGRAMS

Programs for HBCU/MIs are a significant part of the ARO portfolio. Awards in FY12 totaled $18.7 million. These programs are discussed in the following subsections.

A. ARO (Core) HBCU/MI Program

ARO began its HBCU/MI program in 1980 with $0.5 million designed to encourage greater participation of HBCUs and MIs in basic research. The initiative has continued and in recent years has been funded at $1.2 million annually. These funds are made available to the ARO scientific divisions as co-funding opportunities to support HBCU/MI research proposals submitted under the ARO Core Program BAA. In FY12, 8 new starts were awarded totaling over $578K through the ARO Core HBCU/MI Program. The total active award base, including FY12 funding, was 48 awards with a total value of over $2.2 million.

The new-start HBCU/MI research grants are listed below, with the project title followed by the PI, performing organization, ARO PM, and corresponding scientific division.

- *Theoretical Studies of Oxygen Reduction and Proton Transfer in SOFCs and Nerve Agents on Selected Surfaces*, Professor Changyong Qin, Benedict College; Dr. William Clark, Electronics
- *Recognition of In-Vehicle Group Activities (iYGA: Phase-1, Feasibility Study*, Professor Amir Shirkhodai, Tennessee State University; Dr. John Lavery, Mathematical Sciences
- *Rapid and Sensitive THz Bio-Sharing*, Professor Robert Alfano, City College of New York (CUNY); Dr. Dwight Woolard, Electronics
- *A Theoretical Framework for Cyber Defense Operations*, Professor Shouhuai Xu, University of Texas at San Antonio; Dr. Cliff Wang, Computing Sciences
- *Rational Design of Anode Surface Chemistry in Microbial Fuel Cells for Improved Exoelectrogen Attachment and Electron Transfer*, Professor Andrew Schuler, University of New Mexico Albuquerque; Dr. Kurt Preston, Environmental Sciences
- *Organic Matrix Templating and Function in an Ultrahard Biological Composite*, Professor David Kisailus, University of California - Riverside; Dr. Stephanie McElhinny, Life Sciences

The HBCU/MI institutions funded under the ARO Core program were also afforded the opportunity to submit add-on proposals to fund high school or undergraduate student research apprenticeships through HSAP/URAP. Twelve institutions were funded under HSAP/URAP in FY12, totaling approximately $63K. Additional information regarding HSAP/URAP can be found in Section XI: *Youth Science Activities*.

B. Partnership in Research Transition (PIRT) Program

The PIRT Program was established as the second phase of what was previously known as the Battlefield Capability Enhancement Centers of Excellence (BCE). The program's objective is to enhance the programs and capabilities of a select number of high-interest scientific and engineering disciplines through Army-relevant, topic-focused, near-transition-ready innovative research. Furthering ARL's policy of advocating and supporting research at HBCUs, and consistent with the stated mission of the White House Initiative on HBCUs, a secondary objective of PIRT is "to strengthen the capacity of HBCUs to provide excellence in education" and to conduct research critical to DoD national security functions. In FY12, $2.8 million was added to Cooperative Agreements supporting research and student internships at these PIRT Centers:

- *Center of Advanced Algorithms*
  Delaware State University, Dover, DE
  Co-Cooperative Agreement Manager (Co-CAM): Dr. James Harvey, Engineering Sciences Directorate
- *Bayesian Imaging and Advanced Signal Processing for Landmine and IED Detection Using GPR*
  Howard University, Washington, DC
  Co-CAM: Dr. James Harvey, Engineering Sciences Directorate

- *Extracting Social Meaning From Linguistic Structures in African Languages*
  Howard University, Washington, DC
  Co-CAM: Dr. John Lavery, Information Sciences Directorate
- *Lower Atmospheric Research Using Lidar Remote Sensing*
  Hampton University, Hampton, VA
  Co-CAM: Dr. Gorden Videen, Engineering Sciences Directorate
- *Nano to Continuum Multi-Scale Modeling Techniques and Analysis for Cementitious Materials Under Dynamic Loading*
  North Carolina A&T State University, Greensboro, NC
  Co-CAM: Dr. Joseph Myers, Information Sciences Directorate

C. DoD Research and Educational Program (REP) for HBCU/MI

ARO has administered programs on behalf of ASD(R&E) (formerly DDR&E) since 1992. During FY12, 39 grants totaling $17.4 million were made to 34 different HBCU/MIs under the solicitation "*Research and Educational Program for Historically Black Colleges and Universities and Minority-Serving Institutions (HBCU/MI)*." REP aims to: (i) enhance programs and capabilities in scientific and engineering disciplines critical to the national security functions of the DoD, (ii) encourage greater participation in DoD programs and activities, (iii) increase the number of graduates, including underrepresented minorities, in the fields of science, technology, engineering and/or mathematics (STEM), and (iv) encourage research and educational collaboration with other institutions of higher education directed toward advancing the state of the art and increasing knowledge.

Under this program, qualifying institutions were able to submit proposals to compete for basic research grants. In 3Q FY12, BAA W911NF-12-R-0009 was issued for the FY12 DoD REP for HBCU/MI. More than 275 proposals were determined to be eligible under the solicitation. It is anticipated that awards totaling approximately $26 million will be made by 2Q FY13.

D. DoD Instrumentation Program for Tribal Colleges and Universities (TCUs)

ARO was selected to administer the Congressionally-directed program "STEM Research and Veteran Technology Workforce Development Initiatives" for an HBCU institution located in South Carolina. Funding for this FY10 statutory add totaled approximately $1.98 million and was awarded to Benedict College, Columbia, SC in 3Q FY11. Funding for this programs ends in July 2013.

In addition, the John H. Hopps Scholars Program at Morehouse College (funded in FY08) continued to serve approximately 17 scholars during FY12.

X. NATIONAL DEFENSE SCIENCE AND ENGINEERING GRADUATE (NDSEG) FELLOWSHIP PROGRAM

The NDSEG Fellowship Program is an OSD-funded program administered by AFOSR, designed to increase the number of U.S. citizens trained in disciplines of science and engineering important to defense goals. ARO supports the NDSEG Fellowship Program along with ONR, AFOSR, and the DoD High Performance Computing Modernization Program. NDSEG is a highly competitive fellowship awarded to U.S. citizens who have demonstrated a special aptitude for advanced training in science and engineering, and who intend to pursue a doctoral degree in one of fifteen scientific disciplines of interest to the military. NDSEG Fellowships last for three years, and Fellows are provided full tuition and fees at any accredited university of choice, a monthly stipend, and up to $1K/year in medical insurance.

With approximately $5 million available to the Army in FY12, ARO selected 57 NDSEG Fellows from thirteen categories relevant to the Army fundamental research priorities. These awardees began their fellowships in the fall of 2012. Each of ARO's divisions reviewed the applications assigned to NDSEG topic categories within their particular areas of expertise, and selected fellows whose doctoral research topics most closely align with the Army's missions and research needs. The number of Fellows chosen from each discipline was based on the percentage of applicants who submitted topics in that category. The number of fellows chosen from each scientific discipline for the FY12 NDSEG program is shown in TABLE 3.

TABLE 3

FY12 NDSEG fellows by discipline. The table displays the number of NDSEG Fellows chosen in FY12, according to the eleven topic categories relevant to the designated Army research priorities.

Scientific Discipline	NDSEG Fellows Selected in FY12
Biosciences	8
Chemistry	5
Physics	3
Computer and Computational Sciences	6
Mathematics	2
Aeronautical and Astronautical Engineering	3
Civil Engineering	3
Electrical Engineering	6
Geosciences	2
Materials Science and Engineering	4
Mechanical Engineering	6
Cognitive, Neural, and Behavioral Sciences	5
Chemical Engineering	4
TOTAL	**57**

XI. YOUTH SCIENCE ACTIVITIES

ARO Youth Science Programs are sponsored by the Army and have one purpose in common: to increase the number of future adults with careers in science, technology, engineering, and mathematics. These programs accomplish this through a variety of mechanisms, including: providing a work/study laboratory experience, sponsoring hands-on science workshops during the summer, showcasing talented young high school scientists at symposia, and supporting student science fairs nationwide.

The Army's programs for the youth of this nation collectively reach more than 100,000 high school students throughout the United States, Puerto Rico, and DoD Schools of Europe and the Pacific. Students participating in the programs during this past fiscal year were awarded more than $380K in college tuition scholarships, while students, teachers, and near-peer mentors were awarded more than $4 million in stipends for participation in research programs, savings bonds totaling in excess of $25K, and expense-paid trips to international programs.

During the summer of FY12, 228 students served as interns and worked in university laboratories with mentors though the High School Apprenticeship Program (HSAP), Undergraduate Research Apprentice Program (URAP), and the Research and Engineering Apprenticeship Program (REAP). In FY12, 428 students engaged in research experiences in military laboratories through the Science and Engineering Apprentice Program (SEAP) and College Qualified Leaders (CQL) program, and 193 students participated in programs that offered enrichment classes in engineering at universities through the UNITE program. 1,614 middle and high school students experienced hands-on science and technology research activities in Army labs through the Gains in the Education of Math and Science (GEMS) summer program. These programs are described further in the following subsections.

A. Junior Science and Humanities Symposium (JSHS) Program

The JSHS Program promotes original research and experimentation in the sciences, engineering, and mathematics at the high school level and publicly recognizes students for outstanding achievement. By connecting talented students, their teachers, and research professionals at affiliated symposia and by rewarding research excellence, JSHS aims to widen the pool of trained talent prepared to conduct R&D vital to our nation. Forty-eight regional symposia are conducted throughout the U.S. and DoD schools in Europe and the Pacific. Top student winners from each region are invited to attend the national symposium each year. Approximately 9,600 students participate in JSHS through submission of research papers in the regional and national symposia.

B. Research and Engineering Apprenticeship Program (REAP)

REAP is designed to offer high school students the opportunity to expand their background and understanding of scientific research. While originally chartered as a program to identify and support under-represented students in STEM, the program has been expanded to accept applications from all students seeking a first time experience in research. This is accomplished by offering the student an internship during the summer months to participate in a work/study atmosphere with a mentor in a laboratory setting. The experience serves to motivate the student towards a career in STEM by providing a challenging science experience that is not readily available in high school. In FY12, 131 apprentices were placed at 59 hosting universities throughout the U.S.

C. UNITE Program

The UNITE Program is an effective initiative that encourages and assists under-represented students in preparing for entrance into college to study an engineering discipline. High school students are provided the opportunity during the summer months to participate in college-structured summer courses that provide hands on engineering activities, teach problem solving skills, and provide tours of laboratories and engineering facilities. The students are introduced to ways in which math and science are applied to real-world situations and demonstrates how they are related to careers in engineering and technology. A new program structure was created to provide stipends for participating students to offset costs associated with participating and improve our ability to serve students who have previously encountered financial barriers to participation. Nine sites were funded in FY12, seven of which were first time UNITE programs, serving 193 students.

D. Army Awards Program (AAP)

The Army Awards Program provides Army sponsored special awards to students at regional, state, and the International Science and Engineering Fair (ISEF). Each year, ROTC units, Recruiting Battalions, Army Reservists, Army Corps of Engineers Personnel, and Army command/laboratory personnel serve as judges of student projects at hundreds of science fair competitions held throughout the United States and Puerto Rico. By participating in science fairs, the Army is able to encourage and stimulate talented students to consider careers in science and technology while simultaneously exposing these students to Army R&D professionals. In FY12, 1164 students received Army special awards at a science fair.

E. Junior Solar Sprint (JSS) Program

The JSS Program provides students an opportunity to learn engineering and renewable energy concepts and apply them by building and racing solar cars. Students form teams in their local communities, build solar cars with the help of trained mentors, and race them in local competitions. In FY12 the JSS program was reconceived from a north eastern United States regional race sponsorship to a nationally-focused online program. The Army has worked with curriculum and web developers to create an online clearinghouse of JSS resources, including tutorial videos starring Army scientists and engineers talking about the many scientific concepts related to design and build of solar vehicles. Students, teachers, parents, and community organizers throughout the country can access the free resources, advertise their local workshops and races online, and share best practices in teaching/coaching students through the JSS experience. In FY13, the first virtual JSS competition will be held, in which students from throughout the country can upload images of their designs and conduct local time trials to compete for recognition on the Army's JSS website.

F. High School Apprenticeship and Undergraduate Research Apprenticeship Programs (HSAP/URAP)

HSAP/URAP funds the STEM apprenticeship of promising high school juniors and seniors, and undergraduates to work in university-structured research environments under the direction of ARO-sponsored PIs serving as mentors. In FY12, HSAP/URAP awards provided 97 students with research experiences at 31 different universities. ARO invested approximately $353K in the FY12 effort.

G. Science and Engineering Apprentice Program (SEAP) and College Qualified Leaders (CQL)

The U.S. Army sponsors high school and college student internships in research laboratories throughout the Army. Students receive a stipend to spend their summer conducting research. ARO supports this unique vehicle for hiring student apprentices using research funding from participating Army laboratories. In FY12, 154 high school students participated in SEAP and 274 college students participated in the CQL program.

H. Gains in the Education of Math and Science (GEMS)

The GEMS program provides middle and high school students with a unique hands-on science experience in an Army laboratory. Students spend 1-4 weeks learning about Army research and conducting STEM experiments guided by Army scientists and engineers. In FY12, 1,614 students participated at GEMS programs held at twelve Army research laboratories spanning RDECOM, MRMC, and ERDC.

I. Youth Science Cooperative Outreach Agreement (YS-COA)

The YSCOA completed its second year of outreach efforts in FY12. It was awarded on 30 September 2010 to provide support and stimulation of STEM education and outreach in conjunction with DoD and the Army. YS-COA brings together government and a consortium of organizations working collaboratively to further STEM education and outreach efforts nationwide and consists of twelve major components, including the existing ARO Youth Science portfolio (JSHS, REAP, UNITE, JSS, and AAP), the Science and Engineering Apprentice Program (SEAP), College Qualified Leaders (CQL), Gains in the Education of Mathematical Sciences and Science (GEMS), ECybermission Internship Program (ECIP), ARL Intern Program, Teach the Teacher, and a strategic overarching marketing and metrics collection effort.

Virginia Polytechnic Institute and State University has led the consortium of non-profits and academic institutions to execute a collaborative STEM education and outreach program focusing on the Army Educational Outreach Program (AEOP) core objectives, revised in FY12:

- STEM Literate Citizenry: Broaden, deepen, and diversify the pool of STEM talent in support of our Defense Industry Base (DIB)
- STEM “Savvy” Educators: Support and empower educators with unique Army Research and Technology Resources
- Develop and implement a cohesive, coordinated, and sustainable STEM education outreach infrastructure across the Army

The FY12 major accomplishments included conduct of significant program evaluation and implementation of a number of changes. These changes included:

- Dissolution of the ECIP activity in favor of providing more age-appropriate follow-on engagement activities with eCybermission students
- Change in course of the Teach the Teacher program, now called the STEM Teachers Program, to provide summer enrichment opportunities for teachers in the Aberdeen Proving Ground, MD area. This model is being developed in a way that will be replicable in other parts of the country, as needed.
- Development of a new AEOP branding/marketing approach that was approved by ASA(ALT) and will be implemented in FY13
- Addition of eCybermission program to the consortium and identification of a new consortium partner to manage that program
- Establishment of a co-Cooperative Agreement Manager (CAM) representing the RDECOM STEM office

XII. SCIENTIFIC SERVICES PROGRAM (SSP)

ARO established the SSP in 1957. This program provides a rapid means for the Army, DoD, OSD, all branches of the military, and other federal government agencies to acquire the scientific and technical analysis services of scientists, engineers, and analysts from small and large businesses, colleges and universities, academicians working outside their institutions, and self-employed persons not affiliated with a business or university. Annual assistance is provided through the procurement of short-term, engineering and scientific technical services in response to user-agency requests and funding. Through the SSP, these individuals provide government sponsors with scientific and technical results and solutions to problems related to R&D by conducting well-defined studies, analyses, evaluations, interpretations, and assessments in any S&T area of interest to the government.

SSP services are administered and managed for ARO through the Battelle Chapel Hill Operations office located in Chapel Hill, North Carolina on behalf of Battelle Memorial Institute (BMI), headquartered in Columbus, Ohio. Battelle’s responsibilities include the selection of qualified individuals, universities, businesses, and/or faculty to perform all tasks requested by ARO, and for the financial, contractual, security, administration, and technical performance of all work conducted under the program. Over the past 37 years, BMI has administered and managed over 13,000 tasks supporting critical scientific and technical needs in many agencies within the federal government.

SSP awards tasks in a wide variety of technical areas, including mechanical engineering, computer sciences, life sciences, chemistry, material sciences, and military personnel recruitment/retention. In FY12, in addition to the more traditional use of the program, new tasks were initiated to support Warfighters and Combatant Commanders engaged in the Global War on Terror, Operation Iraqi Freedom, and Homeland Security. In FY12, there were a total of 77 new SSP tasks awarded and a modification of the scope and/or funding of 317 ongoing tasks on two SSP contracts. A summary of the agencies served under this program and the corresponding number of FY12 new SSP tasks is provided in TABLE 4.

TABLE 4
FY12 SSP tasks and sponsoring agencies.

Sponsoring Organization	SSP Tasks
Army Research, Development and Engineering Command (RDECOM)	
Army Research Laboratory (ARL)	8
Army Research Office (ARO)	1
Research, Development, and Engineering Centers (RDECs)	
Army Missile RDEC (AMRDEC)	6
Army Material Systems Analysis Activity (AMSAA)	1
Armaments RDEC (ARDEC)	7
Communications-Electronics RDEC (CERDEC)	3
Edgewood Chemical, Biological Center (ECBC)	2
Natick Soldier RDEC (NSRDEC)	2
Space & Terrestrial Communications Directorate (S&TCD)	4
Tank Automotive RDEC (TARDEC)	7
TOTAL: RDECOM	**41**
Army Medical Research and Materiel Command (MRMC)	
Aeromedical Research Laboratory (AARL)	5
Medical Research Institute of Chemical Defense (ICD)	1
TOTAL: MRMC	**6**
Other U.S. Army (USA)	
Headquarters Department of Army (HQ DA)	2
Program Executive Office Combat Support & Combat Service Support	1
US Army Corps of Engineers (USACE)	9
US Army Training & Doctrine Command (TRADOC)	1
US Military Academy (USMA)	6
TOTAL: Other USA	**19**
Other DoD	
US Air Force	4
US Marine Corps (USMC)	4
US Navy	1
Defense Threat Reduction Agency (DTRA)	1
TOTAL: Other DoD	**10**
Department of Health and Human Services (DHHS)	
Centers for Disease Control and Prevention (CDC)	1
TOTAL: DHHS	**1**
TOTAL FY12 SSP Tasks	**77**

XIII. SUMMARY OF PROGRAM FUNDING AND ACTIONS

A. FY12 Research Proposal Actions

The FY12 extramural basic research proposal actions according to each ARO Division are summarized in TABLE 5, below.

TABLE 5

FY12 ARO Research Proposal Actions. The status of research proposals received within FY12 (*i.e.*, 1 Oct 2011 through 30 Sep 2012) is listed based on proposal actions reported through 16 Jul 2013. The table reports actions for extramural proposals in the 6.1 basic research categories: SI, STIR, YIP, HBCU/MI, MRI, MURI, PECASE, and DURIP. The proposals and actions for the FY12 DURIP competition are included, although most of these proposals were received late in FY11.

	Received	Accepted	Declined	Pending	Withdrawn
Chemical Sciences	97	37	43	16	1
Computing Sciences	49	40	1	8	0
Electronics	79	37	29	13	0
Environmental Sciences	31	8	12	11	0
Life Sciences	158	34	92	32	0
Materials Science	68	38	25	5	0
Mathematical Sciences	49	36	7	6	0
Mechanical Sciences	107	38	62	7	0
Network Sciences	68	33	19	16	0
Physics	84	38	30	16	0
TOTAL	**790**	**339**	**320**	**130**	**1**

B. Summary of ARO Core Program Budget

The ARO FY12 Core (BH57) Research Program budget is shown in TABLE 6, below.

TABLE 6

ARO Core (BH57) Program funding. The ARO Core Program FY12 Budget is listed according to each scientific discipline (Division) or Special Program. The FY12 Budget by scientific discipline is reported based on the ARO Director's Budget, while the FY12 Budget for special programs is reported based on the Status of Funds Report as of 30 Sep 2012.

ARO Core (BH57) Program Type	Division or Program Title	FY12 Budget
Scientific Disciplines	Chemical Sciences	$7,744,660
	Computing Sciences	$3,737,859
	Electronics	$5,893,400
	Environmental Sciences	$2,400,538
	Life Sciences	$7,193,553
	Materials Science	$6,501,200
	Mathematical Sciences	$5,868,064
	Mechanical Sciences	$5,965,266
	Network Sciences	$5,349,964
	Physics	$6,864,192
	SUBTOTAL: Core Program Funding by Scientific Discipline	**$57,518,696**
Special Programs	Senior Research Scientist Research Programs	$739,274
	ARL Fellows' Stipends	$75,000
	National Research Council (NRC) Associates Program	$463,006
	HBCU/MI Program*	$1,073,221
	HSAP/URAP	$150,000
	In-House Operations	$15,968,777
	SUBTOTAL: Core Program Funding to Special Programs	**$18,469,278**
TOTAL	**ARO Core (BH57) Program**	**$75,987,974**

* These HBCU/MI Program funds are allocated at the Directorate level, and are matched with Division Core Program funds on a 1:1 basis.

C. Summary of Other Programs Managed or Co-managed by ARO

The FY12 allotments and funding sources for other ARO managed or co-managed programs (*i.e*, not part of the ARO Core Program), are shown in TABLES 7-9.

TABLE 7

FY12 allotments for other Army-funded programs. These programs, combined with the ARO Core (BH57) Program elements shown in TABLE 6, represent all of the Army-funded programs managed through ARO. The FY12 allotment values shown here represent the status of funds on the last day of FY12: 30 Sep 2012.

Other Army-funded Program	FY12 Allotment
Multidisciplinary University Research Initiative	$56,420,936
Presidential Early Career Award for Scientists and Engineers	$6,172,564
Defense University Research Instrumentation Program	$10,201,500
University Research Initiative Support	$2,254,000
MINERVA Program (Projects V72 and D55)	$3,231,000
Strategic Technology Initiatives	$100,000
Army Center of Excellence	$960,000
HBCU/MI – PIRT Centers	$2,215,000
Institute for Collaborative Biotechnologies (ICB)	$11,823,000
Institute for Soldier Nanotechnologies (ISN)	$10,441,000
Institute for Creative Technologies (ICT)	$7,764,000
Army Education Outreach	$2,048,000
Board of Army Science and Technology (BAST)*	$707,000
Small Business Innovation Research (SBIR)*	$4,025,353
Small Business Technology Transfer (STTR)*	$11,170,581
ARO-W Ballston Lease	$58,351
Youth Science Activities	$1,935,000
Research In Ballistics (Project H43)	$976,000
SBIR/STTR Support Services / Contract Support	$1,207,649
TOTAL: Other Army-funded Programs	**$133,710,934**

* In addition to the FY12 allotment shown, FY11 funds were received or reallocated in FY12 for this category, as specified in TABLE 10.

TABLE 8

FY12 allotment for externally-funded programs. FY12 funds received from sources other than Army or OSD are indicated below. The Other Customer Funds category includes funding from a variety of customer sources, such as the Joint IED Defeat Organization (JIEDDO) and the Joint Project Manager, Nuclear, Biological, and Chemical (JPMNBC). The FY12 allotment values shown here represent the status of funds on the last day of FY12: 30 Sep 2012.

External Program	FY12 Allotment
Defense Advanced Research Projects Agency (DARPA)*	$128,648,856
Scientific Services Program (SSP)	$18,066,196
Other Army	$31,954,092
National Security Agency (NSA)	$10,848,297
Defense Threat Reduction Agency (DTRA)	$9,312,544
Simulation and Technology Training Center	$7,714,265
Joint Program Manager NBC Contamination Avoidance	$28,964,774
Other Customer Funds (*e.g.*, JIEDDO and JPMNBC)	$38,829,530
TOTAL: External Programs	**$274,338,554**

* Includes FY11 DARPA funds allotted for FY12.

TABLE 9

OSD direct-funded programs. These funds were allocated directly from OSD to the indicated program.

OSD Direct-funded Programs	FY12 Allotment
SBIR/STTR[1,2]	$610,050
Historically Black Colleges and Universities / Minority Institutions (HBCU/MI)	$26,000,000
Chemical and Biological Defense (CBD) Programs[2]	$0
CBD SBIR[1,2]	$1,397,832
TOTAL: OSD Direct Funding	**$28,007,882**

[1] These SBIR/STTR funds are in addition to Army SBIR/STTR funds; see also TABLES 2 and 7.

[2] In addition to any FY12 allotments shown, FY11 funds were received or reallocated in FY12 for this category, as specified in TABLE 10.

D. Summary of FY11 Funds Received or Reallocated for Use in FY12

TABLE 10

FY11 funds received or reallocated for FY12. In addition to the FY12 allocations listed in TABLES 6-9, these programs were also supported through FY11 funds received or reallocated for use in FY12.

Program Category	FY11 Funds Received in FY12
BAST (Army funds)	$110,329
Army SBIR (Army funds)	$1,445,253
Army STTR (Army funds)	$2,517,996
SBIR/STTR (OSD direct funds)	$1,983,000
CBD Programs (OSD direct funds)	$6,703,506
CBD SBIR (OSD direct funds)	$3,201,437
Other Customer Reimbursable Program	$878,969
TOTAL: FY11 Funds Received or Reallocated in FY12	**$16,840,490**

E. Grand Total FY11 Allotment for ARO Managed or Co-managed Programs

TABLE 11

Summary of FY12 allotment for all ARO managed or co-managed programs. This table lists the subtotals from TABLES 6-9 and the grand total FY12 allotment for all ARO managed or co-managed programs. These totals do *not* include FY11 funds received or allocated in FY12 for certain programs (refer to TABLE 10).

Program Category	FY12 Allotment
Core (BH57) Programs	$75,987,974
Other Army-funded Programs	$133,710,934
External Program Funds	$274,338,554
OSD Direct-funded Programs	$28,007,882
GRAND TOTAL: (all sources)	**$512,045,344**

CHAPTER 3: CHEMICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2012* is to provide information on the programs and basic research efforts supported by ARO in FY12, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Chemical Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY12.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Chemical Sciences Division supports research to advance the Army and nation's knowledge and understanding of the fundamental properties, principles, and processes governing molecules and their interactions in materials or chemical systems. More specifically, the Division promotes basic research to uncover the relationships between molecular architecture and material properties, to understand the fundamental processes of electrochemical reactions, to develop methods for accurately predicting the pathways, intermediates, and energy transfer of reactions, and to discover and characterize the many chemical processes that occur at surfaces and interfaces. The results of these efforts will stimulate future studies and help keep the U.S. at the forefront of chemical sciences research. In addition, these efforts are expected to lead to new approaches for synthesizing and analyzing molecules and materials that will open the door to future studies that are not feasible with current knowledge.

2. Potential Applications. In addition to advancing world-wide knowledge and understanding of chemical processes, research in the Chemical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, results from the Chemical Sciences Program may lead to materials with new or enhanced properties to protect the Soldier from ballistic, chemical, and biological threats. The development of new computational methods may allow the structure and properties of notional (*i.e.*, theoretical) molecules to be calculated before they are created, providing a significant cost savings to the Army. In addition, chemical sciences research may ultimately improve Soldier mobility and effectiveness through the development of light-weight and small power sources, renewable fuel sources, and new energetic materials with improved methods for ignition, detonation, and control.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Chemical Sciences Division coordinates and leverages efforts within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), and the Air Force Office of Scientific Research (AFOSR). In addition, the Division coordinates with other ARO Divisions to co-fund research, identify multidisciplinary research topics, and to evaluate the merit of research concepts. For example, interactions with the ARO Life Sciences Division include developing research programs to investigate materials for use in chemical and biological defense and to understand the biotic/abiotic interface. The Chemical Sciences Division also coordinates efforts with the Materials Science Division to pursue the design and characterization of novel materials through new synthesis and processing methods, the evaluation of bulk mechanical properties, and molecular-level studies of materials and material properties. Research in the chemical sciences also complements research in the Physics and Electronics Divisions to investigate the dynamics of chemical reactions and how chemical structure influences electrical, magnetic, and optical properties. The creation of new computational methods and models to better understand molecular structures and chemical reactions is also an area of shared interest between the Chemical

Sciences and Mathematical Sciences Divisions. Research in the Chemical Sciences Division is also coordinated with research in the Environmental Sciences Division, in which new methods and reactions are being explored for detecting, identifying, and neutralizing toxic materials. These interactions promote a synergy among ARO Divisions, providing a more effective mechanism for meeting the long-term needs of the Army.

B. Program Areas

To meet the long-term program goals described in the previous section, the Chemical Sciences Division engages in the development, identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the identification, evaluation and monitoring of research projects. In FY12, the Division managed research within these four Program Areas: (i) Polymer Chemistry, (ii) Molecular Structure and Dynamics, (ii) Electrochemistry, and (iv) Reactive Chemical Systems. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Polymer Chemistry. The goal of this Program Area is to understand the molecular-level link between polymer architecture, functionality, composition, and macroscopic properties. Research in this program is expected to lead to the design and synthesis of new polymeric materials that give the Soldier improved protective and sensing capabilities, and capabilities not yet imagined. This Program Area is divided into two research Thrusts: (i) Synthesis: Molecular Structure and Composition, and (ii) Properties: From Molecular to Macroscopic. Within these Thrusts, high-risk, high payoff research efforts are identified and supported to pursue the program's long-term goal. Efforts in the Synthesis Thrust focus on developing new synthetic approaches for preparing novel polymers with potentially interesting properties, the design of new polymerizable monomers, and the design and synthesis of polymers with specific responses that are designed into the polymeric material at the molecular level. Research in the Properties Thrust is exploring how changes in molecular structure and composition impact macroscopic properties, focuses on the design of polymer molecular architecture (*e.g.*, location of functional groups) to generate unique and well-defined morphologies, and characterizes molecular-level, multicomponent transport in complex systems.

While these research efforts focus on high-risk, high payoff concepts, potential long-term applications for the Army include light-weight, flexible body armor, materials for clothing that are breathable but also provide protection from toxins, fuel cell membranes to harness renewable energy, and damage-sensing and self-healing materials for vehicles, aircraft, and other DoD materiel. In addition, the efforts in this program may ultimately lead to new, dynamic materials such as photohealable polymers that can be used as a repairable coating and mechanically- or thermally-responsive polymers and composites that can convert external forces to targeted internal chemical reactions (*i.e.*, to convert external force to internal self-sensing and self-repair).

2. Molecular Structure and Dynamics. The primary goal of this Program Area is to understand state-selected dynamics of chemical reactions of molecules in gas and condensed phases across a wide variety of conditions (temperatures and pressures), and to develop theories that are capable of accurately describing and predicting these phenomena. In the long term, these studies may serve as the basis for the design of future propellants, explosives, and sensors. This Program Area is divided into two research Thrusts: (i) Dynamics and (ii) Theory. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high-payoff research efforts that can collectively meet the program's overall goal. The Dynamics Thrust broadly supports research on the study of energy transfer mechanisms in molecular systems (reactive and non-reactive), while the Theory Thrust supports research to develop and validate theories for quantitatively describing and predicting the properties of chemical reactions and molecular phenomena in gas and condensed phases.

The research supported by this Program Area will likely enable many future applications for the Army and general public. These applications include more efficient and clean combustion technology, the development of new tools to study condensed phases of matter, the capability to accurately predict the properties of large, complex chemical systems, and the development of novel molecules for use in energy storage applications ranging from fuels to next-generation explosives.

3. Electrochemistry. The goal of this Program Area is to understand the basic science that controls reactant activation and electron transfer. These studies may provide the foundation for developing advanced power generation and storage technology. This Program Area is divided into two research Thrusts: (i) Reduction-oxidation (Redox) Chemistry and Electrocatalysis, and (ii) Transport of Electroactive Species. These Thrust areas guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. The Redox Chemistry and Electrocatalysis Thrust supports research efforts to discover new spectroscopic and electrochemical techniques for probing surfaces and selected species on those surfaces, while the Transport of Electroactive Species Thrust identifies and supports research to uncover the mechanisms of transport through polymers and electrolytes, to design tailorable electrolytes based on new polymers and ionic liquids, and also explores new methodologies and computational approaches to study the selective transport of species in charged environments.

Research in this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications include the discovery and use of new mechanisms for the storage and release of ions that are potentially useful in future power sources, including new battery or bio-fuel concepts. In addition, studies of electroactive species may enable the development of multifunctional materials that simultaneously have ionic conductivity, mechanical strength, and suitable electronic conductivity over a considerable temperature range, while exposed to aggressive chemical environments.

4. Reactive Chemical Systems. The goals of this Program Area are to explore absorption, desorption, and the catalytic processes occurring at surfaces, and to investigate the structure and function of supramolecular assemblies (*i.e*, complexes of molecules held together by noncovalent bonds). Specific objectives include the discovery of new synthetic approaches to create self-assembled systems and the incorporation of catalytically or biologically active species into these systems. Through the study of these processes and structures, the program seeks to develop a molecular-level understanding of catalytic reactions, functionalized surfaces, and organized assemblies that could lead to future materials for protection and sensing. This Program Area is divided into two research Thrusts: (i) Surfaces and Catalysis and (ii) Organized Assemblies. Within these Thrusts, high-risk, high-payoff research efforts are identified and supported to pursue the program's long-term goals. The Surfaces and Catalysis Thrust supports research efforts on understanding the kinetics and mechanisms of reactions occurring at surfaces and interfaces. Research in the Organized Assemblies Thrust explores the properties and capabilities of self-assembled structures, including their functionality, and ability to respond to external stimuli.

This Program Area supports research that will likely lead to many long-term applications for the Army and the general public. These potential long-term applications include the development of stimuli-responsive materials for Soldier protection, the chemical sensing of hazardous materials, and the controlled release of reactive species for hazardous material destruction.

C. Research Investment

The total funds managed by the ARO Chemical Sciences Division for FY12 were $36.6 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY12 ARO Core (BH57) program funding allotment for this Division was $7.3 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $7.1 million to projects managed by the Division. The Division also managed $5.3 million of Defense Threat Reduction Agency (DTRA) programs, $2.1 million of Defense Advanced Research Projects Agency (DARPA) programs, and $1.2 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $2.5 million for contracts. The Institute for Soldier Nanotechnologies received $12.8 million. Finally, $1.3 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY12 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research projects. Research projects are developed by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts.

The following subsections summarize projects awarded in FY12 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY12, the Division awarded 13 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to advance molecular electronic structure theory and to synthesize and study new supramolecular polymeric materials. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Rodney Bartlett, University of Florida – Gainesville, *The Discovery and Implementation of Accurate Quantum Chemical Methods for Molecular Structure, Spectra, and Reaction Paths*
- Professor Joel Bowman, Emory University, *Theoretical Studies of "Roaming" Reactions*
- Professor Juliet Gerrard, University of Canterbury, New Zealand, *Proteins as Supramolecular Building blocks for Responsive Materials and Nanodevices*
- Professor Craig Hill, Emory University, *New Multi-functional Structures*
- Professor Stephen Klippenstein, University of Chicago, *Effect of Dynamics in the van der Waals Region on the Chemical Kinetics of Nitrogen Containing Molecules*
- Professor Todd Martinez, Stanford University, *Mechanically Trapping Transition States and Reactive Intermediates*
- Professor Stephen Paddison, University of Tennessee - Knoxville, *First Principles Modeling of Cation (H^+, Li^+, and Na^+) Transport in Solid Polymer Electrolytes*
- Professor Stuart Rowan, Case Western Reserve University, *Supramolecular Polymers With Multiple Types of Binding Motifs: From Fundamental Studies to Multifunctional Materials*
- Professor Eugene Smotkin, Northeastern University, Elucidation of Ionomer-Metal Interfacial Structure by Infrared Spectroscopy, *Neutron Reflectivity and Density Functional Theory*
- Professor Randall Snurr, Northwestern University - Evanston, *Computational Analysis of Reactions Between Target Molecules and Functionalized Surfaces*
- Professor Philip Sullivan, Montana State University, *Amphiphilic Block Copolymer Mediated Self-Assembly of Nanocomponents Into Active Metamaterial Structures: Nonlinear Metamaterials*
- Dr. Alan Willey, The Proctor and Gamble Company, *Engineered, Smart and Responsive Biologically Modified Abiotic Surfaces*

- Professor Gleb Yushin, Georgia Tech Research Corporation, *Electrochemical Reactions of Sulfur with Lithium-ion Electrolytes in Carbon Nanopores*

2. Short Term Innovative Research (STIR) Program. In FY12, the Division awarded ten new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to discover and understand fundamental phenomena regarding photoinduced electron dynamics in semiconductor nanocrystals and to gain an in-depth understanding of the morphology and physical properties of polypeptide-grafted brush polymers. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Adam Braunschweig, New York University, *Inducing the Formation of Functional Macroscopic Assemblies Through Programmed Orthogonal Supramolecular Interactions*
- Dr. Calum Chisholm, SAFCell, Inc., *Highly Active ORR Catalysts*
- Professor Wilson Chiu, University of Connecticut - Storrs, *Predicting Carbonate Ion Transport in Alkaline Anion Exchange Materials*
- Professor Russell Howe, University of Aberdeen, *Hydrogen Photo-Production From Ethanol and Water Over Au/TiO_2(110) Rutile Single Crystal*
- Professor Elena Jakubikova, North Carolina State University, *Theoretical Approaches to Describe Ground and Excited State Properties of Earth-abundant Materials*
- Professor Wen Li, Wayne State University, *Time-Resolved Studies of Orbital Orientation in Photodissociation of Small Molecules*
- Professor Yao Lin, University of Connecticut - Storrs, *Pilot Study on the Bulk Properties and Morphology of Polypeptide-Grafted Brush Polymers*
- Professor Brian Long, University of Tennessee at Knoxville, *Redox-Switchable Olefin Polymerization Catalysis: Electronically Tunable Ligands for Controlled Polymer Synthesis*
- Professor Daniel Neumark, University of California - Berkeley, *Attosecond Dynamics and Quantum Dots*
- Professor Tatyana Reshetenko, University of Hawaii - Honolulu, *Separation Method for Oxygen Mass Transport Coefficient in Two Phase Porous Air Electrodes*

3. Young Investigator Program (YIP). In FY12, the Division awarded one new YIP project. This grant is driving fundamental research to develop novel single-molecule probes for the investigation of proteins in near-surface environments at the molecular level. The following PI and corresponding organization was the recipient of the new-start YIP award.

- Professor Joel Kaar, University of Colorado - Boulder, *Probing Enzyme-Surface Interactions via Protein Engineering and Single-Molecule Techniques*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY12 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *20th Conference on Current Trends in Computational Chemistry; Jackson, MS*; 27-29 October 2011
- *Electrochemistry Gordon Research Conference*; Ventura, CA; 8-13 January 2012
- *Batteries Gordon Research Conference*; Ventura, CA; 4-9 March 2012
- *243rd American Chemical Society Symposium on Ionic Liquid Advanced Electrolytes*; San Diego, CA; 25-29 March 2012
- *Materials Research Society Symposium on Functional Materials and Ionic Liquids*; San Francisco, CA; 9-13 April 2012
- *Synthetic Molecular Systems Landscape Workshop*; Arlington, VA; 24-25 April 2012
- *Targeting and Triggering Basic Research Workshop*; Cambridge, UK; 14-16 May 2012
- *IUPAC World Polymer Congress 44th International Symposium on Macromolecules*; Blacksburg, VA; 24-29 Jun 2012
- *Bioinspired Materials Gordon Research Conference*; Davidson, NC; 24-29 June 2012
- *Emerging Computational Methods for Weak Intermolecular Interactions*; Dover, DE; 1-3 August 2012

- *Fuel Cells Gordon Research Conference*; Smithfield, RI; 6-10 August 2012
- *244th American Chemical Society National Meeting, Applied Polymer Science Symposium*; Philadelphia, PA; 19-23 August 2012
- *International Symposium for Polymer Electrolytes*; Selfoss, Iceland; 26-31 August 2012
- *Chemical/Biological Filtration Strategies Working Group*; Arlington, VA; 28-29 August 2012

5. Special Programs. In FY12, ARO Core Research Program funds provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded five new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These projects constitute a significant portion of the basic research programs managed by the Chemical Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Molecular and Optical Properties of Nanophotonic Materials. This MURI began in FY06 and was awarded to a team led by Professor Eric Van Stryland at the University of Central Florida. This MURI is exploring the molecular structure of materials that display properties of high-speed nonlinear optics (NLO).

The field of NLO has enabled breakthrough developments in laser design, controlling light, and remote sensing. The goal of this MURI is to discover the structural components required for creating a new generation of materials that exhibit large NLO-absorption properties. Results from this research may ultimately enable the creation of a new generation of nanophotonic materials that control light at or below nanometer wavelengths, which has the potential to revolutionize the telecommunications industry by providing high-speed interference-free devices on a microchip. In addition, these materials could lead to improved visible-imaging applications (*e.g.*, microscopy) and protective devices that will absorb high-energy light (*e.g.*, visors to protect the Soldier from sunlight or high-powered lasers, without interfering with visibility at dawn or dusk).

2. Mechanochemical Transduction. This MURI began in FY07 and was awarded to a team led by Professor Jeffrey Moore at the University of Illinois, Urbana-Champaign. This research is co-managed by the Chemical Sciences and Materials Science Divisions. The MURI is exploring mechanical-to-chemical energy conversion (*i.e.*, mechano-chemical transduction), including the design, synthesis, and characterization of a revolutionary new class of compounds that could potentially convert mechanical energy to catalyze chemical reactions.

The use of polymers and polymer composites in construction materials, microelectronic components, adhesives, and coatings is well established. Polymer composites can form strong materials for use in civil and government engineering, such as siding materials or armor. Unfortunately, these polymeric materials commonly crack when subjected to mechanical stress (damage), and these cracks can occur deep within the structure where detection is difficult and repair is almost impossible. These cracks are a visible manifestation of the chemical changes (*e.g.*, breaking of bonds) that occur at the molecular level when the structure is damaged. This MURI team is investigating the direct and reversible transduction between mechanical and chemical energy, and the potential to ultimately exploit this process in the design and synthesis of new materials. To meet this goal, the team of investigators is designing, synthesizing, and characterizing revolutionary new class of mechano-responsive molecules, called mechanophores, which are designed to respond to mechanical stress with pre-designed chemical reactions. Based on these results from this project, future molecules could be designed to convert mechanical stress (*e.g.*, structural damage) to useful chemical reactions. Results from this research may ultimately enable the construction of polymer composites that automatically alert the user to when and where a structure has sustained damage, and then self-repair after damage.

3. Molecular Design of Novel Fibers using Carbon Nonotubes. This MURI began in FY09 and was awarded to a team led by Professor Horacio Espinosa at Northwestern University. The focus of this MURI is to understand the molecular properties required for preparing strong fibers using polymers and double-walled carbon nanotubes (DWCNT).

The chief objectives of this research are to (i) develop a model system for predicting the molecular properties necessary for preparing new, high-strength fibers, and (ii) to prepare novel fibers composed of double-walled carbon nanotubes and polymers. The team will use multiscale computer simulations to bridge atomistic (*i.e.*, electronic structure methods and reactive force fields), coarse-grain, and continuum scales to explore and understand DWCNT-polymer interactions, crosslinking effects (bond-breaking mechanisms), and the impact of architecture on fiber strength, elasticity, and toughness. The investigators will use the results to predict fiber precursor properties necessary for optimum strength. The team will use predictive models to develop chemical vapor deposition techniques for producing highly-aligned DWCNT mats with optimized density and surface chemistry. The mats will serve as precursors for fiber formation. These materials will be characterized using *in situ* and *ex situ* microscopy (*i.e.*, assayed during and after reaction completion). The fundamental scientific knowledge uncovered through this research may lead to new approaches for designing and preparing high-strength, flexible fibers that are directly relevant to lighter-weight and flexible personnel armor.

4. Ion Transport in Complex Organic Materials. This MURI began in FY10 and was awarded to a team led by Professor Andrew Herring at the Colorado School of Mines. This MURI team is investigating the interplay of chemical processes and membrane morphology in anion exchange.

Ion transport in complex organic materials is essential to many important energy conversion approaches. Unfortunately, ion transport is poorly understood in terms of its relationship to water content, morphology, and chemistry. While a great deal of research has focused on proton exchange membranes, little work has been performed with anion exchange membranes. This MURI team is studying the fundamentals of ion transport by developing new polymer architectures (*e.g.*, polymer membranes) using standard and novel cations. These new polymer architectures and aqueous solutions containing representative cations will serve as a model system for studies of anion transport and its relationship to polymer morphology. In the longer term, the design and synthesis of robust, thin alkali-exchange membranes, combined with an improved understanding of ion exchange gained through the characterization of these membranes, could enable the development of new classes of fuel cells. If the MURI team can characterize the fundamental processes of ion exchange across these polymer membranes, future fuel cells using similar membranes could harness alkali exchange, resulting in inexpensive, durable, and flexible-source power for the Army and commercial use.

5. Peptide and Protein Interactions with Abiotic Surfaces. This MURI began in FY11 and was awarded to a team led by Professor Zhan Chen at the University of Michigan, Ann Arbor. This MURI is exploring the processes that occur at biological/abiological interfaces.

The objective of this research is to develop a systematic understanding of biological/abiological interfaces and how to design systems for predicted biological structure and function. The MURI team is using a combination of modeling and experimental techniques to understand the interactions of peptides and proteins covalently immobilized on abiotic surfaces. Specifically, the team will be investigating two peptides and one enzyme, with a variety of surfaces, such as self-assembled monolayers, chemically functionalized liquid crystalline films, and chemical vapor deposited polymers. The immobilized biological species will be characterized to determine not only structure but also activity. The investigators will utilize systematic modifications of the surface to probe the effect of chemical composition, morphology, and hydrophobicity on biological structure and function. The role of water will also be probed to determine how hydration affects not only immobilization, but also structure and function. Results from this research may ultimately enable the incorporation of nanostructured abiotic/biotic materials in applications such as sensing, catalysis, coatings, drug delivery, prosthetics, and biofilms.

6. High-Resolution Quantum Control of Chemical Reactions. This MURI began in FY12 and was awarded to a team led by Professor David DeMille at Yale University. This MURI is exploring the principles of ultracold molecular reaction, where chemical reactions take place in the sub-millikelvin temperature regime. This research is co-managed by the Chemical Sciences and Physics Divisions.

The study of ultracold molecular reactions, where chemical reactions take place in the sub-millikelvin temperature regime, has emerged as a new field in physics and chemistry. Nanokelvin chemical reactions are radically different than those that occur at "normal" temperatures. Chemical reactions in the ultracold regime can occur across relatively long intermolecular distances, and no longer follow the expected (Boltzmann) energy distribution. The reactions become heavily dependent on nuclear spin orientation, interaction strength, and correlations. These features make them a robust test bed for long-range interacting many-body systems, controlled reactions, and precision measurements.

The objectives of this MURI are to develop a fundamental understanding of the nature of molecular reactions in the nanokelvin temperature regime and to extend the cooling technique previously demonstrated by Professor DeMille[1] (through a previous ARO award) to other molecular candidates. The researchers will focus will be on the implementation of novel and efficient laser cooling techniques of diatomic molecules, and to understand the role of quantum effects, including the role of confined geometries, on molecules that possess vanishingly-small amounts of thermal energy. This research could ultimately lead to new devices or methods that explicitly use quantum effects in chemistry, such as the precision synthesis of mesoscopic samples of novel molecular compounds, new avenues for detection of trace molecules, and a new understanding of combustion and atmospheric chemical reactions.

7. Coherent Effects in Hybrid Nanostructures. This MURI began in FY12 and was awarded to a team led by Professor Naomi Halas at Rice University. This MURI is investigating nanomaterials and how these materials can control the propagation of electromagnetic (EM) energy.

Fundamental research involving metamaterials, quantum dots, plasmonic nanostructures, and other materials systems during the last decade has demonstrated the unique ability to selectively and actively control and attenuate electromagnetic energy from the far infrared (IR) through ultraviolet (UV) regions. The absorption frequency is dependent on shape, size, orientation, and composition of the nanomaterial. The nanoparticles act as antennae that redirect, focus or otherwise re-radiate the incoming energy. Because this is a resonance phenomenon, the media is generally transparent over a broad frequency range, with one or more resonances that absorb at specific frequencies. A goal in the control of the propagation of EM energy is the design of a material that absorbs over a broad frequency range and is transparent at one or more specific frequencies.

The objective of this research is to develop a fundamental understanding of nanomaterials to control the propagation of EM energy, with a particular emphasis on designing and investigating materials that have a broad spectrum absorption with a narrow, selective window of transmission. The MURI team is using a combination of computational, nanoscale fabrication, and characterization techniques to tailor electromagnetic properties for materials in specific, selected regions of the spectrum. The research team is focusing on designing, synthesizing, and combining nanoparticles and nanoparticle-based complexes to yield nanocomplexes exhibiting optimized coherent effects. This research may ultimately enable the design of materials with precisely-positioned transparency or absorbency windows that will impact Army applications in broadband scattering and absorption.

C. Small Business Innovation Research (SBIR) – New Starts

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY12, the Division managed four new-start SBIR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of two Phase I contracts, one Phase II contract, and one Phase II Chemical Biological Defense SBIR (CBD-SBIR) contract. These new-start contracts aim to bridge fundamental discoveries with potential applications, such as the development of a solid acid electrolyte fuel cell that is hydrocarbon fueled and operates at elevated temperatures, and a system to rapidly and quantitatively identify the presence of spores.

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[1] Shuman ES, Barry JF, DeMille D. (2010). Laser cooling of a diatomic molecule. *Nature*. 467:820–823.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY12, the Division managed seven new-start STTR contracts, in addition to active projects continuing from prior years. These contracts consisted of four Phase I projects and three Phase II STTR projects. These new-start projects aim to bridge fundamental discoveries with potential applications, such as the development of a fuel processor system capable of producing hydrogen from butanol, and the development of new methods for increasing the power density of fuel cells.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY12, the Division awarded one new ARO (Core) HBCU/MI project and two new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The PECASE winners for each calendar year are announced by the White House in the last quarter of the fiscal year. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Attosecond Photon Source to Investigate Ultrafast Electron Dynamics. The objective of this PECASE, led by Professor Wen Li at Wayne State University, is to develop a high-energy attosecond pulse and then to investigate ultrafast electron dynamics in atoms and molecules by attosecond two-photon spectroscopy.

The most fundamental motion in chemical dynamics of atoms and molecules is that of electrons. Investigating electron motions in their most detailed level will provide a significantly-improved understanding of chemical reactions such that a chemical reaction could be effectively predicted or controlled. Because the typical energy differences involved in such electron motions are large, the natural time scale of such electronic dynamics is around a few tens of attoseconds (10^{-18}s). The research team studying sub-femtosecond electron dynamics in molecular systems using a new attosecond pulse spectroscopy. This research may provide an understanding of the electron dynamics involved in such important processes related to the harvesting, storage, and utilization of solar and hydrogen energy. This research may also shed light on the details of how green plants convert solar energy (photosynthesis) into chemical energy (chemical bonds composed of spin paired electrons), which may then lead to the production of artificial photosynthetic systems that can efficiently harvest solar power.

2. Biologically-Patterned Amyloid Scaffolds for Multifunctional and Multiscale Materials. The objective of this PECASE, led by Professor Timothy Lu at the Massachusetts Institute of Technology, is to design multifunctional biological nanowire scaffolds.

Biological systems have a virtually unmatched ability to organize organic and inorganic structures with amazing precision, and at length scales that vary over many orders of magnitude. Despite significant advances in engineering nanomaterials, many challenging hurdles still persist in synthetic biology before the precision of biological systems can be matched in an artificial environment. Challenges include organizing materials from the nanoscale to the microscale and the macroscale, and interfacing biological molecules with abiotic materials. This research project aims to combine synthetic biology with nanotechnology to engineer functional amyloid fibers produced by bacteria into biomaterial scaffolds. Results from this research may ultimately enable the creation of multifunctional materials with far-reaching applications for Army and civilian use, such as sensors, microbial fuel cells, and multi-functional biomaterials.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY12, the Chemical Sciences Division managed seven new DURIP projects, totaling $1.0 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of thin-film deposition methods, photonic reagent control, and self-assembled responsive polymeric nanostructures.

H. University Affiliated Research Center (UARC): Institute for Soldier Nanotechnologies (ISN)

The ISN, located at the Massachusetts Institute of Technology (MIT), carries out fundamental, multidisciplinary, nanoscience research that is relevant to the Soldier. Nanoscience research creates opportunities for new materials, properties, and phenomena as material properties (*e.g.*, color, strength, conductivity) become size dependent below a critical length scale of about 500 nanometers. The research performed at the ISN falls into five Strategic Research Areas (SRAs): (i) Lightweight, Multifunctional Nanostructured Materials (ii) Soldier Medicine, (iii) Blast and Ballistic Threats, (iv) Hazardous Substances Sensing, and (v) Nanosystems Integration. Each SRA is further divided into research themes. Detailed descriptions of each SRA and its corresponding themes are available at the ISN program website (http://mit.edu/isn/research/index.html).

In FY12, the ISN supported 50 faculty, 110 graduate students, and 40 postdoctoral fellows across 12 departments at MIT. The ISN program is unique in that it currently has 18 industrial partners positioned to receive promising technical results and work to bring new products and capabilities to the Soldier, as well as a mechanism for additional industry partners to join and leave the Institute, depending on needs and activities. A U.S. Army Technical Assessment Board and an Executive Steering Board annually review the ISN research portfolio, assessing the goals of the various projects and research results. The ISN and its industry partners are well-situated to perform basic and applied research in response to Soldier needs now and in the future. A total of $12.8 million of program funds was allocated to the ISN in FY12, which was the fifth year of a contract that was renewed in FY07 for a five-year period. Of these FY12 funds, $9.8 million was allocated for 6.1 basic research and $3.0 million was allocated for seven applied-research projects, including two new projects.

I. DARPA Biofuels Alternative Feedstocks

This DARPA program is managed within the Division's Electrochemistry Program. The Biofuels Alternative Feedstocks program is developing affordable alternatives to petroleum-derived JP-8 without using algae and cellulosic biomass. DARPA seeks to develop and demonstrate a technology that can enable the production of JP-8 at less than $3 per gallon at a moderate-scale facility (<50 Mgal/yr).

J. DARPA Limits of Thermodynamic Storage of Energy

This DARPA program is managed within the Division's Electrochemistry Program. DARPA is soliciting innovative proposals to develop revolutionary new approaches to portable energy sources. DoD is critically dependent on portable electronics and, by extension, portable energy sources such as batteries. However, the actual energy output of state-of-the-art battery technologies, such as the BA5590 $LiSO_2$ primary and BB2590 Li-ion secondary systems, fall short of their projected energy capacity under load, limiting the operation of DoD electronic systems that use these batteries to as little as 20% of theoretical capability. This operational inefficiency increases the number of batteries Soldiers must carry in the field and also limits implementation of hybridization and distributed power concepts for DoD ground, aerial, and maritime vehicle platforms. The DARPA Limits Of Thermodynamic Storage of Energy program seeks to address inefficiencies in energy extraction by developing technologies that are capable of delivering the full run time out of a state-of-the-art portable energy source.

K. Fuel-cell Based Squad Battery Charger Quick Reaction Fund

This Quick Reaction Fund Program is managed within the Division's Electrochemistry Program and is coordinated with the ARL Sensors and Electron Devices Directorate (ARL-SEDD), the Communications-Electronics Research, Development, and Engineering Center (CERDEC), and ONR. Current military operations rely heavily on batteries to power portable equipment. Providing batteries to the individual Soldier has become a major logistical challenge to the modern Army. While significant progress has been made in developing alternate power supplies, including prototype individual fuel cells, batteries are expected to remain the primary power source for the individual Soldier for the foreseeable future. If quiet, compact, lightweight and energy-dense chargers were available in sizes appropriate for small-unit operations, then Soldiers could continue using batteries, but reduce their weight burden by a factor of two or more by replacing primary batteries with rechargeable batteries and a high-efficiency battery charger operating on liquid fuels. To address the need for portable battery chargers sized for small squad operation, Protonex Technology Corporation is developing a prototype 125W portable generator based on solid oxide fuel cells. This generator uses low-sulfur kerosene as a fuel and is capable of operating both as a battery charger or directly powering equipment. With a mass of <7 kg, the battery charger fits in a backpack. Using high energy-density kerosene fuel, the charger-based system could save more than 60% of the weight of current solutions. When used to power equipment directly, the fuel cell system saves more than 80% of the weight of the primary batteries. Within this program, Protonex built and delivered prototype systems to both the Army and Navy for testing and evaluation.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Chemical Sciences Division.

A. Integrating Synthetic Biology and Chemistry to Explore Biologically-Patterned Nanowire Scaffolds
Professor Timothy Lu, Massachusetts Institute of Technology, Single Investigator Award

The objective of this research is to design and create multifunctional biological nanowire scaffolds with detailed patterning capabilities that span multiple length scales and can provide novel abiotic-biotic interfaces. The research team has utilized synthetic biology techniques to construct mutated versions of curli fibers (*i.e.*, amyloid fibers produced by *E. coli*) and investigated their behavior on gold surfaces and nanoparticles using a variety of analytical techniques. Quartz crystal microbalance was used to monitor the deposition of the wild-type and mutated curli fibers on gold surfaces, and revealed that wild-type curli has affinity to these surfaces. Amino acid point mutations of the major curli subunit (CsgA) provided additional data as to which residues were responsible for interactions with the golf surface, as well as a potential approach to control these interactions. Circular dichroism (CD) was used to characterize the wild-type curli's structural features independently and in the presence of gold nanoparticles. In FY12, the research team found that structural rearrangement of wild-type curli was minimal when bound to nanoparticles. However, modified CsgA constructs, such as the 7xHis-tagged fiber, changed the CD signal, indicative of a strong curli-nanoparticle interaction. A random-coil structure compared to the wild-type beta-sheet conformation was observed. In order to exploit these interactions, the team explored templating of gold nanoparticles in solution and monitored the results using absorption spectroscopy and transmission electron microscopy (TEM). The team discovered variations in absorbance and size and distribution of nanoparticles on the fiber (see FIGURES 1-2). Based on these initial findings, Professor Lu will continue to investigate other curli fiber mutants and metal surfaces towards understanding fundamental abiotic-biotic interactions that are relevant to sensing, microbial fuel cell, and self-healing material applications.

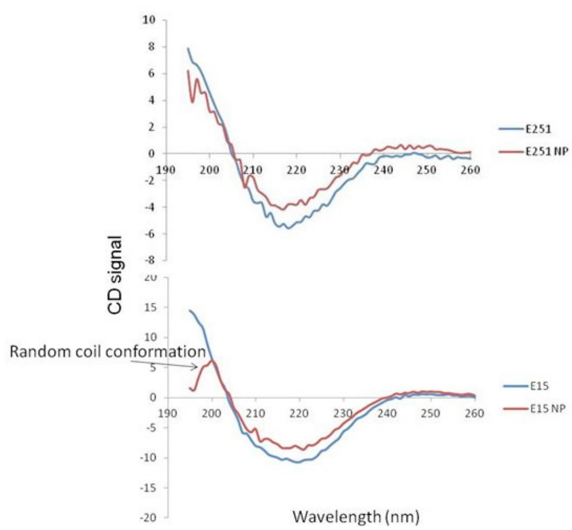

FIGURE 1

Monitoring gold nanoparticle templating on modified curli fibers by absorption spectroscopy. The CD plots compare studies of wild-type curli (E251) versus 7xHis-tagged curli (E15), without and with gold nanoparticles.

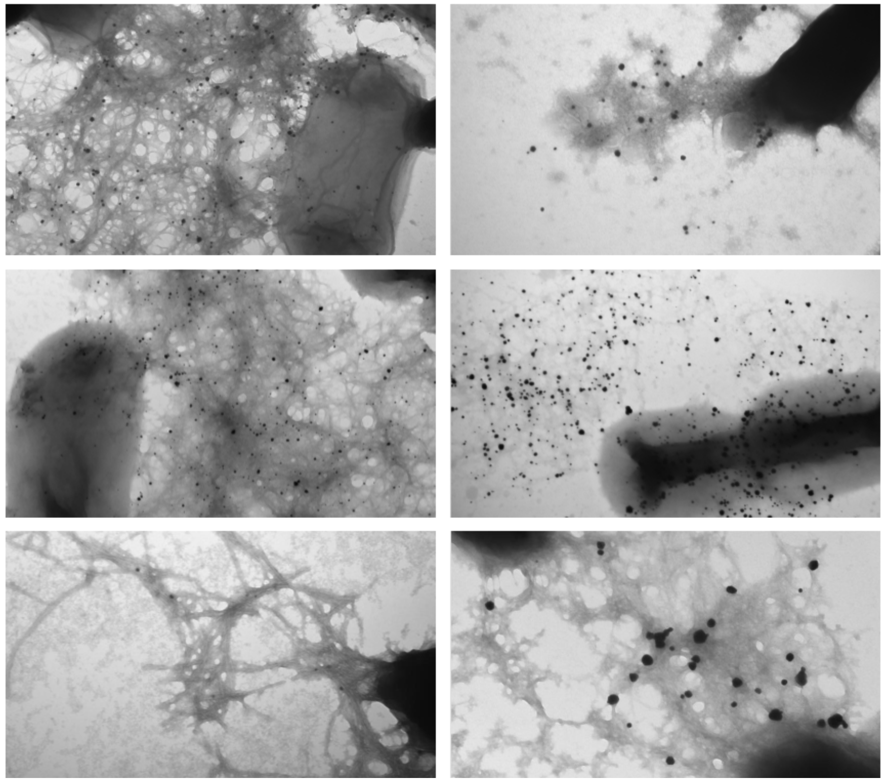

FIGURE 2

Monitoring gold nanoparticle templating on modified curli fibers by TEM. The TEM images reveal mutations in the absorbance, size, and distribution of nanoparticles on the fiber.

B. Precision Morphology in Sulfonic, Phosphonic, Boronic, and Carboxylic Acid Polyolefins

Professor Kenneth Wagener, University of Florida - Gainesville, Single Investigator Award

The objective of this research is to create precision acid and ionomer polymers through systematic variation of the exact position and type of acidic group along the polymer chain backbone in order to examine fundamental changes in morphology. This research will provide a better understanding of structure/morphology/property relationships in a unique set of acid and ion-containing polymers.

To date, the investigators have successfully elucidated the morphology of carboxylic and phosphoric acid-containing polyolefins. In FY12, polyethylene bearing ethyl (aliphatic) sulfonic acid groups precisely placed on every 9th, 15th, and 21st carbon of the polymer backbone were successfully prepared. The major synthetic challenge, the deprotection of the sulfonate ester, was achieved via ethyl ester hydrolysis using sodium hydroxide in dimethyl sulfoxide with mild heating. More specifically, a heterogenous approach was employed where the sulfonate ester polymer was dispersed in DMSO (see FIGURE 3). Upon addition of solid NaOH, the esters were immediately hydrolyzed, resulting in the polymer's complete solubility. The success of this method was also demonstrated by the polymer's solubility in water, as the sulfonate ester precursor is water insoluble.

Success with this synthetic method will generate new, precisely substituted polymers that may possess enhanced barrier or selective permeation properties and will provide new structure/property relationship knowledge that will aid in the design of novel materials.

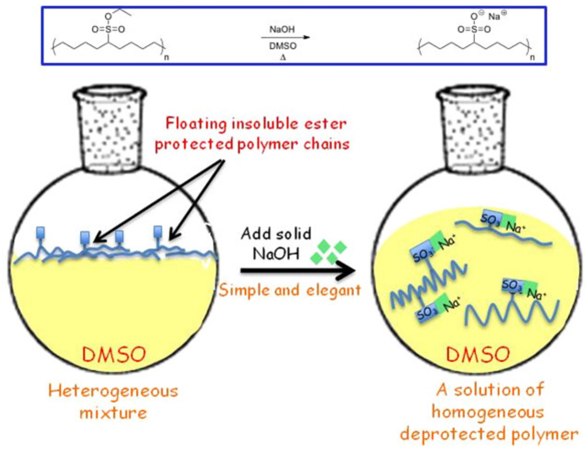

FIGURE 3

Deprotection of sulfonate ester polymer to sodium sulfonate polymer via heterogenous method. The flask on the left shows an insoluble protected polymer, which does not dissolve in DMSO, with the polymer floating on the surface. Upon addition of solid sodium hydroxide, the polymer is "pulled" into the solution by hydrolysis of the ester (as shown in the flask on the right).

C. Novel Colloidal and Dynamic Interfacial Phenomena in Liquid Crystalline Systems

Professor Nicholas Abbott, University of Wisconsin - Madison, Single Investigator Award

Professor Abbott's research focuses on the fundamental understanding of the interfacial phenomena between liquid crystalline (LC) phases and amphiphiles or nanoparticles. Previous research illustrated phase separation of a monolayer of phospholipid, dilauroyl phosphatidylcholine (DLPC), at the LC-aqueous interface. The research team has been exploring whether this phenomenon can be observed with other lipids. The researchers found that dipalmitoyl phosphatidylcholine (DPPC) demonstrated a much more complex phase behavior relative to DLPC. In FY12, Professor Abbott's laboratory discovered that following the initial appearance and growth of homeotropic regions, small planar domains nucleated within, then grew and coalesced over time, nearly covering the entire LC film (see FIGURE 4). Time-dependent data were aligned with what was observed in the optical images: the surface fraction of LC-interface exhibited homeotropic orientation decreases over time while planar anchoring increased.

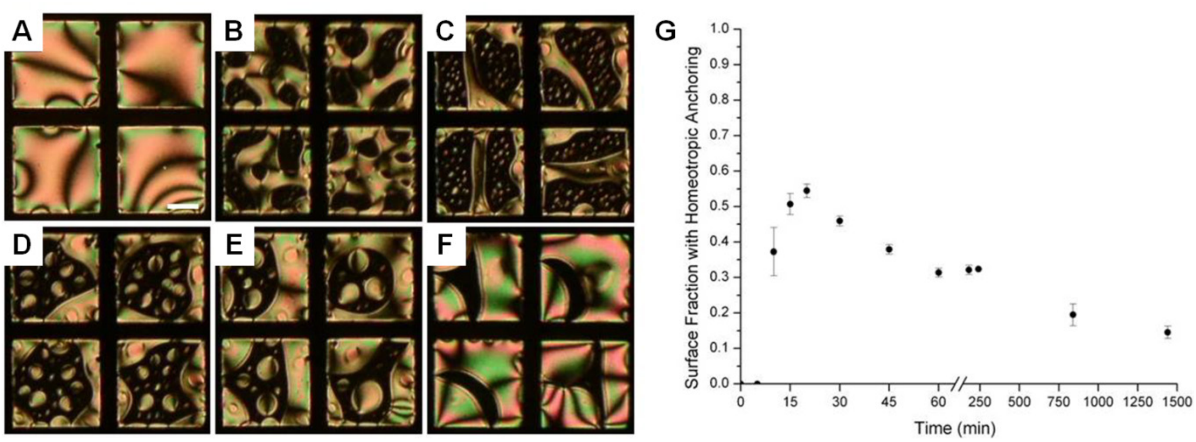

FIGURE 4

Optical images of LC film in a PBS solution. Images were captured at timepoints (**A**) 0 min; (**B**) 10 min; (**C**) 15 min; (**D**) 30 min; (**E**) 60 min; and (**F**) 24 h of contact with 0.1 mM DPPC vesicles. (**G**) The right panel displays a plot of the area fraction of the LC-aqueous interface exhibiting a homeotropic orientation as a function of time.

D. Self-Assembly of Functional Amphiphilic Polymers and Nanoparticles
Professor So-Jung Park, University of Pennsylvania, Single Investigator Award

The objective of this research, led by Professor Park, is to design and synthesize hybrid assemblies that combine the excellent processability and useful mechanical and chemical properties of polymersomes with the unique optical, electrical, and magnetic properties of nanoparticles. Previously, the research the research team fabricated well-defined polymersomes densely loaded with magnetic nanoparticles in the polymersome membrane (superparamagnetic polymersomes). The researchers created the polymersomes through the cooperative self-assembly of amphiphilic polymers of polyacrylic acid and polystyrene (PAA-*b*-PS) and oleic-acid stabilized iron oxide nanoparticles (SEE FIGURE 5A).

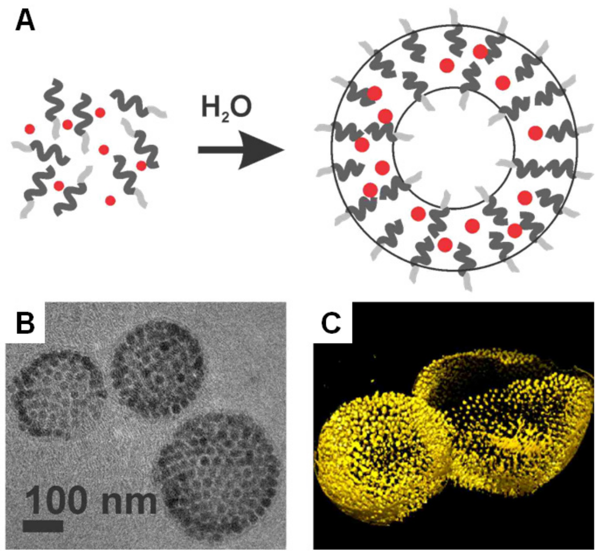

FIGURE 5

Characterization of polymersome structure and properties. Characterization revealed (A) Self-assembly of amphiphilic polymers and nanoparticles into polymersomes, based in part on (B) CryoTEM images of polymersomes loaded with magnetic nanoparticles in the polymersome walls and (C) a TEM tomography image showing the hollow structure of nanoparticle-loaded polymersomes.

In FY12, the researchers further characterized the structure and properties of the polymersome, and investigated the effect of nanoparticle loading on the polymersome formation (see FIGURE 5B-C). The investigators found that the size of polymersomes was controllable by varying the size of nanoparticles. The size-controlled self-assembly of polymersomes was supported by the preferable partitioning of nanoparticles at the inner interface of polymersome membranes and the consequent membrane curvature changes, which is reminiscent of how protein binding and clustering affect the curvature of cell membranes. The nanoparticle-induced self-assembly of polymersomes, therefore, provides a new and reliable way to form size-controlled nanocarriers with the functionality of nanoparticles. The transverse magnetic relaxivity rate (R_2) of the research team's superparamagnetic polymersomes was found to increase with increasing nanoparticle diameter, with the smallest polymersome (241 ± 16 nm) showing R_2 of 555 ± 24 $s^{-1}mM^{-1}$, which is the largest value reported thus far for the size of iron oxide nanoparticles, demonstrating promise for potential future imaging applications.

It is anticipated that these findings will lead to general design principles for the solution-phase self-assembly of nanoparticles and amphiphilic polymers. This research may also allow for the preparation of nanoparticle-encapsulating polymeric materials of desired architectures and properties for applications ranging from nanomedicine to nanofabrication.

E. Discovery of Multi-functional Glass Nanostructure

Professors George Barbastathis and Gareth McKinley, Massachusetts Institute of Technology, ISN (UARC)

Professors Barbastathis and McKinley have discovered a new nanostructured glass surface that simultaneously provides self-cleaning, glare-free, and anti-fogging properties. Although adding specialized coatings to glass can repel water to improve visibility, these coatings have a limited lifetime and cannot simultaneously repel water, prevent fogging, and limit reflective loss. In contrast, certain functionalized surfaces in nature provide unique properties at the macroscale, such as the anti-reflective properties of the moth eye and water-repellant properties of the lotus leaf. Based on these examples in nature, the research team began fundamental studies to understand the mechanical properties of surfaces containing three-dimensional microscopic patterns. The investigators discovered that etching repeating patterns of nanostructured cones onto a glass surface yields properties not possible with surface coatings (see FIGURE 6).

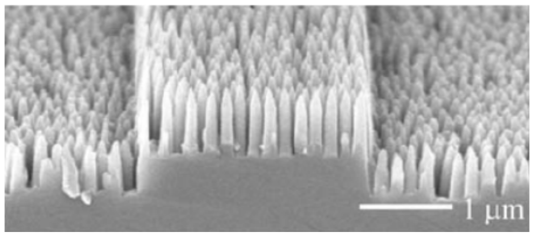

FIGURE 6

Structure of the multifunctional glass surface. The electron micrograph reveals a repeating pattern of nanostructured cones etched onto the glass surface that are approximately 200 nm in diameter and 1 μm in height.

In particular, the new multifunctional glass is almost completely transparent, and the corresponding absence of glare makes it nearly invisible. In addition, the researchers demonstrated that water droplets bounce off the glass surface, fogging is dramatically reduced, and dirt accumulation is minimal (see FIGURE 7).

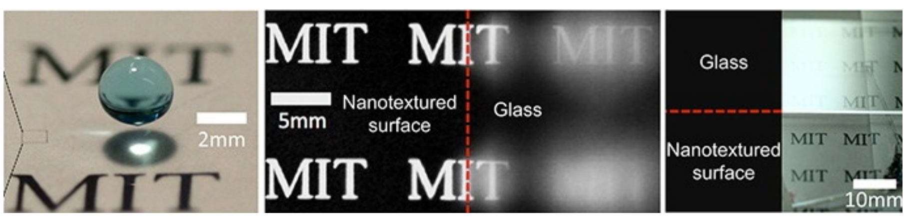

FIGURE 7

Unique properties of the multifunctional glass nanostructure. The nanostructured glass displays many unique properties relative to conventional glass, including superior water repellant (left), anti-fogging (center), and anti-glare (right) capabilities.

If the researchers can improve the stability of these nanostructured cones under environmental conditions then this research may ultimately enable the development of cost-effective and self-cleaning solar cells for remote power production, anti-fogging and anti-glare optics, and windshields and windows with improved performance and safety.

F. Silicon/Carbon Anodes with One-Dimensional Pore Structure

Professor Chunhseng Wang, University of Maryland - College Park, Single Investigator Award

Professor Chunsheng Wang and colleagues have been studying the synthesis and characterization of carbon-tin electrode materials to understand lithium and sodium intercalaction that may ultimately enhance the performance of lithium and sodium batteries.

In FY12, the research team investigated the generation of porous carbon sponges with well dispersed tin nanoparticles using the soft-template technique and achieved a well-controlled pore size (see FIGURE 8). The researchers electrochemically characterized the materials by electrochemically lithiating the Sn to form a Li_xSn alloy. These materials demonstrated excellent cycling stability with the capacity of the porous C/Sn composite in the first delithiation being close to the theoretical capacity of the Sn and carbon composite (see FIGURE 9). The specific capacity of the C/Sn composite gradually decreased to 620 mAh/g during the initial 30 charge/discharge cycles, and then began to increase and stabilized at 1300 mAh/g after 300 cycles. Since the capacity of pure porous carbon continuously increased with the charge/discharge cycles, the initial capacity decline of the porous C/Sn anodes should be attributed to a slight degeneration of the nano-Sn particles. Interestingly, the stabilized capacity of 1300 mAh/g after 300 cycles is much higher than that of the current commercially used graphite and even higher than the theoretical capacity (770 mAh/g) predicted for the composite. A potential long-term application of this research is the development of next-generation batteries with high capacity, high rate capability, and long cycle lives.

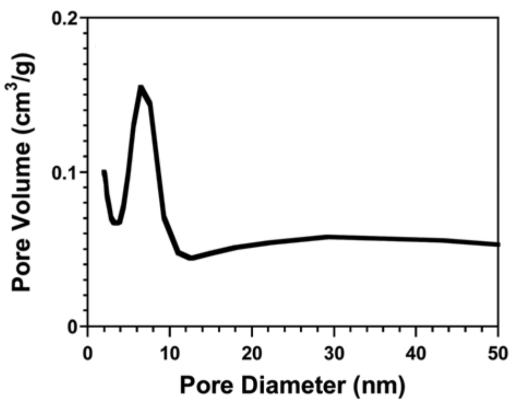

FIGURE 8

Pore-size distribution curve of the porous C/Sn composite. The pore size distribution was analyzed by the Barrett–Joyner–Halenda (BJH) method. The specific surface area of the porous C/Sn composite is $180 m^2/g$ and the pore volume is $0.16 cm^3/g$. The BJH average pore diameter is 7 nm.

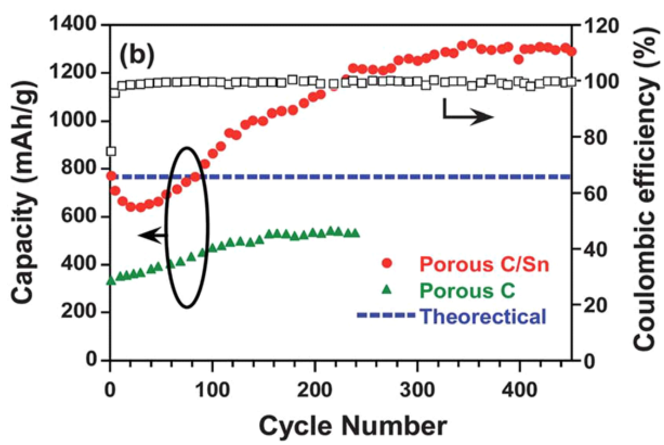

FIGURE 9

Electrochemical Characterizaton of the Porous C/Sn Composite. The plot displays the cycling performance of the porous C/Sn composite (circles), porous carbon without tin nanoparticles (triangles), and the theoretical capacity of the porous C/Sn composite, based on the capacity of pure porous carbon and the theoretical capacity of metallic tin (dashed line). The current density was 200 mA/g, cycled between 0.02 and 3 V.

Professor Wang determined that the increased capacity is due to the reversible decomposition of a gel-like polymer that forms on the C/Sn composite electrode indicating that Sn has a high catalytic activity for the reversible formation of the polymer. This mechanism contributes to an electrode system that is capable of over 450 lithiation cycles, with a reversible capacity above 1300 mAh/g making this an attractive material for use as lithium ion battery anodes.

G. Preparation of Polarized Molecular Hydrogen with Stark-induced Adiabatic Raman Passage

Professor Richard Zare, Stanford University, Single Investigator Award

Dynamics studies for chemical reactions are traditionally carried out under ensemble-averaged (*i.e.*, thermal) conditions. Properties of chemical reactions such as rate constants and activation barriers are then a function of a Boltzmann-averaged thermal distribution of quantum states. Depending on the conditions, the number of available states in the Boltzmann distribution can be quite large.

The objective of this project, led by Professor Zare, is to understand how quantum state selection influences reactive and non-reactive molecular collision dynamics. The investigators have developed a new optical coherent method, called Stark-induced adiabatic Raman passage (SARP), which coherently transfers the population of a molecular ensemble from one quantum state and deposits the entire population into a new, pre-selected rotational-vibrational quantum state. Moreover, the method allows one to select the individual M_J angular momentum sub-level into which to transfer the population. This method allows, for the first time, dynamics studies as a function of the angular momentum vector of a molecule. Such studies will be particularly important for collisional scattering from surfaces, as well as for direction-dependent reaction dynamics. SARP potentially accomplishes complete population transfer to a ro-vibrational state via the Stark-chirped adiabatic passage using nanosecond pump and Stokes laser pulses with a relative delay and an unequal relative intensity.

Professor Zare's laboratory has conducted studies with molecular hydrogen carried out in the collision-free ambience of a supersonically expanded molecular beam (see FIGURE 10). The researchers demonstrated that 60% of the population in the H_2 ($v = 0, J = 0, M = 0$) ground state is transferred to the excited H_2 ($v = 1, J = 2, M = 0$) state using Stark-induced adiabatic Raman passage—a significant improvement from previously recorded few-percent population transfer for isolated homonuclear molecules (see FIGURE 11). Future studies will focus on increasing the efficiency of SARP and investigations of reactive and non-reactive collision dynamics.

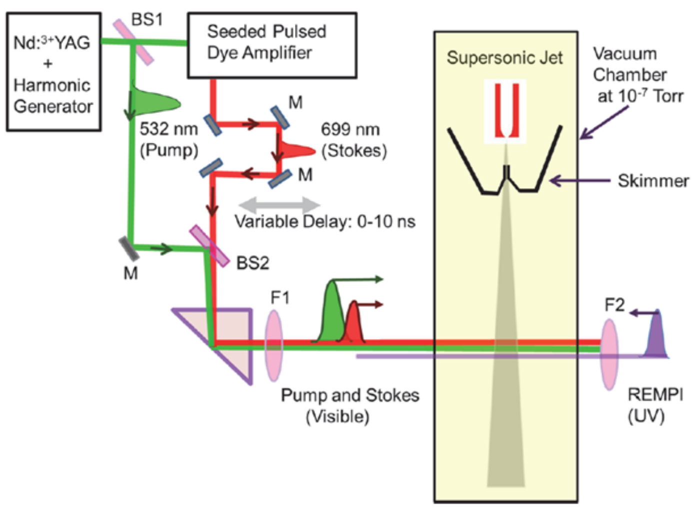

FIGURE 10

Schematic of SARP experiment using partially overlapping pump and Stokes laser pulses. A delay line is formed using mirrors M for temporally-shifted but overlapping pump and Stokes pulses. State detection was accomplished by mass spectrometry with 2+1 resonance-enhanced multi-photon ionization.

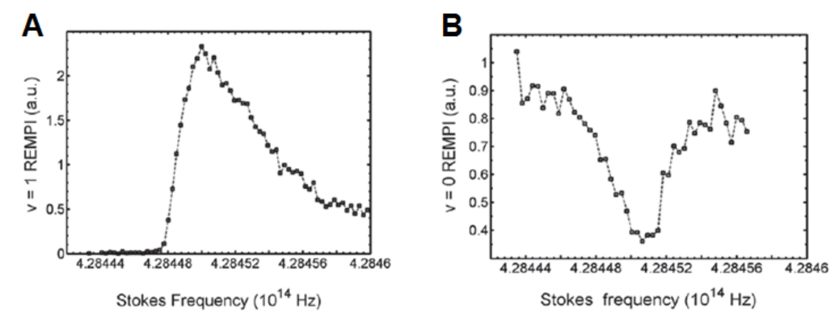

FIGURE 11

REMPI signal versus Stokes laser frequency for the ground state and pre-selected excited state of hydrogen. The Q-branch 2+1 REMPI signal versus the Stokes laser frequency for a relative delay of 6.8 ns between the pump and Stokes laser pulses. (a) REMPI signal from H_2 (v = 1, J = 2, M = 0) state; and (b) REMPI signal from H_2 (v = 0, J = 0, M = 0) state.

H. Decomposition of Pentaerythritoltetranitrate Following Electronic Excitation

Professor Elliot Bernstein, Colorado State University, Single Investigator Award

The objective of this research project is to investigate the molecular relaxation pathways available to polyatomic molecules following electronic excitation under collision-less conditions. In particular, the research focuses on molecules derived from energetic materials. In FY12, the research team completed an experimental and theoretical study of the decomposition of gas-phase pentaerythritoltetranitrate (PETN) [$C(CH_2ONO_2)_4$] following electronic state excitation.

Although PETN has received major attention as an insensitive, high-energy explosive, the mechanism and dynamics of the decomposition of this material have not been clear. The investigators explored the initial decomposition mechanism of PETN using nanosecond energy-resolved spectroscopy and quantum chemical theory, employing the complete active space self-consistent field (CASSCF) methodology. The nitric oxide (NO) molecule was observed as an initial decomposition product from PETN at three UV excitation wavelengths (226, 236, and 248 nm), with a pulse duration of 8 ns. Energies of the three excitation wavelengths coincide with the (0– 0), (0–1), and (0–2) vibrational-electronic bands of the NO $A^2\Sigma^+(\upsilon'=0) \leftarrow X^2\Pi(\upsilon''=0,1,2)$ electronic transition, respectively. A unique excitation-wavelength-independent dissociation channel was observed for PETN, which generates the NO product with a rotationally-cold (~20 K) and a vibrationally-hot (~1300 K) distribution (see FIGURE 12).

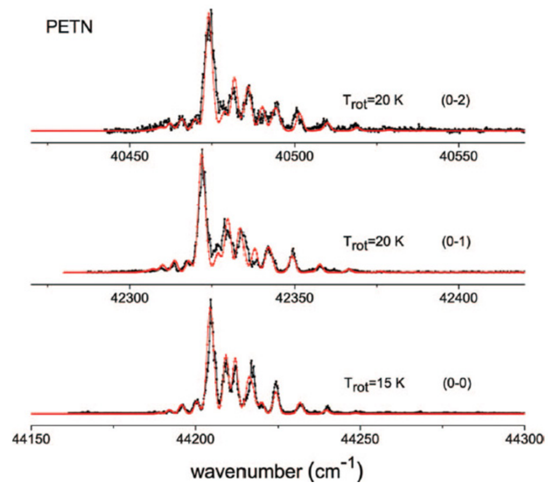

FIGURE 12

Distribution channels of PETN. One-color (1+1) R2PI spectra of the vibronic transitions NO $A^2\Sigma^+(\upsilon'=0) \leftarrow X^2\Pi(\upsilon''=0,1,2)$ of the NO product from the decomposition of electronically excited PETN.

The research team found that potential energy surface calculations at the (CASSCF(6,6)/6-31G(d):UFF) level of theory illustrated that conical intersections play an important role in the decomposition mechanism. Based on these results, electronically-excited S1 PETN returns to the ground state through the (S1/S0) conical intersection, and undergoes a nitro-nitrite isomerization to generate the NO product. The potential energy surfaces are shown in FIGURE 13.

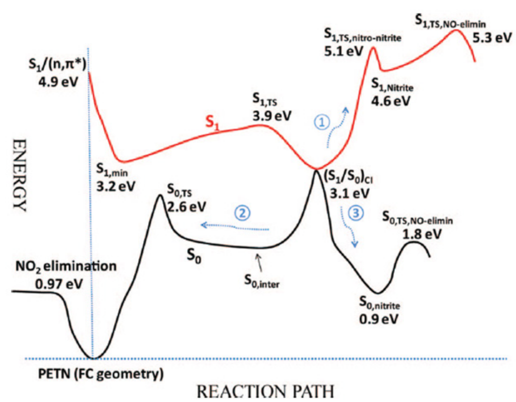

FIGURE 13

Potential energy surfaces of PETN. The schematic one-dimensional projection of the multidimensional potential energy surfaces of PETN was computed at (CASSCF(6,6)/6-31G(d):UFF) level of theory. The labeled relative CASSCF energies of the critical points (minimum, conical intersection, transition state) on the PESs with respect to the FC geometry (S0) are not corrected for zero point energy.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Computational Analysis and Screening of Materials for Capture of Toxic Compounds

Investigator: Professor Randall Snurr, Northwestern University, Single Investigator Award
Recipient: Edgewood Chemical and Biological Center (ECBC)

The objective of the research project, led by Professor Snurr, is to computationally model the interactions and reactions between target molecules and functionalized surfaces. The results of this study could then be used to identify the best sorbent functional groups for removal of toxic industrial chemicals from the air. Professor Snurr has been using quantum mechanical methods to study chemisorption and reactions at ambient conditions on metal-organic frameworks (MOFs), metal oxides, and metal sulfides. The research team found that when various clusters were exposed to ammonia in the presence of water (humidity), the results revealed that metal catechols (metal = Be, Mg, Ca) selectively adsorbed ammonia over water. The observed binding strengths were Be > Mg > Ca. The research by Professor Snurr has transitioned to the ECBC CBR Filtration Team to guide the synthesis of new materials such as MOFs and impregnants with improved filtration properties. Molecular modeling results provided detail on binding positions and interactions with the metal catechols, enabling an optimization of the clusters to provide the strongest binding energy (see FIGURE 14). Similar studies have been carried out with metal sulfide surfaces, but to date only MgS has demonstrated ammonia adsorption over water.

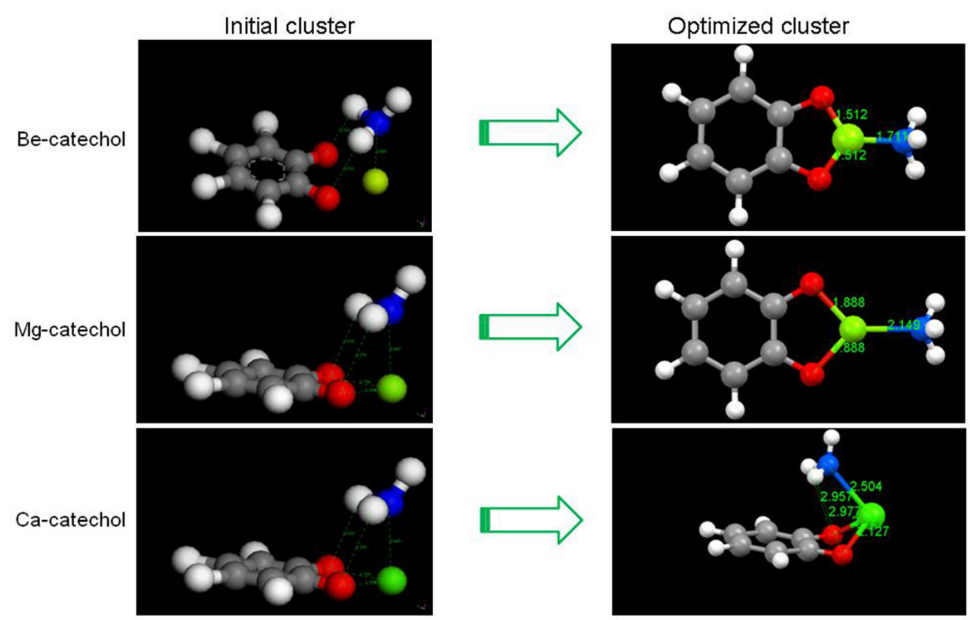

FIGURE 14

Initial and optimized cluster for the strongest binding energy case for selected metal catechols. The metal catechols (metal = Be, Mg, Ca) were found to selectively adsorb ammonia over water

B. Carbon Single-Wall Nanotubes as Electron-Acceptors for Improving Efficiency of TiO_2 Photoexcitation

Investigator: Professor John Yates, University of Virginia, Single Investigator Program
Recipient: U.S. Army Aviation and Missile Research, Development and Engineering Center (AMRDEC)

The objective of this active research project is to investigate the interaction of single walled carbon nanotubes (SWCNTs) with TiO_2 surfaces and determine the effect on charge transport and photoefficiency. Attachment of an electron acceptor molecule, SWNT, to a TiO_2 surface is known to result in electron delocalization and reduction of electron-hole pair recombination. Professor Yates has utilized photoluminescence (PL) to monitor electron-hole pair recombination rate as a function of the SWNT/TiO_2 interface, and has observed a decrease in the PL signal at only 5% loading of SWNTs (see FIGURE 15).

These results have transitioned to a multi-disciplinary research team led by AMRDEC for further investigation of the photocatalytic performance of TiO_2. It is anticipated that placement of TiO_2 near metallic nanostructures will significantly enhance absorption efficiency. The research team will fabricate, characterize, and assess aluminum/TiO_2 core/shell nanoparticles for potential decontamination and bio-remediation technologies.

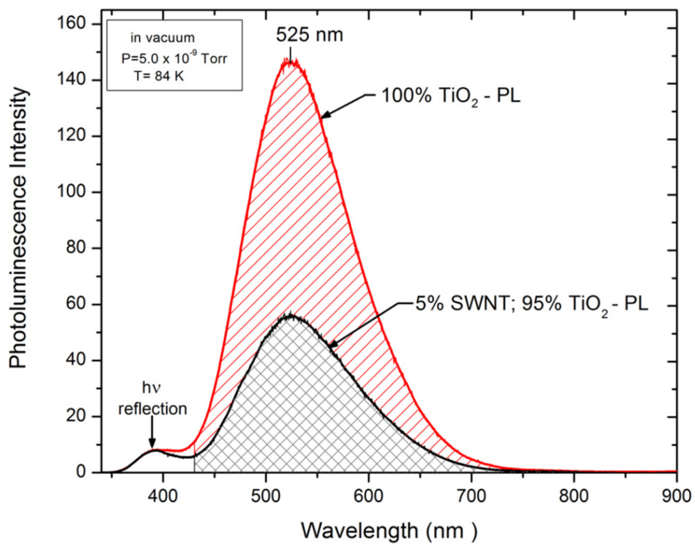

FIGURE 15

TiO_2 photoluminescence effect of interparticle conduction caused by single-wall carbon nanotubes. The plot displays the photoluminescence of 100 % TiO_2 (red spectrum) and 5% SWNT + 95% TiO_2 (black spectrum).

C. Synthesis of Novel Hydrocarbon Soluble Multifunctional Anionic Initiators

Investigator: Professor Jimmy Mays, University of Tennessee at Knoxville, Single Investigator Award
Recipient: National Science Foundation, Partnership for Innovation Program; BBB Elastomers, LLC

Professor Mays and his research team have been using anionic polymerization as a tool to create novel block copolymer architectures, especially branched architectures. They discovered that control of multigraft copolymer architecture can be used to (i) manipulate morphology independent of composition and (ii) to enhance properties of thermoplastic elastomers, including greater elongation at break, more complete elastic recovery, and highly tunable modulus such as in the centipede superelastomer (seE FIGURE 16). Due to the outstanding mechanical properties of this new class of thermoplastic elastomers, the research team has been exploring simpler, one-pot syntheses of the materials. The success of this research effort prompted the formation of a start-up company, BBB Elastomers LLC, which is licensing the technology from the University of Tennessee. The research team has partnered with several small companies to explore potential applications of these novel materials, termed superelastomers. In addition, this effort was recently awarded funding ($600,000 over 2 years) from the National Science Foundation through their Partnerships for Innovation Program to further develop and commercialize this technology.

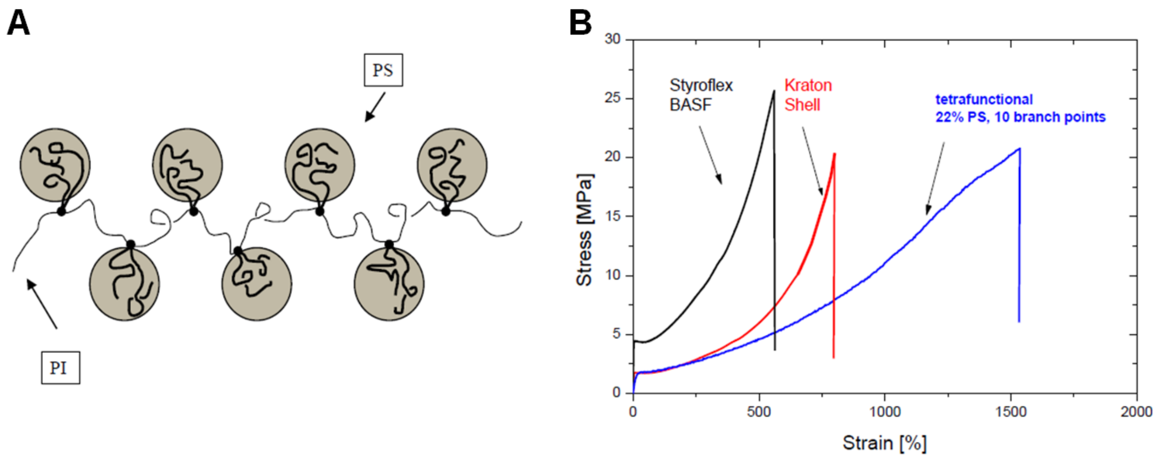

FIGURE 16

Architecture and properties of a centipede superelastomer. (A) Centipede superelastomer with double PS grafts along a PI backbone. This architecture results in better stress distribution and improved elastic recovery. (B) Stress-strain curves of Styroflex, Kraton, and centipede (tetrafunctional) superelastomer.

D. Soldier Power Manager

Investigator: Protonex Technology Corp., SBIR Contract
Recipient: Natick Soldier Research, Development and Engineering Center (NSRDEC); PEO Soldier; Air Force Research Laboratory (AFRL); ONR; United States Marine Corps (USMC)

A previously-completed SBIR contract led by Protonex Technology Corp involved studies of electrolyte membranes and potential uses in powering devices with varying voltage, and current requirements using fuel cells or alternative power sources. Through additional Army and Air Force funding over the following years, combined with DARPA, PEO Soldier, and CERDEC support, this research led to the development, testing, and fielding of the Soldier Power Manager (SPM). The SPM, and the larger-capacity Battlefield Power Manager (BPM) variant, are power-converting devices that can be used to power virtually any piece of portable military/commercial gear from any available battery and to charge any military/commercial rechargeable battery (see FIGURE 17).

FIGURE 17

The Solider Power Manager. This SPM model was field tested in Afghanistan beginning in 2009.

Current military operations rely on batteries to power portable equipment; however, batteries add a significant weight and logistical burden to the Soldier. While significant progress has been made in developing alternative power supplies, including prototype individual fuel cells, batteries are expected to remain the primary power source for the individual Soldier for the foreseeable future. If quiet, compact, lightweight and energy-dense chargers could be developed and made available in sizes appropriate for small-unit operations, then Soldiers could continue using batteries, but reduce their weight burden by a factor of two or more by replacing primary batteries with rechargeable batteries and a high-efficiency battery charger operating on liquid fuels. The SPM fills many of these longstanding Army needs.

Beyond simply a battery charger or a power scavenger, the SPM is capable of actively managing both power inputs and power outputs to ensure compatibility of both the power source and the use device on the fly. As a result, any power source, such as a battery or a photovoltaic source, can be used to power virtually any device carried by the Soldier (see FIGURE 18). Among the capabilities that this provides are the ability to use fuel cells, intermittent sources (*e.g.*, wind, solar), or partially-depleted primary batteries as sources for rechargeable batteries.

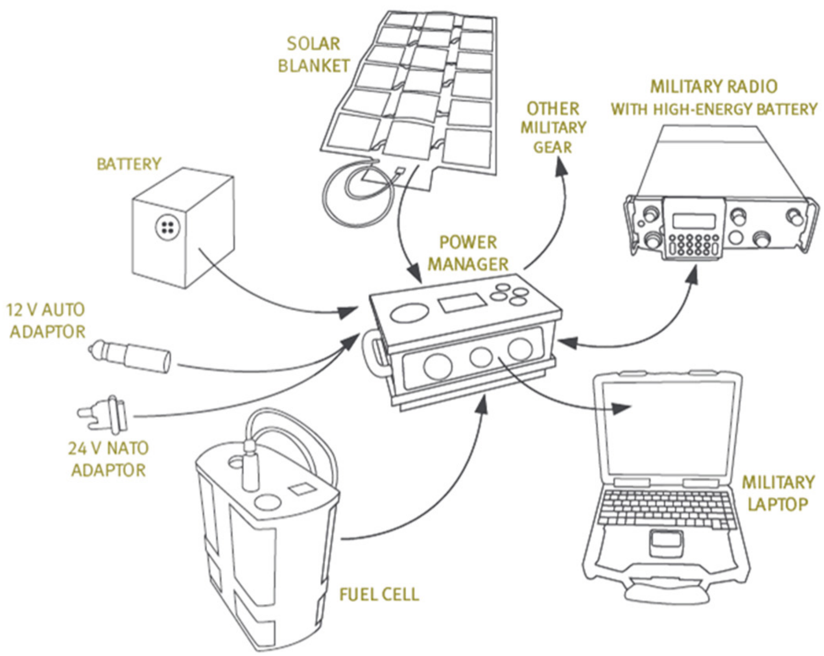

FIGURE 18

Versatility of the SPM and BPM. Using the SPM and BPM, any power source, including batteries, intermittent sources such as wind or solar, or partially-depeleted batteries, can be used to power virtually any device.

The SPM was initially trialed by NSRDEC Fort Dix in Spring 2010, where is was used in a soldier ensemble to monitor and log all power usage throughout the event. The power manager was sent to Iraq and used in a dismounted infantry Limited User Test in late 2010, where it was judged the most valuable new power technology introduced. The successful trial led to an in-theater trial of the SPM in early 2011, where it was again received with enthusiasm, and received excellent After Action Reports.

Based on the results if these trials, PEO-Soldier defined a standard SPM kit, consisting of the power manager itself, and a set of 16 cables and accessories used to charge and power the most commonly used batteries and portable equipment. In addition to follow-on funding by NSRDEC, PEO-Soldier, and others, the power manager also transitioned to other follow-on efforts by a variety of other organizations.

- SPM was used extensively at a FY12 Network Integration Event at Fort Bliss
- AFRL funded more than $3M for the development of derivative power managers specific to AF needs
- USMC funded more than $1M for development of a smaller derivative power manager, and is funding $1.5M for development of a larger derivative power manager
- NSRDEC funded more than $500K for development of a derivative power manager
- ONR funded the $350K development of a specialized cable and accessory kit for use by the Explosive Ordnance Disposal community, and purchased $1.6M of SPM kits in FY12
- USASOC funded development of a SMP kit specific to field medics, and began field-testing kits in FY12
- Navy SEALs purchased derivative SPM kits, which are being evaluated in-theater

E. Portable Fuel Cell System for Logistical Battery Charging
Investigator: Protonex Technology Corporation, OSD Award
Recipient: Army Special Operations Command (SOCOM)

The objective of this research project, led by Protonex Technology Corporation, is to develop a fieldable fuel cell power generator for use as a portable battery charger. The most recent version of this technology is the Protonex M300 (see FIGURE 19). The M300 is a 350-watt fuel cell power system, which uses prepackaged cartridges for methanol/water fuel and has been extensively tested by NSRDEC for safety in use and transport. Each plastic cartridge contains about 1,200 watt-hours of energy, providing equivalent power at about one third the cost, weight, and size of batteries currently in use. The M300 can be used to directly power radios, equipment, or larger battery chargers.

FIGURE 19

The M300 system. This portable fuel cell system provides the ability to charge multiple batteries from a single, lightweight package.

Following the initial development, the M300 was successfully used in training exercises as well as village-sustainment operations in Afghanistan. It is currently in production by Protonex for use by military and other government agencies. The technology transitioned to SOCOM, and with SOCOM funding the M300 was enhanced to permit direct charging of vehicle batteries, like those used in the Special Operations Craft - Riverine (SOC-R) boat (see FIGURE 20).

FIGURE 20

Special Operations Craft - Riverine (SOC-R) boat. In FY12, the M300 was added to the list of installed options on the boat.

The M300 system was able to power each of the SOC-R's power systems and permitted the team to engage in hide missions over eight times as long as possible with existing power systems. Given these successes, SOCOM added the modified M300 to the list of installed option in the boat.

F. Computational Methods for Accurate Prediction of Molecular Interactions in Condensed Phases

Investigator: Professor Christopher Cramer, University of Minnesota, Single Investigator Award
Recipient: U.S. Army Corps of Engineers (USACE), AFRL, NSRDEC, ECBC

Professor Cramer's laboratory has been constructing and validating computational models to predict the vapor pressure of analytes, their solubility in condensed-phase media, and particularly polymer or aqueous polymer solutions, their binding free energies to organic matrices, and the influence of surrounding media or matrices on standard oxidation/reduction potentials and optical properties. Results from Professor Cramer's laboratory have transitioned to software implementing CM*x* charge models and SM*x* solvation models, and made widely available to the modeling community through such freely distributed codes as *AMSOL*, *GAMESSPLUS*, *HONDOPLUS*, *OMNISOL*, and *SMXGAUSS*. The models have also been incorporated into the latest versions of the commercial codes *JAGUAR* and *Q-CHEM*, and the CM5 and SMD solvation models also appear in *Gaussian 09*. Both the models and the codes have found widespread use in the academic computational chemistry community. In addition, the models and codes have transitioned to USACE, AFRL, NSRDEC, and ECBC to enable development of next-generation explosives and propellants, to model interactions of pollutants with the environment and ultimately reduce potential impacts to the soil and air.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Probing Enzyme-Surface Interactions via Protein Engineering and Single-Molecule Techniques

Professor Joel Kaar, University of Colorado - Boulder, YIP Award

The objective of this research project is to design novel single-molecule Förster resonance energy transfer (FRET)-based probes to investigate proteins in near-surface environments at the molecular level. In FY13 protein engineering methods will be used to selectively incorporate non-canonical amino acids at two specific sites in organophosphorous hydrolase (OPH), and fluorescent labels will be conjugated to the new residues via click chemistry. The stability of the orthogonally-labeled OPH in solution will be determined by measuring ensemble-averaged FRET. OPH conformation on model functionalized triethoxysilane surfaces, including methyl, hydroxyl, amino, and poly(ethylene glycol), will be monitored via single-molecule FRET using total internal reflection fluorescence microscopy. Specifically, the team will determine how strongly and in what state the OPH binds (*e.g.*, native, partially folded, or denaturated states). By following the movement of the protein on the surface, surface residence time, adsorption/desorption kinetics, and interfacial diffusion can ultimately be determined.

These novel probes will provide a fundamental understanding of how surface specific, non-covalent interactions influence protein structure and dynamics in real time. In the long term, Professor Kaar's research has broad potential impact in the development of immobilized biocatalysts for decontamination and biosensors, drug delivery, and medical devices.

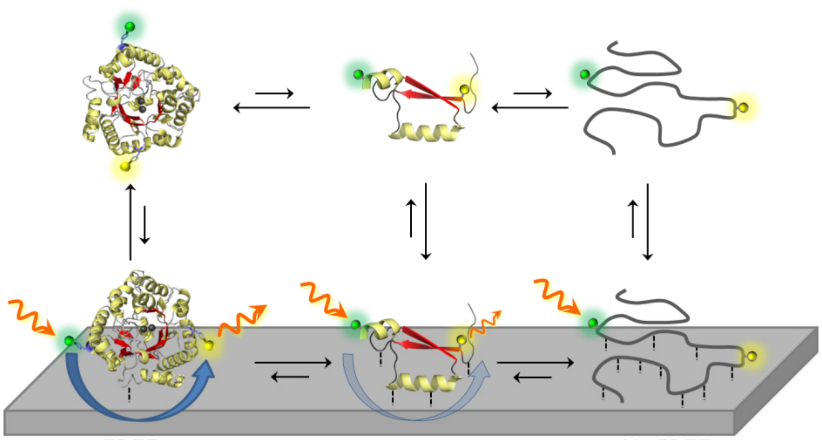

FIGURE 21

Monitoring of the structure of homogenously-labeled OPH on surfaces. It is anticipated that in FY13, the stability and conformation of homogenously-labeled OPH will be monitored using single-molecule FRET using total internal reflection fluorescence microscopy (TIRFM).

B. New Multifunctional Metal-Organic Structures

Professor Craig Hill, Emory University, Single Investigator Award

Professor Hill is investigating new hybrid materials to determine structures that may confer multifunctional adsorbant and catalyst properties. One class of materials that will be investigated is based on polyoxometalate-metal-organic framework (POM-MOF) hybrids. Preliminary data has indicated that the hybrid material has enhanced hydrolytic stability compared to the individual components, as well as higher catalytic activity compared to the free POM catalyst. It is anticipated that in FY13, halide-containing POM-MOFs will be synthesized and characterized, and air-based oxidation of aldehydes, amines, sulfur-containing toxic industrial chemicals (TICs), and chemical warfare agent simulants (CWAs) will be assessed (see FIGURE 22).

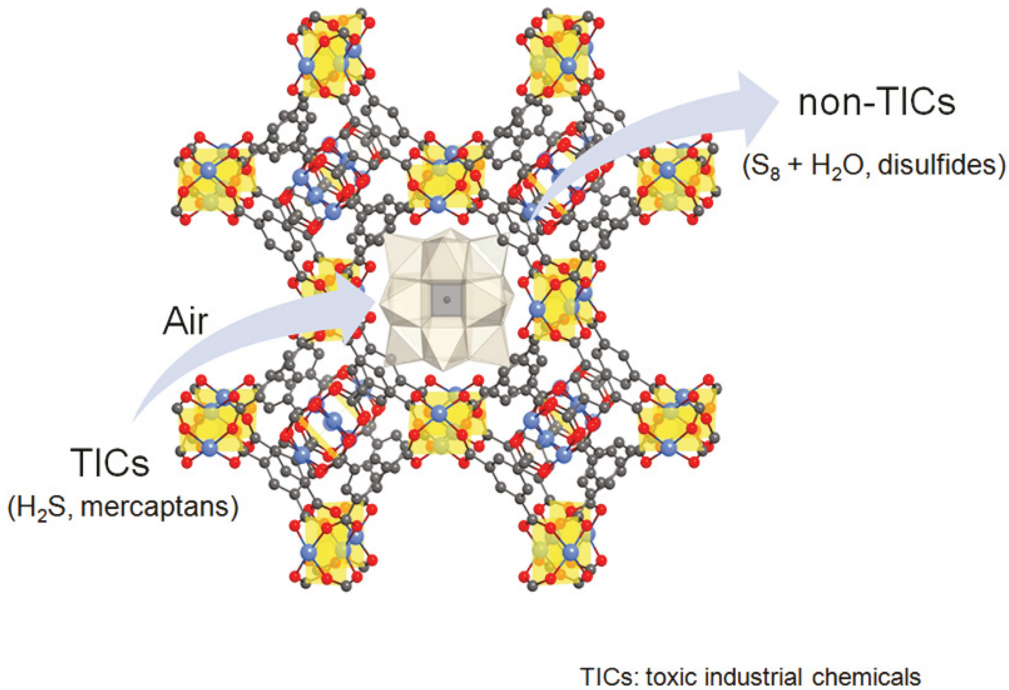

FIGURE 22

POM-MOF hybrid. The image, based on the X-ray crystal structure of a POM-MOF, illustrates the multifunctional properties of POM-MOFs and shows examples of air-based oxidation reactions that can be catalyzed.

Another class of materials that will be pursued is gelating nanoarrays. In these materials, POM catalysts will be covalently linked by various organic connectors into a network that is capable of adsorption and catalytic decontamination of TICs and CWAs (see FIGURe 23). Various methods for POM incorporation into the nanoarray will be explored and mechanistic and kinetic studies will be carried out to fully characterize the catalytic activity and color change associated with simulant exposure. Synthesizing and understanding these multi-functional hybrid materials provides a critical foundation to enable the future development of robust and highly effective catalysts for the detection and decontamination of TICs and CWAs.

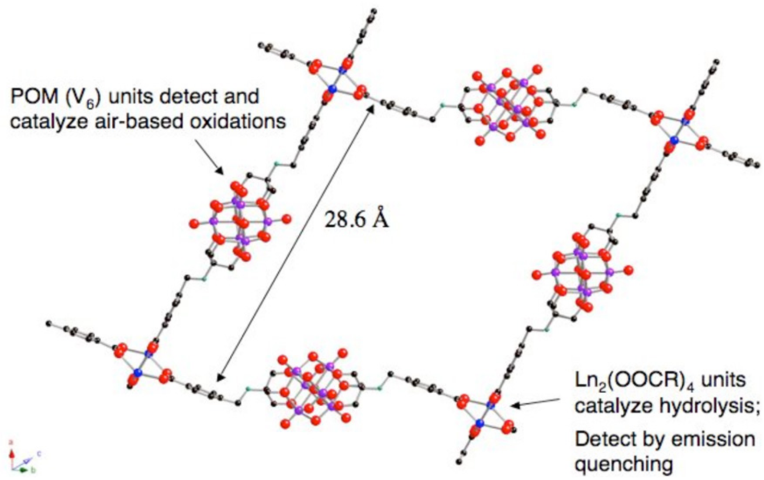

FIGURE 23
Cross-section of pore in gelating nanoarray showing POM-based linker units.

C. Active Microstructured Polymer Systems
Professor Ryan Hayward, University of Massachusetts - Amherst, PECASE Award

The objective of this research project is to understand how the geometry and mechanics of patterned polymer films based on responsive gel materials can be defined to yield structures that undergo controlled transformations between programmed shapes. In FY13, it is anticipated that new approaches will be developed to enable control of both in-plane and through-thickness variations in swelling-induced expansion of gel films. The Hayward laboratory has previously demonstrated control of these two parameters in isolation (see FIGURE 24). However, the ability to independently tune both for the same material system will yield nearly arbitrary control over the three-dimensional shape adopted due to patterned growth. The research team has developed strategies based on modifications to the half-toned lithographic procedure we have recently developed, as well as on multilayer gel films, which will be pursued simultaneously. Furthermore, new material systems will be evaluated that enable the thickness of patterned films to be changed over several orders of magnitude, thereby allowing the strategies demonstrated previously at the millimeter scale to be widely tuned from the macroscopic to the micrometer scale. If successful, this work will establish patterned swelling of thin sheets as a robust and highly versatile method for tailoring three-dimensional shapes adopted by materials.

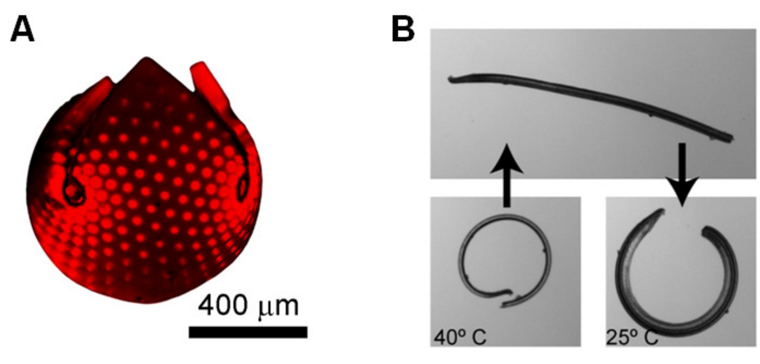

FIGURE 24
In-plane and through-plane variations in swelling-induced gel film expansion. (A) a nearly-closed spherical object formed due to in-plane patterns of growth (defined by the spatial variations in sizes of half-toned dots), and (B) a bilayer film that bends due to differential swelling of the layers represent two mechanisms of swelling-induced gel film expansion.

E. Preparation of Phase-Locked Molecular Quantum States

Professor Richard Zare, Stanford University, Single Investigator Award

The goal of this research is to understand the role of quantum interference in a most fundamental chemical reaction, such as $D + H_2 \rightarrow HD + H$. To pursue this goal, Professor Zare's laboratory, in collaboration with Dr. Nandini Mukherjee, will experimentally prepare a large concentration of H_2, HD, or D_2 molecules in a coherent superposition of rovibrational eigenstates (v, J, M) of the ground electronic surface. Using a new coherent optical technique, developed in the Zare laboratory, called the Stark induced adiabatic Raman passage (SARP), the investigators intend to transfer the entire ($v = 0, J = 0$) ground state population of H_2 or D_2 molecules to a coherent superposition of M states belonging to an excited rovibrational eigenstate ($v > 0, J = 2$), preparing:

$$|\psi(t)\rangle = \sum_M C_M \left|v = 1, J = 2, M\right\rangle.$$

If one could control the phase of the superposition coefficients C_M, then one could control the outcome of a collision experiment. When a large ensemble of target molecules is prepared in a coherent superposition of eigenstates, the ensemble behaves like a multi-slit molecular interferometer in a scattering experiment. Moreover, the investigators will be able to control the multiple slits, thus directing the course of the collision dynamics (see FIGURE 25). Upon demonstration of this goal, SARP will open completely new vistas of reaction dynamics, which will allow the study for the first time of coherent dynamical stereochemistry, where M-state interference instead of M-state averaging occurs.

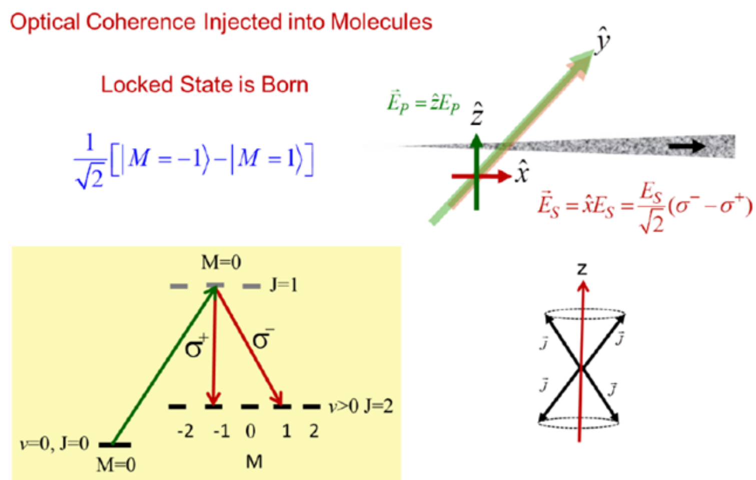

FIGURE 25

A scheme for creating a phase-locked state with M = ± 1. State selection using the S(0) branch Raman pumping of H_2 by combing linearly polarized pump and Stokes laser beams whose vectors are perpendicular to each other. The pump beam is polarized along the z-axis of the laboratory frame. The x-polarized Stokes beam can be expressed as a linear superposition of the right and left circularly polarized beams. The combination of the z-polarized pump with the right (σ^-) or left (σ^+) polarized Stokes beam will enable the selection of $M = \pm 1$ states in $v > 0$, $J = 2$ level, thus preparing the phase-locked state.

F. Understanding Redox Chemistry of Magnesium in Ionic Liquids

Professor Daniel Buttry, Arizona State University, Single Investigator Award

Professor Buttry and colleagues are studying features of the environment of the magnesium ion in ionic liquids that influence the kinetics of the Mg/Mg^{2+} redox couple. In FY12, the team obtained high quality electrochemistry results of Mg/Mg^{2+} in various ionic liquids by determining the sensitivity of the electrochemistry to impurities and other influences of the medium. The team found that water content is a critical element in determining whether or not high quality electrochemistry can be obtained for the Mg/Mg^{2+} redox couple in ionic liquids. When water was present even at very low concentrations, the team observed very poor chemical reversibility of the electrochemical deposition and stripping, which appeared to be due to surface passivation driven by reaction of Mg metal with water, generating an insulating MgO or $Mg(OH)_2$ film.

In FY13, it is anticipated that Professor Buttry will utilize NMR and vibrational spectroscopic methods to characterize the complexation around the Mg^{2+} cation in ionic liquids, study the electrodepoositon of magnesium, and determine the stability of electrodeposition and dissolution of Mg during long-term cycling using different ionic liquids and Mg salts.

G. Mechanochemical Activation of Small Ring Cyclopolymers

Professor Andrew Boydston, University of Washington, YIP Award

The objectives of this project are to synthesize two classes of mechanophores: one in which elongational forces cause bond angle distortions that facilitates mechanically-driven cycloreversion reactions, called "flex-activation" and another in which each arm of a multi-arm star polymer contributes to fragmentation of the central core, called "multi-dimensional activation" (see FIGURE 26). The long-term basic research goals are to understand the effects of polymer structural configurations on mechanochemical transduction efficiency. It is anticipated that in FY13, the research team will synthesize cyclopolymers comprising oxanorbornadiene mechanophores to study "flex-activation" and isocyanurate-based three-arm star polymers to study "multi-dimensional activation." The mechanochemistry of these polymers will be studied using a combination of solution-based techniques such as ultrasonic irradiation, and solid-state experiments involving compression of elastomeric materials containing the mechanophore units. Through their investigations, the research team will determine the extent to which geometric distortion, specifically with the exclusion of bond elongation, can facilitate mechanochemical reactions, and the relative rates of mechanochemical activation in polymers experiencing one- versus two-dimensional elongational forces. If successful, these studies may lead to new materials capable of facilitating energy dissipation, remediation of ballistic impacts, and self-reinforcement for a variety of applications.

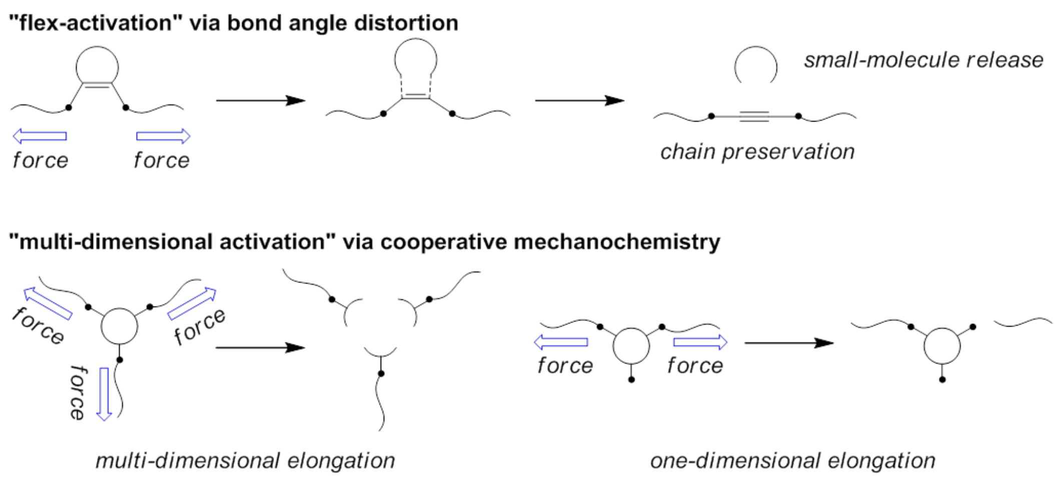

FIGURE 26

Two new classes of mechanophores. The top panel illustrates "flex-activation" for driving a cycloreversion reaction. The bottom panel depicts envisioned modes of reactivity resulting from cooperative two-dimensional activation of a mechanophore, termed "multi-dimensional activation," versus one-dimensional elongation.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

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Program Manager, Polymer Chemistry

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Program Manager, Electrochemistry

Dr. James Parker
Program Manager, Molecular Structure and Dynamics

Dr. Dawanne Poree
Contract Support, Polymer Chemistry

Ms. Wendy Mills
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Contract Support, Institute for Soldier Nanotechnologies and Institute for Collaborative Biotechnologies

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Administrative Specialist

Ms. Jennifer Eaton
Contract Support

Ms. Nicole Elliot-Foster
Contract Support

CHAPTER 4: COMPUTING SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2012* is to provide information on the programs and basic research efforts supported by ARO in FY12, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Computing Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY12.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of the ARO Computing Sciences Division is to provide increased performance and capability for processing signals and data, extract critical information and actionable intelligence, improve decision making, and achieve information dominance to enhance the warfighters' situation awareness. The Division supports basic research efforts to advance the Army and nation's knowledge and understanding of the fundamental principles and techniques governing intelligent and trusted computing systems. More specifically, the Division supports basic research to establish new computing architectures and models for intelligent and trusted computing, to create novel data fusion and extraction techniques for efficient information processing, to create new capabilities in social informatics, and to build resilient computing systems for mission assurance. The results of these research efforts will help gain scientific understanding and keep the U.S. at the forefront of computing sciences research.

2. Potential Applications. In addition to advancing worldwide knowledge and understanding of computing science, the research efforts managed in the Computing Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. This program identifies and addresses the Army's critical basic research problems in the computing sciences where progress has been inhibited by a lack of novel concepts or fundamental knowledge. Computing science is pervasive in nearly all Army systems, particularly Command, Control, Communications, Computing, Intelligence, Surveillance, and Reconnaissance (C4ISR) systems. The number of information sources on the battlefield will grow rapidly; computing and information science research must provide the technology to process this in real-time and ensure that Soldiers and commanders do not experience information overload that could adversely affect their ability to make decisions. Also, in spite of the increased complexity of future battlefield information systems, dependence on them will only increase, therefore they must be extremely reliable and secure. For this reason, computing science is a key technology underpinning future Army operations. Research in this program has application to a wide variety of developmental efforts and contributes to the solution of technology-related problems throughout the Army's Future Force operational goals.

3. Coordination with Other Divisions and Agencies. The Division's research investment strategy is coordinated with partner disciplines and computer scientists at ARO, other directorates within ARL, other Army agencies, and related programs in other DoD and Federal agencies. The Division research portfolio is supported by Army basic research Core funding with substantial additional resources from the Assistant Secretary of Defense for Research and Engineering [ASD(R&E)], including the Multidisciplinary University Research Initiative Program (MURI), and from other agencies, such as the Defense Advanced Research Projects Agency (DARPA.

To effectively meet Division objectives and to maximize the impact of potential discoveries for the Army and the nation, the Computing Sciences Division frequently coordinates and leverages efforts within its Program Areas with Army scientists and engineers and with researchers in other DoD agencies. In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the ARO Life Sciences Division include promoting research to investigate effective human-computer communication mechanisms and developing new metrics and benchmarks for social media analysis. The Division also coordinates efforts with the Network Sciences Division to explore new techniques for robust and resilient mobile ad hoc networks, to establish adversarial models for effective cyber defense, and to investigate fundamental principles for trusted social computing. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas. Each of the Program Areas within the Division balances opportunity-driven research with high risk, high-payoff scientific exploration and needs-driven efforts that look for solutions to the near-term needs of the warfighter.

B. Program Areas

To meet the long-term program goals described in the previous section, the Computing Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY12, the Division managed research efforts within these four Program Areas: (i) Information Processing and Fusion, (ii) Computational Architectures and Visualization, (iii) Information and Software Assurance, and (iv) Social Informatics. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Information Processing and Fusion. The goal of this Program Area is to understand the fundamental principles and to establish innovative theories for data processing, information extraction, and information integration toward real-time situational awareness and advanced targeting. There are three thrusts for this program area: (i) foundations of image and multimodal data analysis, (ii) data and information fusion, and (iii) active and collaborative sensing. With the ubiquitous availability of data acquisition capabilities in future military operations, effective data and information processing is of increasingly critical importance to defense missions. This program emphasizes mathematical theories, methodologies and algorithms for image processing, image understanding, video-based tracking, and data/information fusion. Research efforts support the development of novel representations of multimodal data to enable the understanding of multimodal sensor data and contextual information. Also supported is research on detection of events, actions, and activities to extract activity-based intelligence, especially when the events are rare and no extensive training data is available. Potential applications include detection of improvised explosive devices and persistent surveillance.

The increased capability of electronic systems and the proliferation of sensors are generating rapidly increasing quantities of data and information to the point that system operators and commanders are overwhelmed with data and saturated with information. An area of increasing importance is data and information integration or fusion, especially fusion of data from disparate sensors and contextual information. Research activities address several basic issues of data fusion, including information content characterization of sensor data, performance modeling, and the value of information.

2. Computational Architectures and Visualization. The two main Thrusts of this Program Area are Computational Architectures (CA) and Visualization (V). The goal of the CA Thrust is to discover new effective architectures, computational methods, and software tools for future computing systems with special emphasis on the effect that the technological shift to heterogeneous, multi-core processors will have on newly-developed systems. The goal of the V Thrust is to make very large simulations and the visualization of massive data sets more computationally efficient and more interactive for the user. An overarching theme for both Thrusts is the efficient managing and processing of massive data sets. This is due to the fact that the Army's ability to generate data of all types from the battlefield to the laboratory far outpaces the Army's ability to efficiently manage, process, and visualize such massive amounts of information. The CA Thrust attempts to address this issue by investigating innovative architectural designs of both hardware and software components and their interfaces. The V Thrust addresses the issue by investigating innovative algorithms to render massive data sets and/or massive geometric models and to perform large scale simulations of importance to the Army.

The long-term payoffs of the CA Thrust for the Army include new computer modeling and design concepts (or paradigms) as well as software libraries that take advantage of these new multi-core processors and that are scalable (usable on large-scale complex problems and able to handle massive amounts of data) and accurate (precise enough to predict and detect phenomena of interest) for both the laboratory and the battlefield. A payoff associated with the V Thrust is the development of more efficient, interactive, and physically realistic battlefield, training, and scientific simulations.

3. Information and Software Assurance. The goal of this Program Area is to understand the fundamental principles of robust and resilient systems that can enable the corresponding functions to be sustained under adversarial conditions. The studies guided by this program will enable and lead to the design and establishment of trustworthy computing and communication, regardless of threat conditions. The ARO program on Information Assurance currently has two major Thrust areas: (i) Highly Assured Tactical Information and (ii) Resilient and Robust Information Infrastructure. The goal of the Highly Assured Tactical Information Thrust is to gain new scientific understandings for trustworthy tactical communications and for establishing fundamental principles and models for robust and resilient tactical information processing. The Resilient and Robust Information Infrastructure Thrust promotes research efforts on cyber situation awareness theory and framework, which combines intrusion prevention, detection, response, and recovery together and establishes fundamental scientific principles for building mission-sustaining information systems (*e.g.*, software/hardware, computing/communication systems).

Within these research areas, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. Research in the Resilient and Robust Information Infrastructure Thrust is focused on exploring and establishing resilient computing and survivability principles, and understanding system trade-off among performance, resiliency, and, survivability. The Highly Assured Tactical Information Thrust may lead to the development of novel situation awareness theories and techniques to obtain an accurate view of the available cyber-assets, to automatically assess the damage of attacks, possible next moves, and impact on cyber missions, and also model the behavior of adversaries to predict the threat of future attacks on the success of a mission. The warfighters must have unprecedented situational awareness (including enemy and friendly awareness) at all times. Information assurance must address the delivery of authentic, accurate, secure, reliable, timely information, regardless of threat conditions, over heterogeneous networks consisting of both tactical (mobile, wireless) and fixed (wired) communication infrastructures.

4. Social Informatics. The goal of this Program Area is to quantify technology-based social interaction phenomena, to develop metrics for the quantified phenomena and to develop forensic and predictive analytical and computational models based on these quantifications and metrics. This new Program Area was established in late FY11. The objects of interest will generally be social phenomena (social groups/structure) and socio-cognitive phenomena (human intentions in a social context). The quantification and metrics of interest to this program are those based on domain-scientific principles of social and socio-cognitive science that are at the same time mathematically consistent and computationally feasible. Research of interest to the Program Area includes quantified, analysis-based research about technology-based social interaction phenomena in the following two Thrusts: (i) Quantification and Metrics and (ii) Analytical and Computational Models. Understanding and being able to predict technology-based social networking and social media phenomena will enhance defense in current and future asymmetric conflict, especially in the technology-based component of that defense.

The Quantification and Metrics Thrust focuses on the extraction of information from social media and requires the quantification of and metrics for these phenomena. The metrics by which one measures distance between phenomena will likely be nontraditional. Quantification and metrics need to extend to reliability and accuracy, since falsification and deception are often present at the level of the input into the social medium by a human being. Processing of soft information such as text and voice has been extensively investigated, but insufficiently in the social context that often determines meaning and that can resolve ambiguities.

The Analytical and Computational Models Thrust focuses on analytical and computational models for both forensic and predictive purposes. These models complement the qualitative models of much of sociological research, especially those in the less-investigated area of weak-tie sociology that is important for technology-based social interaction. The models are dependent on the quantification and metrics discussed above as well as on quantitatively expressed social and socio-cognitive principles. Falsification and deception may not be identifiable at the level of input information and may have to be identified by the model. The models should be embedded in applicable sociological and socio-cognitive theory and should not simply be computationally descriptive of social-media phenomena and/or be based only on analogies to physical phenomena.

C. Research Investment

The total funds managed by the ARO Computing Science Division for FY12 were $30.0 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY12 ARO Core (BH57) program funding allotment for this Division was $2.6 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $9.3 million to projects managed by the Division. The Division also managed $1.6 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $2.0 million for contracts. The Institute for Creative Technologies received $14.3 million. Finally, $0.2 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY12 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research projects. Research projects are developed by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts.

The following subsections summarize projects awarded in FY12 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY12, the Division awarded 14 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to discover new compressive sensing techniques, determine new algorithms to detect emergent anomalous spatio-temporal behavior in social networks, and to establish a framework for analyzing and quantifying cyber defense under dynamic environments. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Robert Kirby, University of Utah; *Visualization of Discontinuous Galerkin Based High-Order Methods*
- Professor Partha Pande, Washington State University; *Understanding Millimeter-Wave Wireless Network-on-Chip Architectures*
- Professor Fauzia Ahmad, Villanova University; *Multipath Exploitation and Knowledge Based Imaging Using Compressive Sensing*
- Professor Biao Chen, Syracuse University; *Value Driven Information Processing and Fusion*
- Professor Haibo He, University of Rhode Island; *Incremental Learning and Fusion on Multi-Modal Sensor Data Streams*
- Professor Gonzalo Arce, University of Delaware; *Classification and Recognition Based Compressive Spectral Imaging*
- Professor Alan Yuille, University of California - Los Angeles; *Hierarchical Models for Image Labeling*
- Professor Alfred Hero III, University of Michigan - Ann Arbor; *Emergent Spatiotemporal Behavior in Social Networks*
- Professor David Lazer, Northeastern University; *Weak Ties, Social Media, and Flash Movements*
- Professor Murat Kantarcioglu, University of Texas at Dallas; *A Game Theoretic Framework for Adversarial Classification*
- Professor Kang Shin, University of Michigan - Ann Arbor; *Secure Detection of Mobile Small-Scale Primary Users in Cognitive Radio Networks*
- Professor Yiorgos Makris, University of Texas at Dallas; *Trusted Module Acquisition Through Proof-Carrying Hardware Intellectual Property*

- Professor Ing-Ray Chen, Virginia Polytechnic Institute and State University; *Hierarchical Trust Management of Community of Interest in Heterogeneous Mobile Networks*
- Professor Radha Poovendran, University of Washington; *Modeling and Analysis of Deception Mechanisms in Networks*

2. Short Term Innovative Research (STIR) Program. In FY12, the Division awarded 7 new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to discover novel machine learning methodologies for modeling spatiotemporal dynamics in video, to discover principles for guiding new malware detection methods for mobile devices, and to explore new methods for sensor selection to improve performance of target tracking in sensor networks. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Yun Fu, State University of New York (SUNY) at Buffalo; *Modeling Spatiotemporal Contextual Dynamics with Sparse-Coded Transfer Learning*
- Professor Qiang Ji, Rensselaer Polytechnic Institute; *Modeling Interval Temporal Dependencies for Complex Activities Understanding*
- Professor Qiang Le, Hampton University; *Sensor Management for Target Tracking in Multi-Modal Sensor Networks*
- Professor Vinod Ganapathy, Rutgers, The State University of New Jersey - New Brunswick; *Detecting Malicious Software*
- Professor Michael Jensen, Brigham Young University; *Data-Dependent Fingerprints*
- Professor Gang Qu, University of Maryland - College Park; *Creating Digital Fingerprints in Finite State Machines*
- Professor Neal Patwari, University of Utah; *Assessing RF Environment Using Transceivers in Motion*

3. Young Investigator Program (YIP). In FY12, the Division awarded three new YIP projects. These grants are driving fundamental research, such as studies to create a statistical analysis and data collection framework to identify deviant behavior in social media networks, establish new algorithmic approaches for resilient and robust computing, and to determine a formal foundation for physical disorder-based security primitives. The following PIs and corresponding organizations were recipients of the new-start YIP awards.

- Professor Tyler McCormick, University of Washington; *Understanding Social Media Networks*
- Professor Rakesh Kumar, University of Illinois - Urbana; *Fundamental Algorithmic Techniques for Resilience*
- Professor Farinaz Koushanfar, William Marsh Rice University; *Physical Unclonable Functions Untangled: Novel Analysis, Protocols, and Implementation*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY12 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences or workshops.

- *2012 International Conference on Social Computing, Behavioral-Cultural Modeling, and Prediction*; College Park, MD; 3-5 April 2012
- *ARO Workshop on Sensor Information Estimation and Exploitation*; Ann Arbor, MI; 15-17 April 2012
- *Big Data at Large: Applications and Algorithms*; Durham, NC; 14-15 June 2012

5. Special Programs. In FY12, ARO Core Research Program funds provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded 5 new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Computing Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Sensor Network Structure for Dependable Fusion. This MURI began in FY07 and was awarded to a team lead by Professor Shahi Phoha at the Pennsylvania State University. The goal of this research is to develop theoretical foundations and validation to address: (i) proliferation of multi-source sensor data due to DoD's tactical shift to network-centric warfare, (ii) urban area monitoring demands for fighting the asymmetric warfare, and (iii) collaboration needs of future military devices or systems.

The emphasis of these studies is on dynamically-adaptive fusion, which enables construction of sensor networks to support dependable information fusion. The research is based on fundamental concepts of space-time neighborhoods in the vicinity of events, symbolization, nonlinear filtering, and computational geometry to formulate rigorous mathematical methods and algorithms to capture the causal dynamics of distributed information fusion processes in urban sensor networks. These studies could potentially lead to robust and resilient sensor networks for monitoring a given urban area in support of defense missions.

2. Understanding Brain-to-muscle Signaling. This MURI began in FY08 and is led by Professor Gerwin Schalk at Albany Medical College. The objective of this MURI is to understand the mechanisms of brain nerve-to-muscle signaling so that brain signals can be exploited to provide an accurate, real-time assessment of the user's intentional focus, eye movements, and imagined speech. This MURI is co-managed by the Life Sciences Division, and examines similar, but complementary concepts as the Life Sciences Division MURI led by Professor Michael D'Zmura (see CHAPTER 7: LIFE SCIENCES DIVISION).

This MURI focuses on three research areas: (i) the methods and algorithms for decoding brain signal recordings of brain cortical activity during covert speech, (ii) communication of covertly-spoken thought using an augmented-reality audio system with a spatialized speech channel, and (iii) exploitation of brain signals for interface design and the development of algorithms using only non-invasive recordings. This research could potentially lead to a silent, brain-based communication and orientation system to provide a communication channel between humans and computers and improved human-computer interfaces.

3. Principles for Robust and Resilient Tactical Mobile Ad-hoc Networking Systems (MANETs). Two MURIs in this topic area began in FY08, with one research team led by Professor Vigil Gligor at the University of Maryland and the other led by Professor Prasant Mohapatra at the University of California, Davis. The goal of these MURIs is to use insights from multiple disciplines, such as network science, engineering, mathematical science, and systems theory to develop the analytical models, tools, and mathematical representations for assessing, prescribing, analyzing, and predicting the behavior of robust and resilient mobile ad hoc networks under a total threat spectrum, and to provide security, robustness and resilience for tactical MANETs.

These efforts focus on addressing one of the main research challenges of the Computing Sciences Division, Information and Software Assurance Program, Highly Assured Tactical Information Thrust. The research teams will investigate: (i) mathematical representations and tools for modeling and analysis of resilient and robust MANETs, (ii) theories that explain the MANET layered architecture and cross layer interaction (both intentional and unintentional), (iii) theories that elucidate the relationships and understanding of the trade-offs between fragility and robustness, (iv) interaction of networks, particularly, MANETs, low energy wireless sensor networks, and wired communications networks, and (v) design of MANET survivability algorithms and architecture, resilient management mechanisms, threat spectrum analysis for information applications on MANETs, fault tolerant and attack resilient communication protocols, survivability requirements engineering, and security and trustworthiness in MANETs.

The team led by Professor Gilgor is using a research approach based on the fundamental principles of active protocol monitoring for performance, stability and adversary handling, of employing communication channel diversity for robust end-to-end operation in the face of failures and deliberate attacks, and of exploiting cross-layer interaction for predicting the effects of performance changes caused by layer-specific failures and attacks on end-to-end MANET operation. Design and analysis techniques found in network theory, statistics, game theory, cryptography, economics and sociology, and system theory are used to develop, design and analyze models, tools, and mathematical representations for predicting performance and prescribing resilient, secure MANETs.

The team led by Professor Mohaptra is developing a cross layer architecture that provides comprehensive security and resilience. Depending on the services desired the new architecture will be able to adaptively provide the right trade-offs between performance, security and fault-resilience. The team currently undertakes three parallel but inter-coupled tasks geared towards (i) performing measurements via real deployments and enhancing understanding of layer dependencies and vulnerabilities in mobile ad hoc networks, (ii) building analytical models to characterize the behavioral nuances of these networks, and (iii) designing new cross layer protocols that protect against vulnerabilities and provide the desired robustness.

4. Cyber Situation Awareness. Two MURIs in this topic area began in FY09, with one research team led by Professor Richard Kemmerer at the University of California, Santa Barbara, and the second team led by Professor Peng Liu at the Pennsylvania State University. The goal of these projects is to explore cyber situation awareness theories and frameworks. In the long term, this research may ultimately provide more effective defense against cyber attacks, and may lead to new algorithms and systems that can assist human analysts' cognitive situation-awareness processes and decision making.

Complete situation awareness leads to effective defense and response to cyber attacks, especially those launched by adversaries with state sponsorship. The ability to extract critical information and build intelligence leads to a better capability in attack prevention, detection and response and in sustaining critical functions and services. The team is focusing research in the following key areas: (i) situation (knowledge and semantics) representation and modeling that support multi-level abstraction and transformation of data to intelligence, (ii) information fusion that can effectively combine raw and abstracted intelligence of different confidence levels to support optimal response, (iii) uncertainty management and risk mitigation through probabilistic hypotheses/reasoning and sensitivity control, which uses multi-level statistical analysis to manage incomplete and imperfect situation information, (iv) leverage cognitive science understandings to automate human analysts' cognitive situation-awareness processes (to recognize and learn about evolving situations, to create automated hypothesis generation, and to reason in both pre-attack planning and post-attack response), (v) develop a new framework unifying perception, comprehension, and projection functions and integrating situation recognition, impact assessment, trend analysis, causality analysis, and situation response together, (vi) advanced mathematic models for quantitative analysis and assessment of system assurance, and (vii) rapid repair, recovery and regeneration of critical services and functions as part of automatics response to attacks.

In this research, novel situation awareness theories and techniques are being investigated to obtain an accurate view of the available cyber-assets and to automatically determine the assets required to carry out each mission task. A proposed situation awareness framework that ties together cyber assets, cyber configuration, attack impact, threat analysis and situation visualization under cyber mission is illustrated in FIGURE 1.

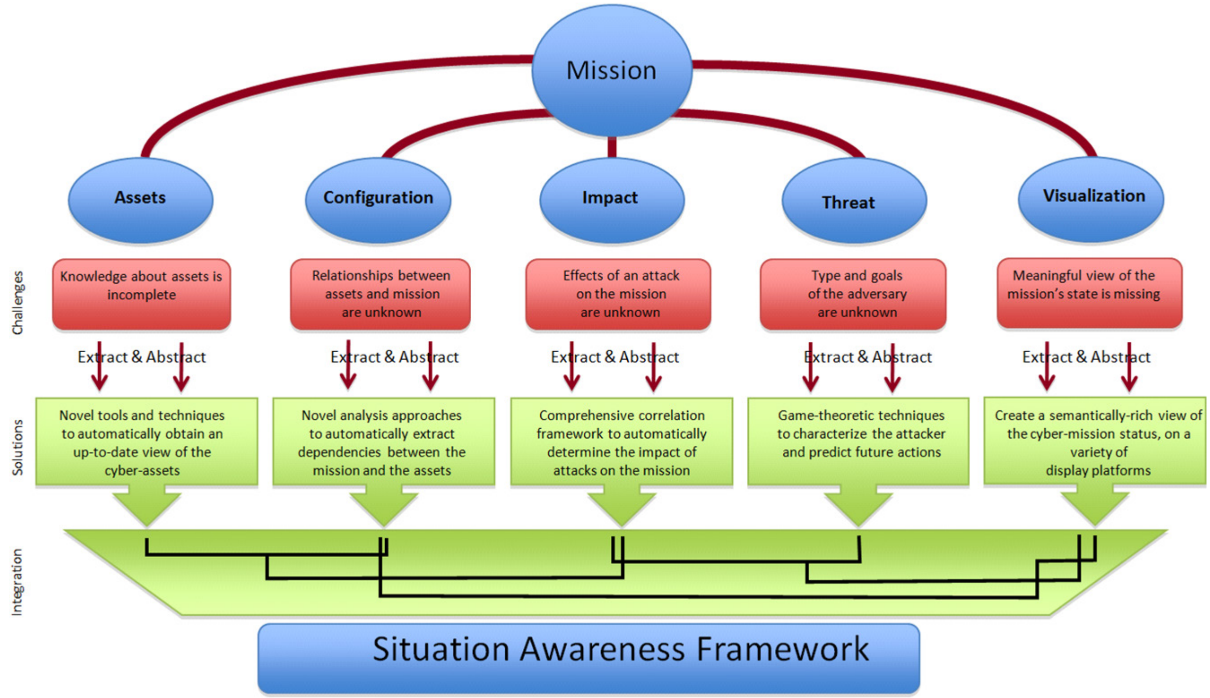

FIGURE 1

Cyber situation framework for attack analysis, prediction, and visualization. This framework incorporates cyber assets, cyber configuration, attack impact, threat analysis, and situation visualization.

5. Principles of Object and Activity Recognition Using Multi-Modal, Multi-Platform Data. This MURI began in FY09 and was awarded to a team lead by Professor Richard Baraniuk at Rice University to gain a fundamental understanding of opportunistic sensing and to create a principled theory of opportunistic sensing that provides predictable, optimal performance for a range of different sensing problems through the effective utilization of the available network of resources.

This project includes four focus areas, aimed at developing a theory of sensing that can provide: (i) scalable sensor data representations based on sparsity and low dimensional manifolds that support dimensionality reduction through compressive sensing, (ii) scalable data processing for fusing image data from multiple sensors of potentially different modalities for activity detection, classification, and learning, (iii) opportunistic optimization, feedback, and navigation schemes for multiple mobile sensor platforms that adaptively acquire data from new perspectives to continuously improve sensing performance, and (iv) experimental validation on real-world inputs, such as multi-camera video, infrared, acoustic, and human language.

6. Value-centered Information Theory. This MURI began in FY11 and was awarded to a team lead by Professor Alfred Hero III at the University of Michigan. The objective of this MURI is to lay the foundation for a new information theory that applies to general controlled information gathering and inference systems and accounts for the value of information. The theory will be built on a foundation of non-commutative information theory, free probability theory, differential geometric representations of information, and the theory of surrogate information measures. This theory will improve the scientific understanding of the fundamental limits of performance and create better algorithms for extracting and exploiting information in distributed sensor systems.

In this effort, research focuses on multiple-modality multiple-sensor fusion problems that use consensus fusion, contextual graphical models, gossip algorithms, and likelihood maps to aggregate information for tracking, surveillance, and other tasks. Topics of interest include resource management in adversarial environments, mobile sensors, and multistage mission planning. Emphasis is placed on creating a powerful theory of actionable information that accounts for value of information and the economic costs of deploying or maneuvering sensors to achieve a particular mission objective. The research comprises three inter-related research themes that collectively address the most critical research challenges in distributed sensing. These thrusts are: (i) information-driven structure learning and representation, (ii) distributed information fusion, and (iii) active information exploitation for resource management. An end-to-end framework will be created that will result in better raw sensor data acquisition and processing, more accurate multi-target tracking, and improved fusion.

C. Small Business Innovation Research (SBIR) – New Starts

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY12, the Division managed two new-start Phase II SBIR contracts, in addition to active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications, including the development of new anti-phishing technology and security products to protect information systems from phishing attacks and cyber intrusions.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY12, the Division managed three new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of one Phase I contract, and two Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications, including the development of fast, efficient and reliable algorithms for imaging change detection, methods and algorithms that effectively utilize hyper/multi-spectral LADAR for improved remote sensing capabilities, and new technology for passive state detection and characterization of soldier stress for automated training applications and improved human-machine interface design.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY12, the Division managed one new ARO (Core) HBCU/MI project, and six new REP awards. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY12.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY12, the Computing Science Division managed eleven new DURIP projects, totaling $1.8 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of sensing through dynamic control of mobile and stationary sensors, large-scale information fusion and data mining, and improved security and performance of large-scale computing infrastructures.

H. University Affiliated Research Center (UARC): Institute for Creative Technologies (ICT)

The ICT, located at the University of Southern California (USC), is a partnership with the Army, the entertainment community, and academia. The objective of the ICT is to conduct basic and applied research and advanced technology development in immersive technologies to advance and maintain the state-of-the-art for human synthetic experiences that are so compelling the participants will react as if they are real. Established in 1999, the ICT brings film and game industry artists together with computer and social scientists to study and develop immersive media for military training, health therapies, education and more. Research projects explore and expand how people engage with computers, through virtual characters, video games and simulated scenarios. The ICT is a recognized leader in the development of virtual humans who look, think and behave like real people. With applications for therapy, leadership, and decision-making, the ICT seeks to redefine the range of skills these systems can address. The ultimate goal of the combined research and development efforts is to harness the power of storytelling to save lives, resources and time. The research performed at the ICT falls into five Strategic Research Areas (SRAs): (i) Immersion, (ii) Graphics, (iii) Virtual Humans, (iv) Social Simulation, and (v) Learning Sciences Tools and Methods. Each SRA is further divided into research themes. Detailed descriptions of each SRA and its corresponding themes are available at the ICT program website (http://ict.usc.edu/research/).

In FY12, the ICT supported 17 faculty, 123 graduate and undergraduate students, 36 postdoctoral fellows, and 10 visiting researchers in such diverse fields as computer science, psychology, cognitive architectures, emotion modeling and interactive media. The ICT program is unique in that it currently has 6.1, 6.2 and 6.3 responsibilities. This fact coupled with the large number of both military and industry collaborators establishes a natural transition pathway for ICT technologies into military simulation and training systems. Also, being based at USC with its own film school and in Los Angeles, the center of the entertainment industry, facilitates collaboration with major movie producers and game makers. In contrast to the ICB and ISN, the ICT is co-managed by ARO and ARL's Human Research and Engineering Directorate (HRED). Funding for the ICT is managed through the ARO while HRED provides technical guidance with ARO support. A U.S. Army Technical Assessment Board and an Executive Steering Board annually review the ICT research portfolio, assessing the goals of the various projects and research results. A total of $14.3 million of program funds were awarded to the ICT in FY12, with $7.3 million allocated for 6.1 basic research, $4.8 million allocated for 6.2 applied research, and $2.2 million allocated for 6.3 advanced technology development, respectively.

I. Congressionally-directed Cyber-security Laboratory (CyLab) at Carnegie Mellon University (CMU)

The CMU CyLab combines the efforts of more than 40 researchers and 100 students from the College of Engineering, the School of Computer Science, the H. John Heinz III School of Public Policy, and the Computer Emergency Response Team (CERT) Coordination Center. In the area of information assurance, current research is carried out under six themes: (i) Resilient and Self-Healing Systems, (ii) User Authentication and Access Control, (iii) Software Measurement and Assurance, (iv) Information Privacy, (v) Threat Prediction Modeling, and (vi) Business and Economics of Information Security. The CMU CyLab is working closely with ARO to discover breakthrough technologies that can secure and protect the computing and communication capabilities of the Army. Successful results from these research efforts will contribute to the development of a highly assured, efficient, and survivable information system for future combat forces. The Cylab did not receive funding in FY12; research efforts were carried out under a no cost extension.

J. Congressionally-directed Cyber-Threat Analytics (Cyber-TA) Research Consortium

The mission of the consortium is to explore and develop advanced capabilities to defend against large-scale network threats and to create new technologies to enable next-generation privacy-preserving digital threat analysis centers. Currently, the consortium is led by SRI International, a non-profit research institute. The consortium consists of nine universities, two non-profit research organizations, and three small businesses, with more than 20 researchers participating. The project thrusts focus on: (i) privacy-preserving schemes for internet-scale collaborative sharing of sensitive information and security log content, (ii) real-time Malware-focused alert correlation analyses, including contributor-side correlation applications with repository-side reassembly, and (iii) new threat-warning dissemination schemes to rapidly inform large-scale multi-enterprise environments of new attack patterns and malware mitigation strategies that take advantage of the collaborative data correlation analysis. The researchers have already developed cutting-edge technologies and new tools that have been deployed to protect DoD information infra-structure. Most recently they developed effective analysis tools and counter-measures against the latest wave of intelligent attacks, such as the Conficker computer worm. The consortium did not receive funding in FY12; research efforts were carried out under a no-cost extension.

K. Congressionally-directed Secure Open Source Institute (SOSI)

A national center was established at North Carolina State University in FY08 to carry out research and develop trustworthy open source systems, techniques, and tools. The goal of the center is to develop a new computing architecture called a Secure Virtual Computing Architecture (SVCA) that will provide on-demand and secure delivery of a generalized computing environment (from a plain desktop, to classroom sized group of users, to cluster of servers, to high-performance computing) to an authenticated and authorized user located anywhere in the world. The system will be engineered such that there is mutual trust between the system, user data, and the users themselves. Several industry partners (*e.g.*, Red Hat, IBM, Cisco, and Nortel) are collaborating with researchers to facilitate technology transfers and conduct joint research. The researchers at the center have recently focused on developing cost effective security solutions for virtual computing and cloud computing. The SOSI did not receive funding in FY12 and research efforts were carried out under a no cost extension.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Computing Sciences Division.

A. Analysis and Understanding of Crowd Behavior

Professor Mubarak Shah, University of Central Florida, Single Investigator Award

The objective of this project is to develop a new paradigm for the visual analysis of sequences of crowded scenes. Professor Shah and his research group have established a new framework for crowd behavior analysis from moving cameras using Lie algebra. The method involves a novel motion segmentation algorithm adapted for the purpose of detecting regions of coherent motion in a video sequence of crowds. Even though this framework is proposed for crowd videos, its application is not limited and it can readily be applied to other application domains. This approach has achieved promising results on a challenging set of real life videos of crowds, where no existing method is applicable (see FIGURE 2). The regions of coherent motion are computed based on the observation that coherent motion induces temporally smooth sequences of affine transformation between small patches of videos. The similarity between two affine transformations can however only be quantified after converting them to a linear space (*e.g.*, by using Lie algebra).

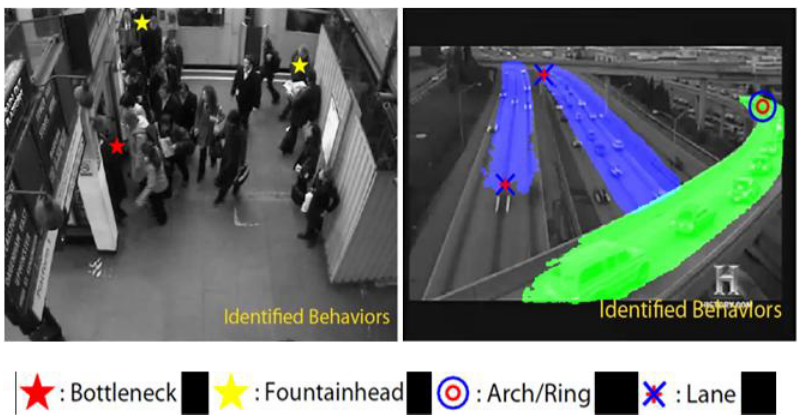

FIGURE 2

Visual analysis of crowded scenes. Scenes from real video sequences, each showing the behaviors that are detected by the stability analysis method.

This research has also established a novel tracking method tailored to dense crowds which does not require modeling of crowd flow and, at the same time, is less likely to fail in the case of dynamic crowd flows and anomalies by minimally relying on previous frames. The method automatically identifies prominent individuals from the crowd that are easier to track based on discriminative appearance. Therefore, instead of the conventional simultaneous data association paradigm for the tracking problem, this method employs a sequential one, where the order of preference is based on the ability of an object or human to distinguish itself from its neighbors.

B. Verifying Volume Rendering Using Discretization Error Analysis

Professor Robert Kirby, University of Utah, Single Investigator Award

In past years, significant efforts in visualization research have been dedicated to direct volume rendering (DVR), which is now widely used in different disciplines of science. For many of these disciplines high accuracy and precision is of major importance, for instance in image-based medical diagnosis or material science. Unfortunately, until now very little research has been dedicated to verifiable volume rendering, which would allow one to assess the correctness of volume rendered images. The objective of this project is to create and implement visualization techniques that act on high-order data directly, that are interactive and have quantifiable visualization error. In FY12, Professor Kirby developed concepts for verifiable volume rendering which exploit discretization error analysis. The approach is based on an analysis of the volume rendering integral which serves as a basis for most DVR algorithms. Professor Kirby can mathematically derive the expected behavior from the discretization of the volume rendering integral and can then verify existing implementations through convergence analysis, by comparing their actual behavior to the expected behavior (see FIGURE 3). This is demonstrated through a CT scan of a carp rendered by a popular open source software system for 3D computer graphics, image processing, and visualization called The Visualization ToolKit (VTK). In the original VTK rendering artifacts are present that are not in the scanned data but are due errors made by VTK. Using his verifiable volume rendering techniques, Professor Kirby was able to both detect and correct these errors. This is the first instance of a provably correct, mathematically sound approach for the verification of DVR algorithms that can be easily implemented in practice.

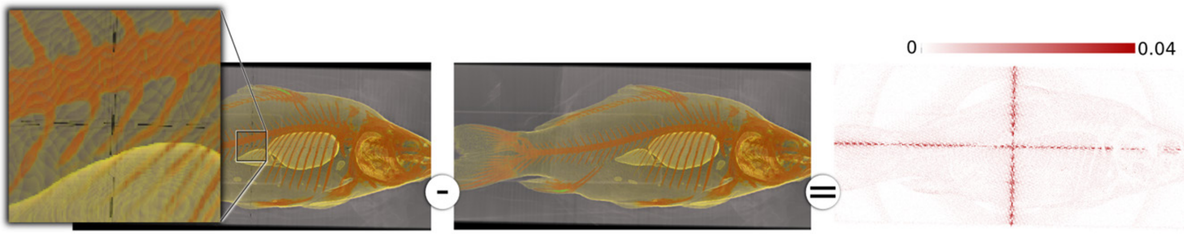

FIGURE 3

Rendering by the Visualization ToolKit (VTK). The panels display a CT scan of a carp, rendered with VTK 5.6.1. On the left, artifacts (dark lines) are incorrectly displayed by VTK. In the middle, the results after fixing the issues using verifiable visualization techniques are displayed; the artifacts are no longer visible. The difference image is shown on the right.

C. Robust Location Distinction using Temporal Link Signatures

Professors Neal Patwari and Sneha Kasera, University of Utah, Single Investigator Award

The objective of this project is to develop an analytical method to utilize changes observed on channels between pairs of transceivers for environment sensing, and to develop an experimental methodology to collect wideband channel data for verification of the analytical model. The physical characteristics of a wireless link between a transmitter and a receiver are determined by a number of factors including interference, signal-to-noise ratio, and very importantly, multipath behavior. The multiple paths (multipath) between the transmitter and the receiver are caused by the reflections, diffractions, and scattering of the radio waves interacting with the physical environment. Each path has a different length, so a wave propagating along that path takes a different amount of time to arrive at the receiver. Each path has attenuation caused by path losses and interactions with objects in the environment, so each wave undergoes a different attenuation and phase shift. Given the heterogeneous and changing nature of most real-world environments (other than free space), the physical behavior of the wireless links is different at different locations and at different times. Thus the physical characteristics of a wireless link can be used as its signature.

The PIs have used a measured temporal link signature to uniquely identify the link between a transmitter and a receiver. When the transmitter changes location, or if an attacker at a different location assumes the identity of the transmitter, the link distinction algorithm reliably detects the change in the physical channel. This detection can be performed at a single receiver or collaboratively by multiple receivers. Over 9,000 link signatures at different locations over time have been recorded (see FIGURE 4). The analysis of the link signatures leads to the conclusion that temporal link signatures can be used to develop a robust location distinction method, with a very good accuracy and a low rate of false alarm.

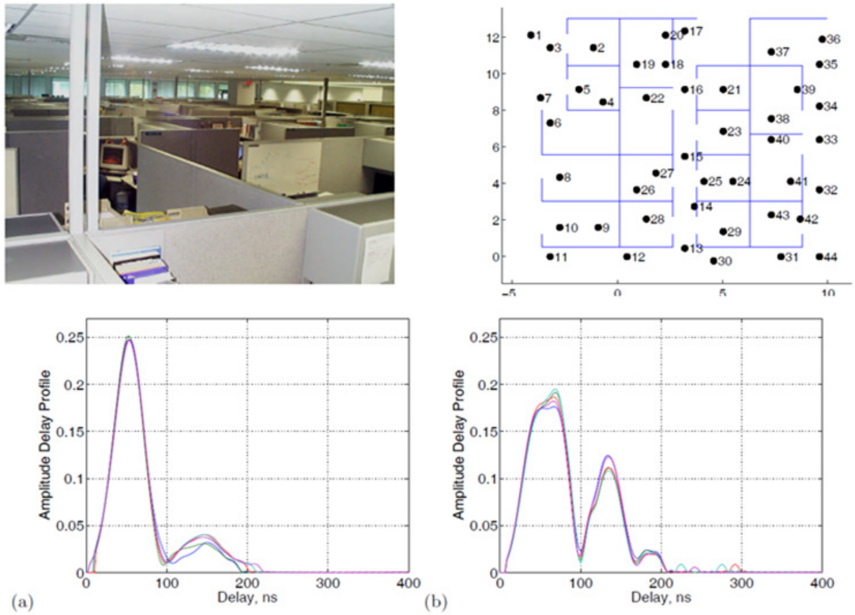

FIGURE 4

Test bed setup and two captured link signatures. Over 9,000 link signatures at different locations over time were recorded. The analysis of the link signatures led to the conclusion that temporal link signatures can be used to develop a robust location distinction method, with a very good accuracy and a low rate of false alarm. The top left and top right figures show the testbed setup within the lab. The bottom left and bottom right figures show distinct channel signatures for two separate wireless links.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. High-Level Visual Inference to Improve Vision-based Mobile Robot Localization

Investigator: Professor Jason Corso, The State University of New York (SUNY), YIP Award
Recipient: ARL Computational and Information Sciences Directorate (ARL-CISD)

The objective of this project is to create a semantic framework of high-level scene and object understanding for vision-based navigation of autonomous ground systems. Professor Jason Corso at SUNY - Buffalo has created a novel approach to stairway detection. Autonomous mobile robots have traditionally been restricted to exploring single floors of a building or outdoor areas that are free of abrupt elevation changes such as curbs and stairs. This effort removes the restriction by using geometric cues from depth data to detect ascending stairwells. This method can operate at the frame rate of the sensor when deployed on a mobile platform, so that a mobile robot that is capable of traversing stairs will be able to explore an environment and map the space (*e.g.*, with Simultaneous Localization and Mapping) while simultaneously localizing the stairwells that exist in the environment within the map. This approach leverages a number of image processing techniques including Canny edge detection and probabilistic Hough transform to detect lines in the depth image representing discontinuities. Stairwells will exhibit multiple parallel discontinuities. These candidate lines are filtered to isolate a set that are parallel (or nearly so) and localized as a group in the image. Finally, a plane is fit to the detected stair edge lines to confirm that the detected stair edges lie on an inclined plane at a traversable angle. The detector has been deployed on an iRobot Packbot equipped with a Microsoft Kinect depth sensor in a variety of natural environments, and has proven to succeed in addressing the needs of a robotic system for autonomous exploration. This approach is computationally efficient, robust to stair size, appearance, and viewing angle, highly accurate, and applicable to depth imagery captured both indoor and outdoor. This system was evaluated extensively during field tests with ARL at Camp Lejeune, and has subsequently transitioned to ARL-CISD.

B. Scalable Techniques for High Resolution Elevation Data Analysis and Modeling

Investigators: Professor Pankaj Agarwal, Duke University, Single Investigator Award
Recipients: Engineering Research and Development Center (ERDC), Topographic Engineering Center (TEC), and Scalgo, Inc.

Army terrain data is massive and dynamic, with different point densities and accuracies. There are many difficulties to overcome when dealing with such data, for example: the sets cover large geographical areas; sampling errors and random noise make extraction of relevant features difficult; accessing data from disk or network is a bottleneck; extracting features on the terrain and tracking them in a time-series data is expensive; and optimization problems are usually intractable. The goal of this project is to provide enhanced terrain modeling and analysis capabilities by developing sophisticated techniques that function with massive non-standard datasets, such as point clouds, and that produce a confidence level for the results.

In FY12, Professor Agarwal and co-PI Professor Helena Mitasove at North Carolina State University presented results of this research to various Army research organizations, including the Army Corps of Engineers (ACE) Engineering Research and Development Center (ERDC), and the Topographic Engineering Center (TEC). The presentations led to transitions and collaborations for further research. Researchers at ERDC worked with Professor Agarwal and Professor Helena Mitasove with two follow-on projects to extend the novel and innovative methods and software developed at Duke for spatial digital elevation models (DEMs) to include time as a parameter (i.e., spatio-temporal DEMs). The results of this research will lead to computational tools for working with spatio-temporal data at a desired resolution and save computation and communication cost, while retaining the meaning of the data and preserving the feature information. The PIs also started a company called Scalgo that develops software for terrain modeling and analysis based on this research. The software is being used by more than 100 organizations worldwide.

C. Automated Network Service Discovery
Investigator: Professor Peng Ning, North Carolina State University, MURI Award
Recipients: ARL-CISD, IBM

The objective of this project is to create a novel approach to automatically discover dependencies between network services. Enterprise networks today host a wide variety of network services, which often depend on each other to provide and support network-based services and applications. Understanding such dependencies is essential for maintaining the well-being of an enterprise network and its applications, particularly in the presence of network attacks and failures. In a typical enterprise network, which is complex and dynamic in configuration, it is non-trivial to identify all these services and their dependencies. Several techniques have been developed to learn such dependencies automatically. However, they are either too complex to fine tune or cluttered with false positives and/or false negatives. NCSU researchers have created a suite of novel techniques and developed a new tool named NSDMiner (which stands for Mining for Network Service Dependencies) to automatically discover the dependencies between network services from passively collected network traffic, which has transitioned to ARL-CISD and IBM for futher study. The new system has two appealing properties. First, it only uses passively observed network traffic as input, and thus does not rely on application behavior or configuration files to identify dependencies. Second, it is not restricted to only known services, and does not need any input about the existing network services and server infrastructure. NSDMiner is non-intrusive; it does not require any modification of existing software, or injection of network packets. More importantly, NSDMiner achieves higher accuracy than previous network-based approaches. On a performance ROC curve, when the false positive rate is below 20%, the dependence detection rate is at least 10 times better than previous schemes. Experimental evaluation, which uses network traffic collected from the NCSU campus network, shows that NSDMiner outperforms the two best existing solutions significantly. In addition, NCSU and ARL-CISD published a joint paper on this new technique in FY12.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Multipath Exploitation and Knowledge-Based Imaging Using Compressive Sensing

Professor Fauzia Ahmad, Villanova University, Single Investigator Award

The objective of this research project, to be pursued in collaboration with Professor Moeness Amin at Villanova University, is to create a compressive sensing based approach to radar imaging that will enable fast data acquisition in wideband ground-based and airborne radar imaging systems for urban sensing applications. The capability of compressive sensing to reconstruct a sparse scene from far fewer measurements provides a new perspective for data reduction in through-the-wall radar imaging without compromising target detection, localization, or imaging quality. It is anticipated that in FY13, techniques to provide persistent surveillance in urban environments will be integrated with wall clutter mitigation methods, developed models of target multipath, and algorithms for urban imaging. This will yield reduced cost, simplified hardware, and efficient sensing operations that allow fast super-resolution imaging of sparse scenes, thereby culminating in quick turnaround actionable intelligence. In the long term, this research will establish new methods to achieve the following goals: (1) utilization of valuable system resources more effectively for enhanced target detection through knowledge-based processing; (2) establishing appropriate change detection models and determination of possible approximations that permit application of compressive sensing to benefit the detection paradigm of moving targets behind walls and in enclosed structures; (3) exploitation of the rich multipath nature of the indoor environment for a compressive sensing based imaging radar and characterization of the improvement in stationary target detection performance; and (4) accomplishing single sensor based detection and localization of non-cooperative unknown targets in a swift manner with as few measurements as possible.

B. Millimeter-Wave Wireless Network-on-Chip Architectures for Multi-Core Systems

Professor Partha Pande, Washington State University, Single Investigator Award

The Network-on-Chip (NoC) is the communication backbone of modern systems-on-chip that integrates large numbers of embedded cores on a single die. Existing NoCs employing planar metal interconnects suffer from high latency and power consumption due to multi-hop links used in inter-core data exchanges. The goal of this project is to address the latency and power consumption problems by investigating novel wireless NoC (WiNoC) architectures that replace multi-hop wired interconnects with high-bandwidth single-hop long-range millimeter-wave wireless links. The specific objectives of this effort are to:

- Design small-world WiNoC architectures with long-range wireless links that maximize throughput and minimize latency, power and area; evaluate the performance of WiNoC architectures using various traffic patterns; and compare performance with other emerging architectures such as 3D, photonic and RF interconnect-based NoCs
- Design highly efficient on-chip wideband antennas and millimeter-wave wireless transceivers for high throughput on-chip data transfer; and fabricate, test and evaluate prototype wireless links including on-chip antennas and transceivers

This research could transform the design of NoCs for large multi-core systems-on-chip by eliminating the constraints associated with long wired interconnects. Many military applications require both high performance computing and low power consumption. These applications will benefit immensely from the WiNoC's improved data throughput and reduced overall power consumption.

It is anticipated that in FY13, the researchers will design the network architecture and then evaluate its performance through rigorous simulation in the presence of various realistic traffic patterns. As the industrial collaborator, Intel will provide the PIs with application-specific traffic models to validate the performance of the WiNoCs.

C. Will the Revolution be Tweeted? Weak ties, Social Media, and Flash Movements
Professor David Lazer, Northeastern University, Single Investigator Award

The goal of this project is to leverage social media to explore how groups of users reach consensus when no explicit external hierarchy or consensus mechanisms (such as voting) are present. Specifically, the project will explore how social media may provide the necessary weak ties to facilitate rapid global coherence in a population with an inclination to mobilize, in part because social media facilitates the rapid emergence of informal leaders. The project will examine the role that social media plays in enabling such global coherence by analyzing digital traces from Twitter, Facebook, and the blogosphere. This research involves four primary research thrusts focused on (i) how forums of discussion are agreed upon, (ii) how linguistic norms to facilitate discussion and to serve as a shibboleth for group members are established, (iii) how information is propagated between users (how different relationship types affect information propagation), and (iv) how group behavior is coordinated. It is anticipated that in FY13, preliminary results about three items related to the first thrust will be available, namely, identification of related hashtags, modeling user–hashtag behavior, and validation of hashtag models.

D. RF Environment Sensing Using Transceivers in Motion
Professor Sneha Kasera, University of Utah, STIR and DURIP Awards

Multi-static RF localization technologies, such as radio tomographic imaging and MIMO radar, offer the potential to locate moving people and objects over wide areas, even through entire buildings, using changes observed in the RF channel between pairs of transceivers. Recent research has typically assumed that transceiver devices are static, but it would be advantageous in many applications to use mobile devices, such as swarms of autonomous robots. Mobile transceivers introduce a fundamental ambiguity between small-scale fading and the desired temporal fading signal. The objective of this project is to develop an analytical model that can effectively identify temporal fading changes (the "signal" in environmental monitoring) while offsetting the small-scale fading due to a transceiver moving. It is anticipated that in FY13, new methods will effectively quantify and measure the temporal fading on the channel with mobile transceivers. Experiments using wideband, multiple antenna transceivers, such as those using OFDM-MIMO will be carried out to verify the validity and precision of the temporal fading quantification model.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Cliff Wang
Division Chief
Program Manager, Information and Software Assurance

Dr. Mike Coyle
Program Manager, Computational Architectures and Visualization

Dr. Liyi Dai
Program Manager, Information Processing and Fusion

Dr. John Lavery
Program Manager, Social Informatics

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Dr. Randy Zachery
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Dr. Bruce West
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Dr. Ellen Segan
Science Advisor to the 18th Airborne Corps

Ms. Anna Mandulak
Contract Support

C. Administrative Staff

Ms. Debra Brown
Directorate Secretary

Ms. Diana Pescod
Administrative Support Assistant

CHAPTER 5: ELECTRONICS DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2012* is to provide information on the programs and basic research efforts supported by ARO in FY12, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Electronics Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY12.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of research in the ARO Electronics Division is to gain new fundamental knowledge in phenomena that involve charged particles. More specifically, the Division supports basic research to discover and control the relationship of nanostructure and heterostructure designs on charge transport and carrier recombination dynamics, to understand and improve the stimulus-response properties of electronic materials/structures, to leverage nanotechnology for enhanced electronic properties, to comprehend and mitigate distortion and noise, and to explore ultra-fast, solid state mechanisms and concepts. The results of these efforts will stimulate future studies and help keep the U.S. at the forefront of research in electronics by revealing new pathways for the design and fabrication of novel electronic structures that have properties that cannot be realized with current technology.

2. Potential Applications. Electronics research is relevant to nearly all Army systems; therefore, research under this program provides the underlying science to a wide variety of developmental efforts and contributes to the solution of technology related problems throughout the full spectrum of the Army's "System of Systems." Research in electronics can be divided into five areas: (i) multimodal sensing for detection, identification, and discrimination of environmental elements critical to decision-makers in complex, dynamic areas, (ii) ubiquitous communications for multimode and secure communications in all situations including high data rates, transmission over long distances and complex terrain paths, as well as problems associated with short range networked systems, (iii) intelligent information technology that enhances the creation and processing of information, (iv) optoelectronic warfare, which involves the use of electromagnetic (EM) radiation from radio frequency (RF) to ultraviolet (UV), to interrogate, disrupt, and defeat hostile electronic and threat systems, and (v) power electronics for electronic circuits and components that require less power and/or operate in extreme conditions.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Electronics Division frequently coordinates and leverages efforts within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). Moreover, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, sensing is a research element of all ARO Divisions, and the Electronics Division serves as the focal point for ARO sensing research. Specific interactions include joint projects with the Physics Division that promote research for physics-based understanding of semiconductor materials, non-reciprocal materials and devices, propagation effects, and stimulus response effects in condensed matter. The Electronics Division also coordinates efforts with the Materials Science Division to pursue the design and characterization of new materials and structures, the evaluation of electrical properties, and the study of electronic processes at the molecular level. This Division complements its research initiatives in the Chemical Sciences Division to include research to understand how chemical changes and chemical structures influence electrical, magnetic, and optical properties and investigations of high frequency spectroscopic techniques for use in chemical defense, especially explosive detection. The Life Sciences Division's Program Areas also interface with electronics research in areas of biological detection as well as interfacing to biological organisms. Lastly, creating computational methods and models for target recognition and understanding nano-molecular structures and carrier transport shared research goals between the Electronics and Mathematical Sciences Divisions.

B. Program Areas

To meet the long-term program goals described in the previous section, the Electronics Division engages in the identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY12, the Division managed research efforts within four Program Areas: (i) Solid State and High Frequency Electronics, (ii) Electromagnetics, Microwaves, and Power, (iii) Optoelectronics, and (iv) Electronic Sensing. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have long-term objectives that collectively support the Division's overall objectives.

1. Solid State and High Frequency Electronics. The goal of this Program Area is to conduct research into quantum phenomena, internally and externally induced perturbations, and novel transport and optical interaction effects in nano-scale electronic structures. This Program Area is divided into two research Thrusts: (i) Nanoelectronic Engineering Sciences, and (ii) Teraherz-frequency and Ultra-fast Electronics. These Thrust areas guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. Nanoelectronic Engineering Sciences' research efforts involving nano-devices and molecular-level electronics and addresses issues related to the design, modeling, fabrication, testing and characterization of novel electrically and magnetically-controlled electronic structures. The research program on ultra-fast and terahertz frequency electronics includes a strong component for sensing science at very high frequencies.

2. Electromagnetics, Microwaves, and Power. The goal of this Program Area is carry out basic research leading to the creation of a transmit/receive system that will receive and demodulate any electromagnetic signal from any direction, modulate and transmit any electromagnetic signal in any direction, reconfigure to implement a variety of radio and sensor functions, adapt to the ambient environment, and respond to changing requirements. This Program Area is divided into three research Thrusts: (i) Electromagnetics and Antennas, (ii) RF Circuit Integration, and (iii) Power Efficiency and Control. Research efforts within these Thrusts include studies of the generation, transmission, and reception of high frequency microwave and millimeter wave radiation, as well as specific technical problems at high frequency (HF), very high frequency (VHF), and ultra-high frequencies (UHF). This includes studies of the coupling of electromagnetic (EM) radiation into and out of complex structures, active and passive antennas, transmission lines and feed networks, power combining techniques, EM wave analyses of electrical components, and EM modeling techniques that advance mixed-signal design to the state of current digital design. The research efforts within this Program Area may lead to the discovery of novel active and passive devices and components with improved dynamic range, linearity, bandwidth, and loss performance. Army applications of this technology include communications (both tactical and strategic), command and control, reconnaissance, surveillance, target acquisition, and weapons guidance and control.

3. Optoelectronics. The goal of this Program Area is to discover and control novel nanostructure and heterostructure designs for the generation, guidance, and control of optical/infrared signals in both semiconductor and dielectric materials. The research in this program may enable the design and fabrication of new optoelectronic devices that give the Soldier high-data-rate optical networks including free space/integrated data links, improved IR countermeasures, and advanced 3D imaging. This program has three Thrust areas: (i) High Speed Lasers and Interconnects, (ii) Ultraviolet and Visible Photonics, and (iii) Mid-infrared Lasers. The research topics involve efforts to overcome slow spontaneous lifetimes and gain dynamics, low carrier injection efficiency, poor thermal management, and device size mismatches. Novel light emitting structures based on III-V compounds, wide bandgap II-VI materials, rare-earth doped dielectrics, and silicon nanostructures are being investigated along with advanced fabrication and characterization techniques. Nanotechnology is exploited to allow interfacing of optoelectronic devices with electronic processors for full utilization of available bandwidth. Electro-optic components are being studied for use in guided wave data links for interconnections and optoelectronic integration, which are all requirements for high speed full situational awareness. In addition, emitters and architectures for novel display and processing of battlefield imagery are also important.

4. Electronic Sensing. The goal of this Program Area is to extend the underlying science behind action-reaction relationships in electronic materials and structures as well as understand target signatures. This Program Area is divided into two research Thrusts: (i) Photonic Detection and (ii) Thermal, Mechanical, and Magnetic Effects. The scientific objective of the Photonic Detection thrust is to understand and control the direct conversion of light to charge in infrared materials and structures. This includes the design and fabrication of novel detector structures, such as superlattice or barrier structures, as well as novel plasmonic effects. An important element in this Thrust area is the reduction of performance limiting defects in semiconductor material and structures through lattice matching and other methods. Development of novel characterization techniques is also explored to determine the fundamental issues behind carrier transport, lifetimes, and noise. The Non-Imaging Sensing Thrust strives to uncover the underlying relationships behind signature phenomenology and use it to guide sensor development and decision techniques. The Thermal, Mechanical, and Magnetic Effects thrust modalities include acoustic, magnetic, infrasound, and "passive" environmental signals such as radio or TV broadcasts as well as thermal effects for infrared detection. Efforts in the this Program Area seek to give the Soldier 100% situational awareness of vehicles, personnel, weapon platforms, projectiles, explosives, landmines, and improvised explosive devices (IEDs), in day/night, all weather, and cluttered environments through natural and man-made obstructions.

C. Research Investment

The total funds managed by the ARO Electronics Division for FY12 were $42.8 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY12 ARO Core (BH57) program funding allotment for this Division was $6.0 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $5.0 million to projects managed by the Division. The Division also managed $20.4 million of Defense Advanced Research Projects Agency (DARPA) programs, and $2.2 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $5.2 million for contracts. Finally, $4.0 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY11 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research projects. Research projects are developed by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts.

The following subsections summarize projects awarded in FY12 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY12, the Division awarded 18 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to determine the potential of flexoelectric nanostructures for multimodal sensing, address the critical needs of energy efficient ultra-high speed data transmission applications, and characterize scientifically important systems at THz frequencies. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Les Atlas, University of Washington; *Complementary Correlation: Audio Analysis and Enhancement*
- Professor Gregory Belenky, SUNY at Stony Brook University; *Investigation of the III-V Barrier Photo Detector Heterostructures for Spectral Range Above 10 um*
- Professor Elliott Brown, Wright State University; *1550-nm Extrinsic-GaAs Photomixers, Arrays and Spectrometers*
- Professor Gary Brown, Virginia Polytechnic Institute and State University; *Investigations of Wave Scattering and Propagation Over Rough Dielectric Surfaces*
- Professor Dennis Deppe, University of Central Florida; *WDM Nanoscale Laser Diodes for Si Photonic Interconnects*
- Professor Milton Feng, University of Illinois - Urbana; *Low noise Energy Efficient Micro-cavity Transistor Laser for 50 Gb/s direct modulation*
- Professor Jean-Pierre Leburton, University of Illinois - Urbana; *Self Consistent Ambipolar Transport and High Frequency Oscillatory Transient in Graphene Electronics*
- Professor Xiaoning Jiang, North Carolina State University; *Flexoelectricity in Nanostructures: Theory, Nanofabrication and Characterization*
- Professor Zetian Mi, McGill University; *Ultrahigh-Speed Electrically Injected 1.55 um Quantum Dot Microtube and Nanowire Lasers on Si*
- Professor Rao Mulpuri, George Mason University; *Ultra-fast Microwave Annealing to Increase Acceptor Activation in In-situ and Ion-implantation Doped ZnO*
- Professor Unil Perera, Georgia State University; *Band Structure and Band Offset Characterizations of Semiconductor Heterojunctions*

- Professor Inna Ponomareva, University of South Florida - St. Petersburg; *Terahertz Nanoscience of Multifunctional Materials: Atomistic Exploration*
- Professor Manijeh Razeghi, Northwestern University - Evanston Campus; *Capacitance-Voltage (CV) Measurement of Type-II Superlattice Photodiodes*
- Professor Ronald Reano, Ohio State University; *RF Energy Interaction With Electro-Optic Materials*
- Professor Roman Sobolewski, University of Rochester; *Ballistic deflection transistors for THz amplification*
- Professor Michael Steer, North Carolina State University; *Time-Frequency and Non-Laplacian Phenomena at Radio Frequencies*
- Professor Judy Wu, University of Kansas; *Fundamental Physics of Carbon-based Nanostructures*
- Professor Weidong Zhang, North Carolina State University; *First Principal And Hybrid Molecular Modeling Development*

2. Short Term Innovative Research (STIR) Program. In FY12, the Division awarded seven new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to determine physical limits of extremely non-degenerate two photon absorption in terms of frequency and intensity and to determine the advantages of the tunable epsilon-near-zero (ENZ) materials for optical modulators using slot waveguides with ultra-compact dimensions and investigate the physics of antenna field null generation. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Mohammod Ali, University of South Carolina; *Foundations of Broadband Multifunctional Metamaterials Inspired by the Analogy of Formation*
- Professor Michael Aziz, Harvard University; *Deep Impurity Band Silicon For Subbandgap Photodetection*
- Professor Boris Gelmont, University of Virginia; *Stability and Physical Accuracy Analysis of the Numerical Solutions to Wigner-Poisson Modeling of Resonant Tunneling*
- Professor Vrinda Haridasan, Physical Devices LLC; *Antenna Field Nulling of Radio Frequency Interference: Basic Physics*
- Professor Zhaolin Lu, Rochester Institute of Technology; *Ultracompact Electro-Absorption Modulators Based On Novel Materials*
- Professor Kathleen Melde, University of Arizona; *Exploring New RF Circuit Structures with Embedded Patterned Substrate Layers*
- Professor Eric Van Stryland, University of Central Florida; *Extremely Non-Degenerate (END) 2-Photon Detection*

3. Young Investigator Program (YIP). In FY12, the Division awarded two new YIP projects. These grants are driving fundamental research, such as studies to determine the electrochemical mechanism of new material, discover new synthesis approach for class of polymers, and characterize properties of new cool class of compounds. The following PIs and corresponding organizations were recipients of the new-start YIP awards.

- Professor Mona Jarrahi, University of Michigan - Ann Arbor; *Fundamental Properteries and Capabilities of Plasmonic Antennas for Efficient Interaction with Nanoelectronics*
- Professor Lin Zhu, Clemson University; *Innovation in Broad-Area Diode Laser Array Architecture: Grating-Confined Zigzag Modes*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY12 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *36th International Conference on Infrared, Millimeter, and Terahertz Waves;* Houston, TX; 2-7 October 2011
- *International workshop on 6.1 Å II-VI and III-V materials and their integration;* Tempe, AZ; 8-9 November 2011
- *11th International Workshop on Finite Elements for Microwave Engineering;* Estes Park, CO; 4-6 June 2012

- *Advanced Research Workshop on Future Trends in Microelectronics: Into the Cross Currents;* Corsica, France; 25-29 June 2012
- *2012 Nanostructure Fabrication GRC*; Biddeford, ME; 15-20 July 2012
- *3rd Summer Institute on Complex Plasmas;* South Orange, NJ; 30 July - 8 August 2012
- *11th International Conference on Infrared Optoelectronics: Materials ad Devices (MIOMD-XI);* Evanston, IL; 4-8 September 2012
- *Antenna Applications Symposium;* Monticello, IL; 18-20 September 2012

5. Special Programs. In FY12, ARO Core Research Program funds provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded 11 new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

C. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Electronics Division; therefore, all of the Division's active MURIs are described in this section.

1. Stimulus-Response Properties of Uncooled Infrared Materials. This MURI began in FY06 and was awarded to a team led by Professor Mark Horn at Pennsylvania State University. The goal of this research is to gain knowledge of the physics and chemistry of disordered materials useful for uncooled infrared detection and quantify their fundamental and technological attributes and limitations.

The main focus of this research is on vanadium oxide (VO_x) and amorphous silicon germanium (a-$Si_{1-x}Ge_x$:H) but other novel materials are also being explored, such as the spinel family and zinc oxide (ZnO). A combination of theory, microanalysis, optical measurements, and feedback to growers is employed to unravel the mysteries of the structure, absorption mechanism, and transport properties in these largely disordered materials. During the previous year it was shown that the substrate plays a major role in the crystallinity and phase of the VO_x growing on top of it. It is hoped that the knowledge gained from this MURI can be used to make improvements in materials to fully exploit their capability for uncooled infrared-detector applications. Understanding the dynamics of the materials at the molecular level will provide a quantitative fundamental base toward achieving the goal of an infrared camera for every Soldier.

2. Near and Far-Field Interfaces to DNA-Guided Nanostructures from RF to Lightwave. This MURI began in FY10 and was granted to a team led by Professor Peter Burke at the University of California - Irvine. The goal of this research is the broad-spectral-based (RF to Lightwave) electromagnetic interrogation and interfacing to novel biological-based nanostructures that include DNA tiles, nanotubes and nanowires for the purposes of defining new scientific and technology concepts at the nanoscale in the context of electronic signal application and extraction for novel sensing applications.

The specific aims of this research are the development and application of nanowire and nanotube antenna architectures for realizing optical, THz and RF spectroscopy with highly localized, nanoscale spatial resolution that will allow for single molecule spectroscopy to be performed on self-assembled DNA superstructures that have been designed and fabricated to incorporate novel sensor functionality. Here, a significant scientific opportunity exists for the use of on-chip source/detector architectures with very little signal attenuation (due to their nanoscale proximity), allowing for unresolved spectral features that were previously masked by severe water absorption to be discovered, characterized, and exploited across the entire spectrum from DC to Lightwave, especially in the THz domain. The research and technology developed has the potential to define an entirely new methodology for interfacing to the nanoscale in the context of electronic signal application and extraction. This technology would enable pioneering studies in biological-based molecules and systems and contribute new insights and discoveries in bio-molecular electronics with relevance to future sensing, data processing and computation. The anticipated high-importance impact areas include (i) neuron signal science and phenomenology, (ii) bio-based sensing of chemical, biological, radiological and explosive agents, (iii) novel bio-molecular devices for RF-THz-IR-optical digital/analog applications, and (iv) novel diagnostic and treatment methodologies for bio-medical applications. One of the results in the past year was the demonstration of a prototype DNA-based computational device with variable input.

3. Defect Reduction in Superlattice Materials. This MURI began in FY11 and was awarded to a team led by Professor Sun Lien Chuang at the University of Illinois - Urbana Champaign. The team consists of researchers from Arizona State University, Georgia Tech, and the University on North Carolina - Charlotte. The objective of this project is to determine and understand the relationship between minority-carrier lifetimes and classes of defects in superlattice materials and to formulate strategies for growth and post processing to eliminate or mitigate defects.

This research effort includes an in-depth study of the origins and structural, electrical and optical properties of defects, in-situ and ex-situ probing of defects during growth and fabrication, an investigation of defect reduction techniques, a study on ways to minimize the impact of defects on performance, and testing of results through fabrication and characterization of superlattice structures and devices. Understanding defects at the basic level in these superlattice materials will promote advancements in lasers and modulators as well as infrared detectors. For detectors, lifetime improvements will allow the next generation of focal plane arrays with increased long wave resolution, much larger array formats, broader spectral range into the very long wave infrared, and higher operating temperature to reduce life cycle costs. One of the important accomplishments during the year was the demonstration of record long minority carrier lifetimes in a Ga-free InAs/InAsSb type-II superlattice material.

D. Small Business Innovation Research (SBIR) – New Starts

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY12, the Division managed four new-start SBIR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of two Phase I contracts, one Phase I Chemical Biological Defense SBIR (CBD-SBIR) contract, and one Phase II contract. These new-start contracts aim to bridge fundamental discoveries with potential applications, including the development of a biosensor nanofluidic platform for integration with a terahertz spectroscopic system and novel techniques to reduce dislocation density in long wave infrared HgCdTe epitaxial layers grown on alternate substrates.

E. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY12, the Division managed six new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of one Phase I contract, and five Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications, including the development of DNA nanostructures with built-in functionality, a state-of-the-art terahertz imaging spectrometer capable of sub-wavelength resolution and high sensitivity to trace amounts of chemical and biological agents, and high-performance lasers that are beam combined through a waveguide coupling design.

F. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY12, the Division managed one new ARO (Core) HBCU/MI project and seven new REP awards. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

G. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY12.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY12, the Electronics Division managed nine new DURIP projects, totaling $1.4 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies in the areas of infrared radiation detection, nanophotonics, and graphene science and technology for electronic devices.

I. DARPA Nanoscale Architectures for Coherent Hyper-Optic Sources (NACHOS) Program

The DARPA NACHOS officially ended Phase III in late FY12. The goal of this ARO-managed program was to demonstrate a sub-wavelength electrically injected semiconductor laser in all 3 dimensions was achieved, and the laser worked continuous-wave at room temperature. Such lasers far exceed the state-of-the-art in terms of size, and many potential applications exist both for future Army and non-military systems. Further improvement in the efficiency of such nanolasers may result in their effective use in nanoscale photonic sensor platforms. Another area of potential benefit would be in chip-scale optical interconnects. The most notable achievements were made in the groups of Professors Ning and Fainman at Arizona State University and the University of California – San Diego both in terms of laser size and electrical injection operating temperature.

J. JTO Multidisciplinary Research Initiative (MRI) Programs in High Energy Lasers

ARO currently manages nine MRI programs for the High Energy Laser Joint Technology Office in Albuquerque (managed by OSD). Six of those are new MRIs and three of those were awarded through ARO's Electronics Division (the others through Materials and Physics). The three ongoing MRIs are led by professors at the University of New Mexico, the University of Central Florida (Center for Research in Electro-Optics and Lasers), and Clemson University. Their respective foci are in three different areas: optical techniques for characterizing high power handling optical coatings and methods for improving their reliability, uses and fundamental material loss improvement and beam combining techniques with volume Bragg gratings, and solid core photonic crystal fiber laser development for larger core sizes and suppressed acoustic mode interference. ARO continues to play a significant role in leading the MRI programs by organizing kickoff meetings and program reviews, particularly on the fiber laser efforts, to review progress and aid in technology transition and the development of new research programs. The ARL Computational and Information Sciences Directorate (ARL-CISD) and the ARL Sensors and Electron Devices Directorate (ARL-SEDD) participate in HEL-JTO program evaluation through annual reviews.

K. DARPA High Power Efficient and Reliable Lasers (HiPER) I Program

The DARPA HiPER Program was funded to understand the thermal management limitations in diode bars toward creating kW level power outputs from single laser bars. The program at the Science Research Laboratory (SRL), which is managed by ARO, successfully determined how to extract heat from laser bars to such an extent as to make the heterostructure itself the limiting factor in the performance of high power laser bars. An add-on effort based on these results will complete four additional tasks in twenty four months. The start of this effort will begin after month three of the present award. In the First add-on Task, SRL will set-up and test the Micro Cooling Concept (MCC) impingement cooler to verify its thermal resistance and waste heat removal potential. This task will culminate in the experimental demonstration of waste heat removal of 2.5 kW/cm^2, thermal resistance of < 0.25 K/W and optical power extraction of 170 mW/µm. The second add-on Task will focus on the attachment of 3.6 mm kW LD bars on an impingement cooler with the goal of demonstrating a high-brightness of kW/bar-cm. The last experimental task will be the design, fabrication and test of a narrow 1.8 mm impingement cooler. The main goal of the add-on effort is to extend the methods developed by the PI to laser diode bars capable of kW/Bar-cm output power. Work at SRL on this and the related efforts are tied to ARO and DoD goals of developing higher power, more efficient laser diodes and is being coordinated with ARL-SEDD and another ARO single investigator program for potential transition.

L. DARPA High Power Efficient and Reliable Lasers (HiPER) II Program

The objective of this work is to develop compact, efficient and bright laser-diode (LD) sources that will result in extremely light-weight and inexpensive high-energy lasers (HELs) for the U.S. military. The SRL technologies developed in the HiPER I program will increase the power-to-weight ratio of LD pumps for HELs. This program follows on the previous DARPA/ARO funded program, HiPER I. HiPER II takes the thermal modeling efforts of HiPER I and pushes the entire pump module forward to create an array of modules that will be used in the DARPA Adaptive Photonic Phased Locked Elements (APPLE) Program together with RIFL (Revolution in Fiber Lasers) Program. ARO is involved in this program by providing assistance in leveraging technical knowledge of many related JTO-HEL programs and DARPA's APPLE program. ARL-CISD is a co-PI in the new APPLE program, which uses fiber lasers to achieve beam steerable laser arrays. Integrated diode laser bars may provide further miniaturization to such systems. Progress has continued with the program this year resulting in an additional ARO managed program also under this heading to make 1.8 kW pump modules for use in the DARPA EXCALIBUR fiber laser program.

M. DARPA High Power Laser Diode Facet Passivation Program

Another follow-on program to HiPER II is a result of discoveries that catastrophic optical mirror damage (or COMD) continues to plague laser bar power limits. ARO led discussions with Science Research Lab (SRL) which led to this ARO/DARPA effort as well as an ARO/DARPA SBIR. DARPA and ARO began a program to systematically study and understand the optimal facet passivation. ZnSe is known to be used in a number of laser diode commercial products, but other opportunities exist for better lattice matching and thermal expansion matching. Much of the effort will focus on using materials similar to those used in the laser itself. DoD will benefit from these studies as they help identify the best materials and processes to complete the passivation, which may lead to further improvements in power handling.

N. Edgewood Chemical Biological Center (ECBC) Program in Nanoelectronic Architectures for THz-Based Bio-sensing

ARO and ECBC jointly lead and support novel research programs that are advancing the state-of-the-art in nanoelectronic engineering in application areas that have relevance to national defense and security. One fundamental research area that is presently being emphasized is the investigation of new bio-molecular architectural concepts that can be used to achieve rapid, reagent-less detection and discrimination of biological warfare (BW) agents through the control of multi-photon and multi-wavelength processes at the nanoscale. This program supports multiple ARO single-investigator projects with the support of DTRA to develop new devices and nanoelectronic architectures that are effective for extracting THz signatures from target bio-molecules. Emphasis will be placed on the new nanosensor concepts and THz/optical measurement methodologies for spectral-based sequencing/identification of genetic molecules.

O. DARPA Efficient Linearized All-Silicon Transmitters ICs (ELASTx) Program

The goal of the ELASTx program is to enable monolithic, ultra high power efficiency, ultra high linearity, millimeter-wave, silicon-based transmitter integrated circuits (ICs) for next-generation military microsystems in areas such as radar and communications. The ARO Electronics Division currently co-manages two university grants within this program that are exploring quasi-optical power combining of Doherty amplifiers, and asymmetric multilevel outphasing of large numbers of transistor amplifiers. The program will lead to revolutionary increases in power amplification efficiency while simultaneously achieving high linearity for digitally modulated signals. Prototype ELASTx amplifiers are being tested by scientists in ARL-SEDD for potential use in Army radar and communications systems.

P. DARPA Microscale Plasma Device (MPD) Program

The goal of the MPD program is to support fundamental research in the area of microplasma device technologies and substrates for operation in extreme DoD-relevant environments. The ARO Electronics Division currently co-manages two grants within this program that will develop fundamentally new fast-switching microplasma devices, develop modeling and simulation design tools, and demonstrate the generation of a plasma with an extremely high charge density (10^{20} - 10^{22} unbound electrons per cubic centimeter) in a sealed cell with solid walls. This charge density is four to six orders of magnitude larger than is achieved in current microplasma research and is comparable to the carrier density in metallic materials. Research results will be communicated to ARL-SEDD Electronics Technology Branch scientists in order to identify opportunities for technology transfer. If successful, the MPD program will provide proof-of-concept for fast-switching microplasma devices that may enable new sources of radiated energy at sub-millimeter wave and terahertz frequencies, the enabling science behind new high resolution imaging radar and covert communication systems.

Q. DARPA High Frequency Integrated Vacuum Electronics (HiFIVE) and THZ Electronics Programs

The long-term vision for the DARPA THZ Electronics program is to develop the critical device and integration technologies necessary to realize compact, high-performance electronic circuits that operate at center frequencies exceeding 10^{12} cycles per second (*i.e.*, 1 THz). The DARPA HiFIVE program will develop a compact, efficient source of electromagnetic energy capable of generating 100 W with 5 GHz bandwidth at 220 GHz using innovative cold cathode and micromachining technologies. The ARO Electronics Division and ARL-SEDD Electronics Technology Branch co-manages projects within these programs with a goal of using silicon micromachining and MEMS processes to produce precision interaction structures scaled for these extremely small wavelengths. These programs have a high potential impact on military sub-millimeter wave communications, ECM, and radar systems, which is directly responsive to future Army needs in C4ISR and ground mobile wireless communications.

R. DARPA Advanced Wide FOV Architectures for Image Reconstruction and Exploitation (AWARE)

ARO is currently managing two seedling projects in the DARPA AWARE program: one at George Mason University and the other at IRDT Solutions, Inc. These projects were awarded as Cooperative Agreements and require substantial collaboration with ARO-SEDD researchers. Both projects are endeavoring to reduce defects in mercury cadmium telluride devices grown on silicon substrates. George Mason will develop an ultrafast microwave anneal material in an attempt to reduce defects for short wave HgCdTe grown on silicon. The effect of the anneal on impurity activation and ohmic contacts will also be investigated. IRDT Solutions, Inc. will build an automated multi-wafer mercury vapor annealing apparatus that will facilitate the thermal cycle anneal process for HgCdTe wafers. This equipment will be delivered and installed at ARL's Adelphi Lab Center for use by SEDD researchers. The goal of the DARPA AWARE program is to increase field of view, resolution and day/night capability at reduced size, weight, power, and cost (SWaP-C) for advanced imaging systems.

S. DARPA Compact Mid-Ultraviolet Technology (CMUVT) Program

The DARPA CMUVT program was initiated due to advances from Sensor Electronic Technology and Nitek funded by ARO SBIR Phase IIs using sapphire substrates coupled with advances at Hexatech (Morrisville, NC) and Crystal IS (Troy, NY) on AlN substrates to push light-emitting diodes (LED) and laser diode technology in the 225-275 nm region toward usable levels for water purification and biosensing. The goals of the program include 20% wall-plug efficiency LEDs in the 250-275 nm regime and laser diodes with wavelengths less than 250 nm with 5% wall-plug efficiency. In 2012, great advances were made on the LED side with SET producing wall-plug efficiencies exceeding 10% at approximately 275 nm. For the ARO managed program at Photon Systems, Inc., which focuses on approaches to pump AlGaN heterostructure lasers with electron beams, DARPA chose to significantly cut the program. However, this component of the program was continued at a much reduced level due to difficulties in the initial attempts to get lasing from heterostructures grown on SiC. As a result, Photon Systems is pursuing alternate growth methods to improve efficiency and to initiate lasing. Coordination with ARL-SEDD occurs through ARL co-management of the CMUVT program with DARPA, ARO, and others. ARL-SEDD has also been active in collaborating within the CMUVT effort.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Electronics Division.

A. PN Nanojunctions in Compound Semiconductors

Professor Gary Wicks, Rochester University, Single Investigator Award

The objective of this project is to demonstrate the failure of doping and the success of surface-control to create n- and p type conductivities and operational pn junctions in small diameter (typically less than about 60 nm) nanowires. Attempts to make smaller semiconductor devices eventually run into limits where devices fail to operate because bulk behavior vanishes, leaving only surface effects. At such small sizes, doping fails to create n- and p-type conductivities because the surface Fermi level pinning, not doping, dominates electrical properties. At present there is a minimum size limit for functional semiconductor devices, which occurs when bulk conductivity vanishes and only surface conductivity remains. In the past year, different diameter mesa pn junctions were grown as shown in the inset in FIGURE 1. The researchers found that as mesa cross sections were made smaller, bulk-dominated behavior gave way to surface-dominated behavior at a temperature dependent crossover point. Future outgrowths of this research will enable shrinking of devices beyond present minimum size limits, opening the door to a wide collection of operational devices on the scale of tens of nanometers and smaller, such as nano-rectifiers, nano-LED's, nano-photodetectors, and nano-bipolar-transistors.

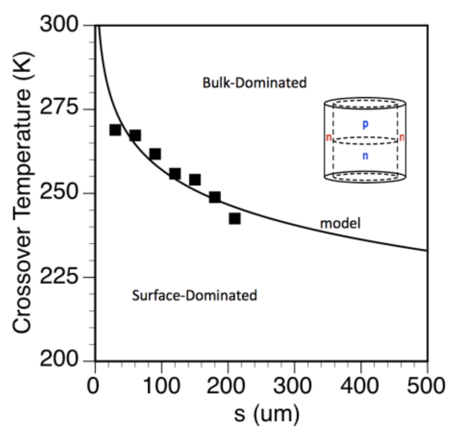

FIGURE 1

Bulk-surface crossover temperatures for InAs pn mesas. This plot shows the crossover point from bulk-dominated to surface-dominated current transport in InAs. Surface-dominated behavior extends up to higher temperatures in smaller devices.

B. Terahertz and Microwave Devices Based on the Photo-Excited Low Dimensional Electronic System

Professor Ramesh Mani, Georgia State University, Single Investigator Award

The objective of this project is to conduct follow-on research based on discoveries from an earlier ARO-supported project related to research studies of microwave/terahertz- photoexcitation-induced transport physical phenomena in the GaAs/AlGaAs, graphite, and graphene systems, with the goal of advancing the capability in the upper microwave and lower-terahertz bands. In FY12, Professor Mani made the first experimental observation of spin resonance by electrical detection in a graphene nanostructure.[1] The work was done in conjunction with Professor W. De Heer's group at the Georgia Institute of Technology that provided state of the

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[1] Mani RG, Hankinson J, Berger C, et al. (2012). Observation of resistively detected hole spin resonance and zero-field pseudo-spin splitting in epitaxial graphene. *Nat. Commun.* 3:996

art epitaxial graphene. The measurements examined epitaxial graphene prepared by heat treating SiC wafers. Small chips were prepared for Hall measurements by electron beam lithography. The devices included Gold-palladium contacts. The samples were cooled to liquid helium temperatures and excited with microwaves over the 10-50 Ghz band, and the electrical response was detected both in the presence and absence of microwave excitation. Most surprisingly, the devices exhibited a strong microwave response indicating that a graphene device may be used as a microwave power sensor. The reason for the strong electron heating, unlike in GaAs/AlGaAs is not yet understood; nevertheless, it turns out that heating is reduced under spin resonance conditions and this helps to detect the spin resonance. A second interesting and unexpected result of the experiment was that there occurred two spin resonance branches in this system. This effect was attributed to the breaking of the spin- and sublattice- degeneracy in the honeycomb graphene system. In such a picture, the measurements reveal the sublattice splitting in the epitaxial graphene system.

C. Vertical Cavity Transistor Lasers

Professor Milton Feng, University of Illinois - Urbana-Champaign, Single Investigator Award

The objective of this project is to develop a three-port vertical cavity transistor laser (VC-TL) to address the critical needs of energy efficient ultra-high speed data transmission applications. In FY12, the first VC-TL was made and demonstrated by Professor Feng's laboratory.[2] This work was the culmination of a three-year effort that led to a follow-on proposal with the goal of exploring the carrier dynamics achievable in such a regime. Prior to FY12, the researchers were able to achieve lasing in the edge-emitting, or more standard diode laser geometry. Given the significant process and prior fabrication work, he was able to achieve a vertical cavity regime with similar physics as the edge-emitter. VC-TLs have potential to become the laser of choice for optical interconnects due to the smaller emitting area. Advantages in heat dissipation and carrier injection area may translate into faster modulation speeds albeit with flat frequency responses also. VC-TLs of the future may reach scale sizes of around 100 nm, but with no need for special driver circuitry and with data rates approaching 100 Gbps. Use of VC-TL for various intra-chip, inter-chip, and board to board functions for data communications could enable unprecedented data parallelization and overall efficiencies. Both system level efficiencies of the circuits and optical interconnects as well as modulation energy efficiencies will be pursued in a follow on program, as well as more development of the theory of multi-junction emitters. Operation from electrical and optical functions and combined electrical-photonic interactions could lead to advanced circuitry with faster speeds and greater ability to interface with circuits and longer range "Si photonics" technologies.

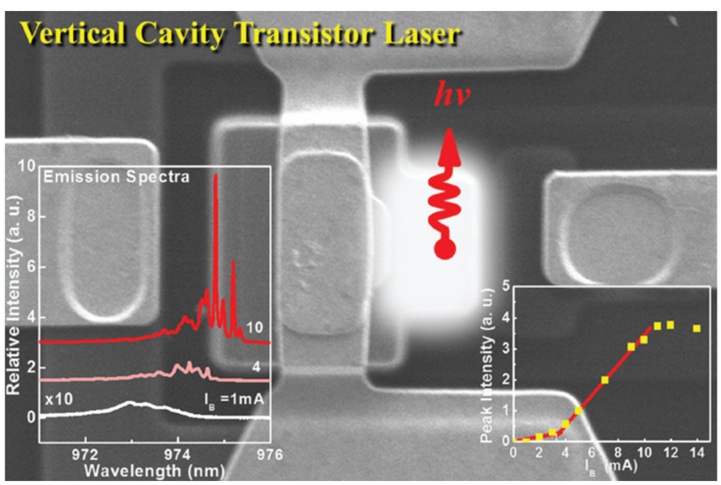

FIGURE 2

Top view of a vertical cavity transistor laser. The bright spot shows the emission that is normal to the page. The insets show emission spectra and peak intensity versus base current. *[Wu et al., 2012]*

[2] Wu MK, Feng M, Holonyak N Jr, k, Jr. (2012). Voltage modulation of a vertical cavity transistor laser via intra-cavity photon-assisted tunneling. *Appl. Phys. Lett.* 101:081102.

D. Expedient Computation of Electromagnetic Radiation Coupling to Integrated Electronics

Professor Andreas Cangellaris, University of Illinois - Urbana-Champaign, Single Investigator Award

The objective of this project is to develop a methodology to calculate the coupling of electromagnetic radiation to electronic components consisting of packaged circuit boards. The challenges are the complexity of the small circuit features, which are too complex to address with standard software EM models, and the variability and even unknown nature of the internal circuit and material features along with the properties of the interfering EM field. Professor Cangellaris and his group have developed powerful statistical macromodels that treat the variability and unknown properties of the circuits as stochastic variables and solve for the mean and variance of the parameters of interest. They have demonstrated the superiority of the stochastic collocation (and generalized polynomial chaos expansion) method in comparison to the Monte Carlo and stochastic Galerkin methods, in solving the stochastic problem. They have demonstrated promising results exploiting the quasi-periodic nature of some of the internal componentry (*e.g.*, layered materials in the circuit board) by modeling it as a periodic structure with random variability. They have developed and demonstrated an effective, efficient methodology to address the stochastic modeling of EMI coupling to interconnects on PCB's accounting for randomness in both interconnect routing and incident EM field. These results will be incorporated in a comprehensive model of the external, internal, and circuit board coupling, which will provide significant capability for computer-aided assessment of the immunity of electronic devices to EMI occurring through unanticipated paths and the exploitation of coupling paths and types of signals that can be used for the intentional jamming, interrogation, and manipulation of enemy electronic devices.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Advanced Microstructure Characterization of HgCdTe

Investigator: Professor David Smith, Arizona State University, Single Investigator Award
Recipients: Communications-Electronics Research, Development and Engineering Center (CERDEC), ARL-SEDD, BAE Systems

Professor Smith is using advanced electron microscopy methods, including high-resolution imaging, nanoprobe spectroscopy, and nanoscale elemental mapping, to study infrared mercury cadmium telluride (HgCdTe) material growth and processing. In FY12, samples of HgCdTe(211)/ CdTe(211)/ GaAs(211)B were grown by MBE at NVESD and characterized in Professor Smith's lab. Observations of the GaAs/CdTe interface have revealed the atomic-scale structure of the stepped GaAs surface and showed larger defective regions, most likely voids, that are attributed to polishing damage of the as-received GaAs(211) wafers (see FIGURE 3). Most recent studies of this system have included observations of the CdTe(211) upper surface before and after deposition of thick HgCdTe(211) epilayers.

This project involves a Cooperative Agreement between Arizona State University, ARL-SEDD, and the CERDEC Night Vision and Electronic Sensors Directorate (CERDEC-NVESD) wherein the Army researchers are supplying unique samples for microanalysis. In addition, Professor Smith's characterization results such as those described above are transitioning to Army laboratories to refine the growth process.

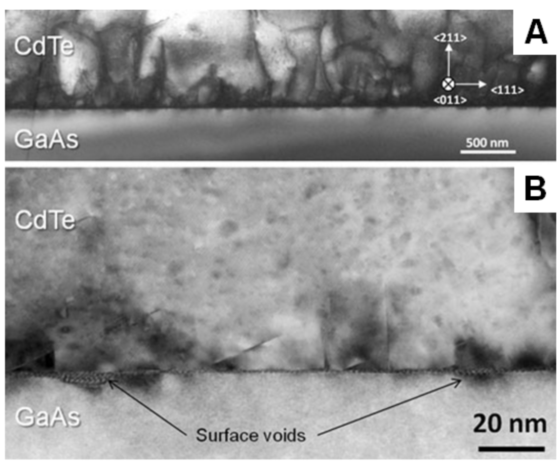

FIGURE 3

Cross-section bright-field TEM images of the CdTe/GaAs interface. The panels reveal (**A**) top-surface GaAs defects possibly related to polishing damage on as-received GaAs(211) wafers, and (**B**) higher-magnification that identifies polishing damage as "surface voids." The depth of the surface voids is similar to that seen by AFM.

B. Extremely Compact Efficient Laser Sources (HiPER II)

Investigator: Dr. Jonah Jacob, Science Research Laboratory (SRL), DARPA Award
Recipients: Massachusetts Institute of Technology Lincoln Laboratory, ARL-CISD, SVT Assoc.

The Science Research Laboratory, under the direction of Dr. Jonah Jacob, was a research performer in the ARO/DARPA Program (HiPER II), which brought increased understanding and capability to laser diodes. This research led to two follow-on efforts involving small businesses and MIT Lincoln Laboratory. A key discovery from Dr. Jacob and colleagues included improved cooling and packaging of laser diodes with the ability to sustain 600 W continuous wave per bar (600 W CW/bar). This result far exceeds current technology of only 80-

100 W. These results transitioned to new programs (ARO/DARPA SBIR and ARO/DARPA MTO BAA) that aim to achieve higher breakdown threshold levels at the mirrors. The laser bars have transitioned to SVT Assoc., one of the small business partners within the ARO/DARPA SBIR, to explore making better mirrors and pushing the capabilities of the laser bars to higher power levels.

C. Uniform, Large-Area $BaSrTiO_3$ Growth and Novel Material Designs to Enable Fabrication of High Quality, Affordable, and Performance Consistent Phase Shifters

Investigator: Professor David Boyd, California Institute of Technology; Single Investigator Award
Recipients: ARL Weapons and Materials Research Directorate (ARL-WMRD), CERDEC, Agile Materials and Technologies, Inc.

On-the-move (OTM) Army radio communications systems require agile antennas to maintain pointing accuracy in spite of disruptive vehicle motion during rapid movement over rough terrain. Phased array antenna technology can meet the agility requirement, but the biggest barrier is the cost of the phase shifters. The objective of this project was to design and fabricate proof-of-concept phase shifters based on advanced thin film materials and to transfer the resulting technology to the Army. This cost can be traced to fabrication and material costs and to costs associated with non-uniformity between devices. Professor Boyd's laboratory has demonstrated highly uniform growth recipes using their unique MOCVD reactor, which can control each component of the precursor flux in real time using real time absorption measurements of the vapor before it reaches the substrate. The researchers have developed the growth and science protocols for novel recipes of compositional grading and heterostructure layering to promote enhanced environmental insensitivity, increased phase shift per device, and increased device yield. They also developed unique control software and in-situ diagnostics for these device structures.

In the course of the project the MOCVD reactor design, the associated software, and the growth and fabrication recipes transitioned to ARL-WMRD. Close collaboration was maintained with CERDEC and Agile Materials and Technologies, Inc. (CERDEC's industry partner for phase shifter development). The technology is being transferred to CERDEC's Affordable Directional Antenna and Pointing Technologies ATO and Electronic Thin Film Materials for OTM Advanced Antennas TPA.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Increased Lifetime Beyond Radiative Limit Using Carrier Separation

Professor Yong-Hang Zhang, Arizona State University, STIR Award

One of the key parameters for photodetectors is the carrier life time, which determines the dark current and ultimate device performance. It is highly desirable to have a semiconductor with a very high absorption coefficient like that in direct bandgap semiconductors but very low recombination rate like that in the indirect semiconductors. Professor Y-H Zhang is exploring a novel idea to realize synthetic semiconductor structures by taking advantage of spatial separation of electrons and holes to minimize the three recombination processes (SRH, radiative and Auger). The goal of this research is to combine the high absorption found in direct bandgap semiconductors with the long lifetimes in indirect bandgap semiconductors, which will be attempted by growing layered structures consisting of a set of alternating semiconductor superlattice and heterostructure layers (see FIGURE 4). The photogenerated carriers are thermalized to different layers, which act as electron and hole conduction channels. It is reasonable to anticipate that both types of carriers can be easily transported to the corresponding contacts with reduced recombination rate and thus enhanced carrier long lifetime. In FY13 the research team will test this thesis using different designs to create spatially separated electron and hole pathways to enhance carrier recombination lifetimes.

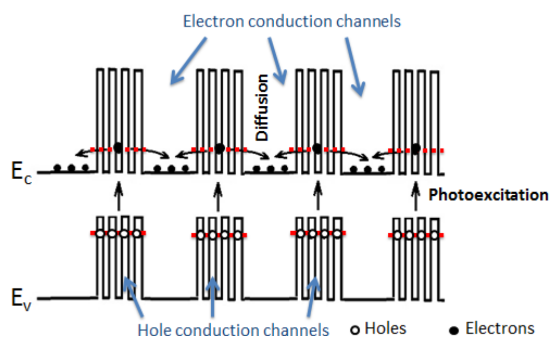

FIGURE 4

Schematic of proposed structure consisting of InAsSb and T2SL layers and spatial separation processes of the photogenerated electrons and holes. Upon photoexcitation, electrons are transported to contact in the electron conduction channels (InAsSb), while holes are transported to contact in the hole-conduction channels.

B. Time-Frequency and Non-Laplacian Phenomena at Radio Frequencies

Professor Michael Steer, North Carolina State University, Single Investigator Award

In FY13, this project will explore approaches to extend the conventional analysis, such as fractional calculus in the time domain and non-integer Laplacian analysis, as well as coupled physics descriptions of electro-thermal and acoustic-electro effects. The intent is to establish the fundamental understanding and fundamental concepts that will enable computer aided design tools and reduced order circuit models which can address these difficult phenomena and result in electronic systems with lower levels of cosite interference and reduced flicker noise effects. This would significantly impact military radar, radio, sensors, and electronic warfare capabilities.

The objective of this project is to invent and extend radio circuit theory to include diffusive and multi-scale, multi-physics analysis in order to address a range of phenomena that cannot be treated or even understood using traditional methods and concepts of circuit analysis. It is well known that some cosite interference phenomena cannot be understood or predicted by the tradition concept of sum and difference frequency intermodulation products. Since this cannot be understood using traditional concepts, it cannot be remediated except to avoid certain frequency band combinations. Similar phenomena accompany situations of high power jamming by an adversary and of intentional manipulation of circuits using inserted signals. Another poorly understood phenomenon is the interference due to flicker noise (1/f noise) in oscillators, which rapidly increases as the noise frequency approaches the frequency of oscillation and which mixes to produce spurious frequencies that limit the detection of desired signals or the range that can be resolved. Recent advances have identified chaotic behavior as a possible source of the flicker noise. Interference is also observed in systems which are supposedly linear, which is called "passive intermodulation distortion." Professor Steer has also characterized modulation phenomena resulting from the electro-thermal effects of thermal relaxation in very small electronic components and acoustic-electrical effects of mechanical vibrations on antenna elements. He has also observed diffusion effects in circuits, such as the very long term transitions in filters as they charge and discharge. These phenomena cannot be explained, understood, or controlled by conventional circuit design approaches, such as traditional Laplacian analysis, which miss significant physics.

C. Self-Consistent Ambipolar Transport and HF Oscillatory Transient in Graphene Electronics

Professor Jean-Pierre Leburton, University of Illinois - Urbana-Champaign, Single Investigator Award

The objective of this project is to explore the onset of hot electron-induced plasma oscillations in various kinds of graphene layer devices and define new methods for investigating the ambipolar nature of the transport, by determining the condition required for emission of electromagnetic radiations in the THz frequency regime. Professor Leburton's laboratory will focus on high-frequency current oscillations in graphene layers, induced by hot carriers, both electrons and holes interacting with OP during transient excitations by a constant electric field. This theoretical effort will use a Boltzmann-Poisson approach that solves self-consistently the Boltzmann equation for the distribution of both kinds of charge carriers, while accounting for space charge effects through the Poisson equation. The methodology relies on a large signal model for solution of the spatio-temporal Boltzmann equation developed by the PI. It is anticipated that in FY13, this research will lead to new modeling and simulation approaches to semi-classical transient regime in single- and double-layer graphene.

D. Enhanced Light Emitters based on Metamaterials

Professor Vinod Menon, CUNY - Queens College, Single Investigator Award

The objective of this project is to build on prior work where Professor Menon's laboratory developed hyperbolic metamaterial (HMM) reflectors that enhance the spontaneous recombination rate across a broad spectral band. It is anticipated that in FY13, Professor Menon will determine whether the HMM can be used in a real light emitter, potentially enabling high-speed data communications. Other uses for this type of HMM reflector published in *Science* include use of the increased density of states of the photons for sub-wavelength lasers since the superlattice-like materials can support deeply sub-wavelength optical modes.[3] In a prior YIP award, Professor Menon demonstrated flexible lasers based on layered polymers. His experience with quantum dots as related expertise with periodic structures will play a role in his pursuits with HMMs. For example, he will study use of Fano resonance structures using silver nanocylinders to enhance in and out coupling of light to the cavity.

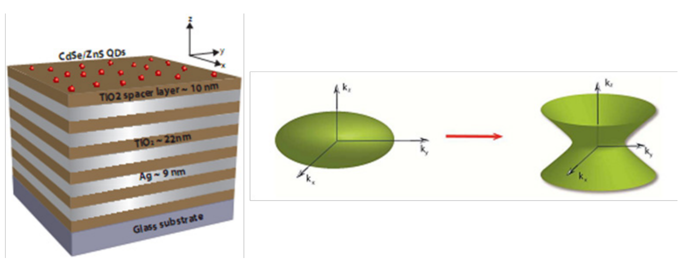

FIGURE 5

Hyperbolic metamaterial formed by TiO_2/Ag superlattice with CdSe/ZnS quantum dots to enhance spontaneous lifetime over a broad bandwidth. The wavevector diagrams show the difference between a typical dielectric material and a hyperbolic metamaterial.

[3] Krishnamoorthy HNS, Jacob Z, Narimanov E, et al. (2012). Topological transitions in metamaterials. *Science* 336:205-209

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. William Clark
Division Chief
Program Manager, Electronic Sensing

Dr. Michael Gerhold
Program Manager, Optoelectronics

Dr. Dev Palmer
Program Manager, Electromagnetics, Microwaves, and Power

Dr. Dwight Woolard
Program Manager, Solid State and High Frequency Electronics

B. Directorate Scientists

Dr. Thomas Doligalski
Director, Engineering Sciences Directorate

Mr. George Stavrakakis
Contract Support

C. Administrative Staff

Ms. Pamela Robinson
Administrative Support Assistant

CHAPTER 6: ENVIRONMENTAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2012* is to provide information on the programs and basic research efforts supported by ARO in FY12, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Environmental Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY12.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Environmental Sciences Division supports basic research to advance the Army and Nation's knowledge and understanding of the atmosphere, the terrestrial domain of the natural environment, and habitation therein by the Soldier. Specifically, the goals of the Division are to develop first-principle knowledge of the physical, chemical, and biological basis of atmospheric and terrestrial processes at Army relevant spatial and temporal scales, as well as to improve our fundamental understanding of the lower atmosphere, air-land interface, and near-surface environment, and their dynamic behavior and complexity at those scales. The research results stimulate future studies and seek to maintain U.S. dominance at the forefront of research in military-relevant areas of the environmental sciences.

2. Potential Applications. The research efforts managed by the Environmental Sciences Division provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO in the environmental sciences will impact and leverage environmental factors in favor of the Army to take advantage of environmental weakness of adversary systems, optimize the design of new systems, and ensure mission sustainability. The capability to understand at a fundamental level the atmosphere and remotely sense and interpret Earth's surface features (both natural and anthropogenic) is critical for mission success.

3. Coordination with Other Agencies. Because the natural environment is by nature a highly complex and dynamic system characterized by complicated feedbacks, multidisciplinary approaches are fundamental to environmental science and are addressed in every aspect of this Division's basic research program. For this reason, the basic research program is developed in conjunction with the ARL Computational and Information Sciences Directorate (ARL-CISD) Battlefield Environment Division and the laboratories of the U.S. Army Corps of Engineers (USACE), the Army Communications-Electronics Research, Development, and Engineering Center, Night Vision and Electronic Sensors Directorate (CERDEC-NVESD) Countermine Division, and the Army Engineer School. The program is also coordinated with related programs in other Department of Defense agencies, including the Navy, Marine Corps, Air Force, the Defense Advanced Research Projects Agency (DARPA), the Strategic Environmental Research and Development Program (SERDP), and the Environmental Security Technology Certification Program (ESTCP). Across the U.S. Government, coordination with the Environmental Protection Agency (EPA), National Aeronautics and Space Administration (NASA), National Oceanic and Atmospheric Administration (NOAA), National Science Foundation (NSF), Department of Agriculture - Agricultural Research Service occur as a matter of standard operations.

B. Program Areas

To meet the long-term program goals described in the previous section, the Environmental Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The

Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY12, the Division managed research efforts within these three Program Areas: (i) Atmospheric Science, (ii) Terrestrial Sciences, and (iii) Habitation Science. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Atmospheric Science. The objective of this Program Area is to explore and understand the constituents, processes, and effects of the atmospheric boundary layer over land. This understanding is mission critical since intelligence planning for the battlefield depends on a full and timely knowledge of atmospheric conditions and their effects on operations, weapon systems, and the Soldier. Knowledge of the atmosphere and its effects on Soldiers and sensor systems are essential for command and control as well as visualization of the battlefield at all echelons. The ultimate goal of this Program Area is to uncover methods and tools for the Army to address the wide spectrum of conditions and influences within the atmospheric boundary layer on Army operations and systems. Extremely close coordination of this Program with ARL-CISD Battlefield Environment Division (BED) was facilitated through the vehicle of a developmental assignment to ARO of a BED Program Manager.

2. Terrestrial Sciences. The goal of this Program Area is to improve the fundamental understanding of terrain and land-based phenomena. By investigating the broad spectrum of terrain and land-based phenomena that affect the Army, the long-term applications of discoveries made through this program will significantly enhance the Army's ability to fully achieve its Future Force vision for full-spectrum operations. The achievement of this vision will require a sustained investment in Terrestrial Sciences basic research that addresses the scientific challenges identified as capability gaps for the Army's Future Force, together with those issues understood to be critical to the stewardship of Army installations necessary to insure the sustainability of Army training and testing lands and the remediation of Army contaminated sites. Because the natural environment is, by nature, a highly complex and dynamic system characterized by complicated feedbacks, there is an increasing need for multidisciplinary approaches to address the multifaceted problems that are addressed by the ARO Terrestrial Sciences basic research program. This extramural research program is developed in conjunction with the laboratories of the USACE Engineer Research and Development Center (ERDC), the Countermine Division of CERDEC-NVESD, and the Army Engineer School, with input from land managers at several Army installations.

3. Habitation Science. The goal of this Program Area is to explore engineered biological processes, membrane processes for water purification, resource reuse and transformation. Research efforts within this program are exploring radically new unit operations with the potential to maximize recovery of usable energy via physical, chemical and biological processes. Such operations need to simultaneously minimize system mass, volume and power while controlling the amount, composition and release of reaction by-products. This Program Area also coordinates efforts, and leverages funding with other agencies, including Product Manager Force Sustainment Systems, USACE, and DARPA. Potential long-term applications of the research efforts managed within this Program Area include systems that continuously accommodate troop populations of variable size and perform equally well in urban and remote locations under a wide range of climates with maximum recovery of usable energy via physical-chemical and biological processes.

C. Research Investment

The total funds managed by the ARO Environmental Sciences Division for FY12 were $4.1 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY12 ARO Core (BH57) program funding allotment for this Division was $2.8 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $0.2 million to projects managed by the Division. The Division also managed $0.8 million of Defense Advanced Research Projects Agency (DARPA) programs. Finally, $0.3 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY12 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research projects. Research projects are developed by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts.

The following subsections summarize projects awarded in FY12 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY12, the Division awarded 14 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to explore and understand the constituents, processes, and effects of the atmospheric boundary layer over land, explore engineered biological processes, resource reuse and transformation, and membrane processes for water purification. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Largus Angenent, Cornell University; *Conversion of Biomass Into n-caproate*
- Professor Ben Balsley, University of Colorado - Boulder; *High-Resolution Atmospheric Studies During the Matterhorn Campaigns*
- Professor Rafael Bras, Georgia Technical University; *Maximum Entropy Principle as a Unifying Theory for Characterization and Sampling of Multi-scaling Processes in Hydrometeorology*
- Professor Hui Cao, Yale University; *Real-Time, High-Throughput Bio-Aerosol Sampling System based on Negative Polarization of Backscattering*
- Professor George Emmitt, Simpson Weather Associates, Inc.; *Deployment of an airborne DWL during Materhorn and validation of the ARO ADLAATS*
- Professor David Fritts, G & A Technical Software, Inc.; *Turbulence Fine Structure, Intermittency, and Large-Scale Interactions in the Stable Boundary Layer and Residual Layer*
- Professor Thomas Vonder Haar, Colorado State University - Ft. Collins; *DoD Center for Geosciences/Atmospheric Research*
- Professor Yong-qing Li, East Carolina University; *Characterization of Atmospheric Biological Particles Using Confocal Raman Spectroscopy and Optical Trapping*
- Professor Eric McDonald, Desert Research Institute - Las Vegas; *Soil and Terrain Analysis of Vehicle Mobility*
- Professor Andreas Muschinski, Northwest Research Associates, Inc.; *Measurement Science of the Intermittent Atmospheric Boundary Layer*
- Professor Richard Raspet, University of Mississippi; *Measurement and Prediction of Infrasonic Wind Noise in Forests*

- Professor John Regan, Pennsylvania State University; *Whole-Cell Modeling and Integrated Experimentation of Bioelectrochemical Systems*
- Professor Jie Shan, Purdue University; *Topographic Exploitation*
- Professor Charles Toth, Ohio State University; *Exploitation of Full-Waveform LiDAR*

2. Short Term Innovative Research (STIR) Program.

No new starts were initiated in FY12.

3. Young Investigator Program (YIP). In FY12, the Division awarded one new YIP project. This grant is driving fundamental research to investigate a new digital holographic method to image flowing aerosol particles in situ and to establish the feasibility of an interferometric infrared-probe technique to characterize their composition. The following PI and corresponding organization was the recipient of the new-start YIP award.

- Professor Matthew Berg, Mississippi State University; *Digital Holographic Interferometry for Airborne Particle Characterization*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY12 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Symposium on the Applications of Geophysics to Engineering and Environmental Problems;* Tuscon, AZ; 24-29 March 2012
- *Exploration Workshop: Concepts in Electromagnetic Scattering for Particulate-Systems Characterization*; Memphis, TN, 18-19 May 2012

5. Special Programs. In FY12, ARO Core Research Program funds provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded three new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

C. Multidisciplinary University Research Initiative (MURI)

No projects were active in FY12.

D. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY12.

E. Small Business Technology Transfer (STTR) – New Starts

No new starts were initiated in FY12.

F. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY12, the Division managed one new ARO (Core) HBCU/MI project. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

G. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY12.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY12, the Environmental Sciences Division managed four new DURIP projects, totaling $0.2 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies to explore including studies to explore fluvial processes, improved infrastructure design, maintenance and protection and behavior of micro/nano-particles in the terrestrial environment.

I. DARPA Materials with Novel Transport Properties (MANTRA) Program

The ARO Environmental Sciences Division is serving as agent for the DARPA MANTRA program. The goal of this program is to demonstrate a prototype seawater desalination system that produces high rates of potable water from seawater while achieving two orders of magnitude reduction in size and weight and one order of magnitude reduction in power compared to existing systems. The research supported in this program focuses on investigating and designing large-area membranes with substantially reduced defects for improved fluid transport by increasing the use of CNTs or other gatekeeper molecules in the membrane, while preserving the salt rejection at 98%. However, research pursuing evolutionary improvements to the existing state of practice for the rapid development of more advanced membrane concepts is excluded. This program will move to competition between phase two prototypes during FY13.

J. Global Military Operating Environments: Linking Natural Environments, International Security and Military Operations

The goal of this Congressionally-mandated project was to explore military testing and training in support of the Army Yuma Proving Ground Natural Environments Test Office. Five distinct research efforts were pursued: (i) Multiple Master Environmental Reference Sites (MERS) for comprehensive characterization of soil processes were established at sites that represent prevalent terrain conditions critical for military operations and testing (*i.e.*, different military operating environments; MOE), (ii) data analysis of the established MERS was initiated to evaluate the temporal dynamics of energy fluxes under both natural and disturbed conditions in different climatic regimes, (iii) techniques and methods for incorporating data on soil and soil surface processes and conditions in the development and testing of technologies for the detection and defeat of IEDs were studied and a set of recommended approaches developed, (iv) terrain conditions at primary testing and training installations were characterized to determine terrain analogs for areas of current and future strategic interest, and (v) a military environments reference database was created that compiles soil and terrain data and related literature to increase availability of global terrain data to the testing and training community. This effort concluded in FY12.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Environmental Sciences Division.

A. Acoustic Tomography of the Atmospheric Surface Layer

Professor Vladimir Ostashev, University of Colorado, Single Investigator Award

The Boulder Atmospheric Observatory (BAO) acoustic tomography array was built and an algorithm was developed that allows robust and accurate reconstruction of temperature and wind velocity fields in acoustic tomography of the atmospheric surface layer (ASL). The main goal of this project has been to employ the BAO array for detailed studies of the temperature and wind velocity fields in the ASL. Particular objectives of the project are to process and analyze the data recorded during a joint experiment; to upgrade capabilities of the BAO acoustic tomography array for 3D tomography and 2D tomography with reciprocal sound transmission; to achieve near real time reconstruction of the temperature and wind velocity fields; to carry out joint experiments with the BAO acoustic tomography array and other meteorological instrumentation; to continuously operate the BAO acoustic tomography array; and to continue theoretical studies of acoustic tomography of the ASL. There is close collaboration with several organizations, including NOAA/ESRL, CRREL, ARL, and OSU. The proposed research will establish the BAO array as a unique permanent facility for remote sensing of temperature and wind velocity in the ASL.

FIGURE 1 shows the tower and microphone configuration, in addition to one of the speaker towers, of the BAO acoustic tomography array that is currently the only operational array for acoustic tomography in the ASL. Speakers and microphones at the upper level of the BAO acoustic tomography array have been used in transmission and reception of acoustic signals, thus enabling 2D, horizontal slice tomography. This feature of the array allows continual monitoring of the temperature and velocity fields inside the tomographic volume or area. All previous arrays for acoustic tomography were dismantled after a short time of operation.

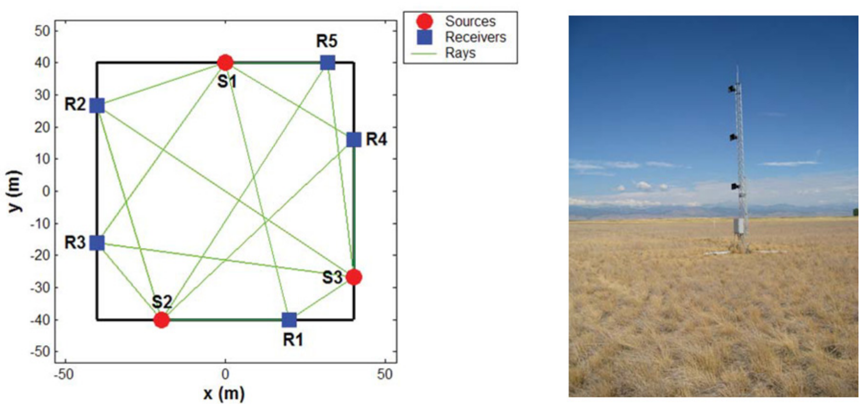

FIGURE 1

BAO acoustic tomography array. (left) The location of eight towers of the BAO acoustic tomography array in a horizontal plane. Green lines indicate sound propagation paths from speakers (red circles) tomicrophones (blue squares). (right) A speaker tower of the BAO.

The array enables measurement of the travel times of sound signal propagation between different speakers and microphones, which constitute the tomography array. The results in reconstruction of the temperature and wind velocity fields in the acoustic tomography experiment at the BAO are shown in FIGURE 2. The BAO tomography array can be used for testing theories of line-of-sight sound propagation through a turbulent atmosphere, including theories of broad-band propagation and temporal coherence, which are yet to be developed. In such experiments, the tomography array could provide information about both atmospheric turbulence and fluctuations in acoustic signals propagating through the turbulence.

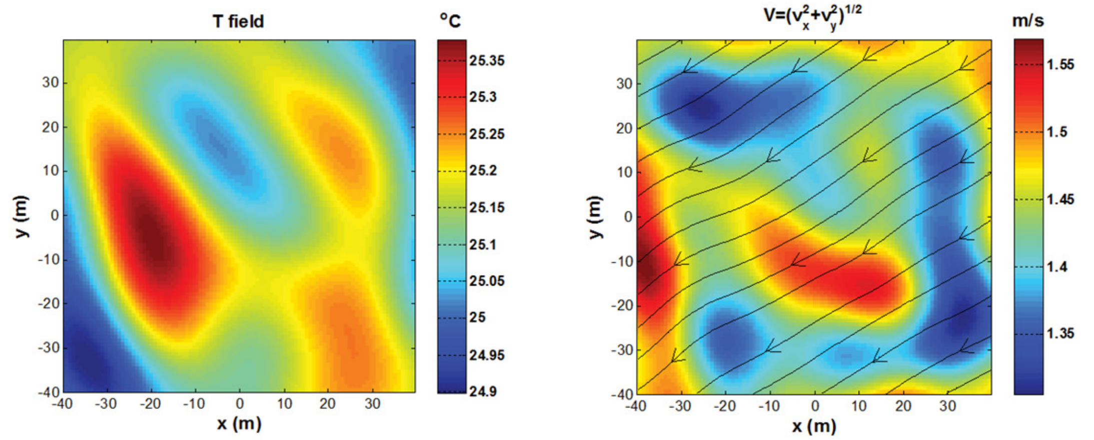

FIGURE 2

Temperature and wind velocity fields in the acoustic tomography experiment at the BAO. (left) Temperature field reconstructed with TDSI in the acoustic tomography experiment at the BAO. (right) Magnitude of the wind velocity reconstructed with TDSI in the acoustic tomography experiment at the BAO. Arrows indicate the direction of the wind velocity vector.

B. Measurement Science of the Intermittent Atmospheric Boundary Layer

Professor Andreas Muschinski, University of Massachusetts - Amherst, Single Investigator Award

The goal of this project is to explore the fundamental processes occurring within the intermittent atmospheric boundary layer. One goal of this research is to review, refine and generalize the theoretical foundations to analyze and interpret the optical and in-situ data that was collected during a field experiment at the BAO site near Erie, CO. The researchers demonstrated that the optical angle-of-arrival fluctuations observed with a large-aperture telescope equipped with a moderately fast CCD camera can be used to retrieve, with high sensitivity and accuracy, path averages of the vertical temperature gradient, as well as the transverse wind velocity, the temperature structure parameter along a horizontal propagation path (200 m path length, 1.7 m above ground level) in the atmospheric surface layer. FIGURE 3 shows a comparison of optically derived and sonically measured velocities measured using tower 1 of the Boulder Atmospheric Observatory (BAO). Very good agreement was achieved, demonstrating the abilities of the optical technique.

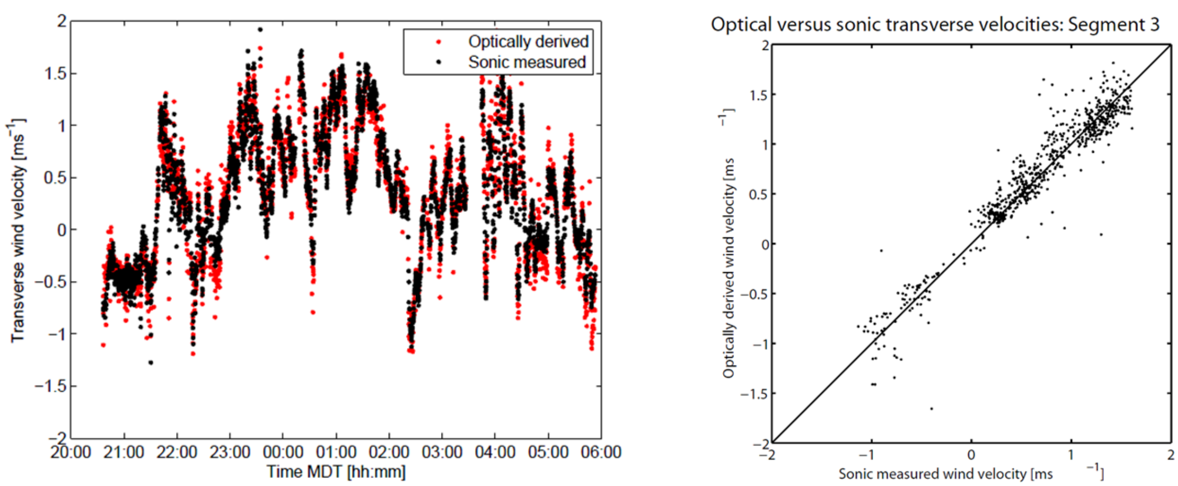

FIGURE 3

Comparison of optically-derived and sonically-measured velocities. (left) Optically derived and sonically measured velocity time series retrievals using time-delay-to-peak method (Tower 1). Red dots correspond to the velocity obtained by the time-delay-to-peak method, while the black dots correspond to the sonic measured velocity at 1.77m AGL. (right) Correlation between the optically derived and sonically derived methods.

Within this project an optically derived method was developed to obtain wind velocities using statistical techniques. The optically retrieved time series of (i) temporal fluctuations of the path-averaged, vertical temperature gradient, of (ii) the path-averaged, beam-transverse horizontal velocity component, and of (iii) the path-averaged temperature structure parameter were found to agree very well with in-situ reference measurements. In addition, the researchers demonstrated that temperature structure parameters and lateral wind velocities can be effectively retrieved from optical angle of arrival statistics estimated from test-light image centroids.

C. Measuring and Modeling Hydrologic Fluxes and States from Aquifer to Atmosphere at Multiple Scales
Professor Warren Barrash, Boise State University, DEPSCoR Award

The objective of this project is to develop data assimilation methods to improve predictions of soil moisture content at scales ranging from meters to kilometers. The data collected from the field at a range of spatial and temporal scales makes use of previously installed instrumentation in semi-arid and riparian environments. These data and those from laboratory studies were used in conjunction with ecohydrologic models, in part for model calibration and verification. Additionally, this work is advancing the use of data assimilation in hydrological models. At the time of this report, eight manuscripts have been submitted and one paper has been published.

Working towards the goal of data assimilation into models, the researchers conducted a number of monitoring studies and focused heavily on data assimilation. Noteworthy accomplishments are listed below.

- *3D transient hydraulic tomography in unconfined aquifers with fast drainage response:* explores the use of 3D transient hydraulic tomography in an unconfined aquifer using numerical simulation.
- *A simplified approach for estimating soil carbon and nitrogen stocks in semi-arid complex terrain:* presents an approach to using remotely sensed data to provide information on nutrient distribution.
- *Hydrologic data assimilation with a hillslope-scale resolving model and L-band radar observations:* improves the ability to determine soil moisture at a higher resolution than is currently possible, using remotely acquired data.

D. Design and Control of Omnidirectional Unmanned Ground Vehicles
Professor Karl Iagnemma, Massachusetts Institute of Technology, Single Investigator Award

Omnidirectional wheels are currently used in a variety of vehicles, such as mobile robotic bases and wheelchairs. A drawback of these wheel designs (roller wheel and mecanum wheels) is that they are complex, with numerous roller, axle, and bearing elements. The objective of this project, which ended in FY12, was to study the design and control of ultra high-performance unmanned ground vehicles with omnidirectional motion capability. In FY12, the research team developed an entirely novel omnidirectional vehicle with anisotropic friction wheels in which the wheel has a series of bendable "nodes" on its circumference, each of which is made of two materials with differing friction properties: one material exhibits high friction, and the other exhibits low friction (see FIGURE 4). The high friction section of the node generates a high traction force, while the low friction section enables the wheel to passively slide. The wheels are arranged such that the wheel exhibits high traction in its driving direction (much like a conventional tire), but low traction when sliding laterally. Exploiting this "anisotropic friction" property, the wheel enables a vehicle to realize omnidirectional motion (*i.e.*, the vehicle can move any direction within the plane—forward, back, or laterally), and such a prototype was developed (see FIGURE 5). While many other omnidirectional wheel drives exist, the newly developed wheel is simpler than any other existing design because the wheel is composed of a single, moldable element.

Two experimental tests, an omnidirectional mobility test and a traction performance test, were performed in which the newly developed vehicle's performance was compared with that of vehicles using currently used omnidirectional wheels. It was found that the vehicle with the proposed wheels has similar omnidirectional motion characteristics to a vehicle with conventional omnidirectional wheels. The proposed wheel was found to grip to the ground with its high friction property, enabling the vehicle to generate much larger traction force than conventional wheels do. Thus, a significant improvement by the proposed wheel over the conventional omnidirectional wheel was found to be the high traction performance while having equivalent omnidirectional mobility. In addition, the proposed wheel consists of single, moldable element and no mechanical components such as bearings and axles, which allows for a reduction in design complexity and potential for decreased production cost and increased robustness. The newly developed wheel will be able to enhance a mobility performance of an omnidirectional vehicle requiring both high traction performance and omnidirectional motion (*i.e.*, for vehicle towing or for environment such as sloped ground).

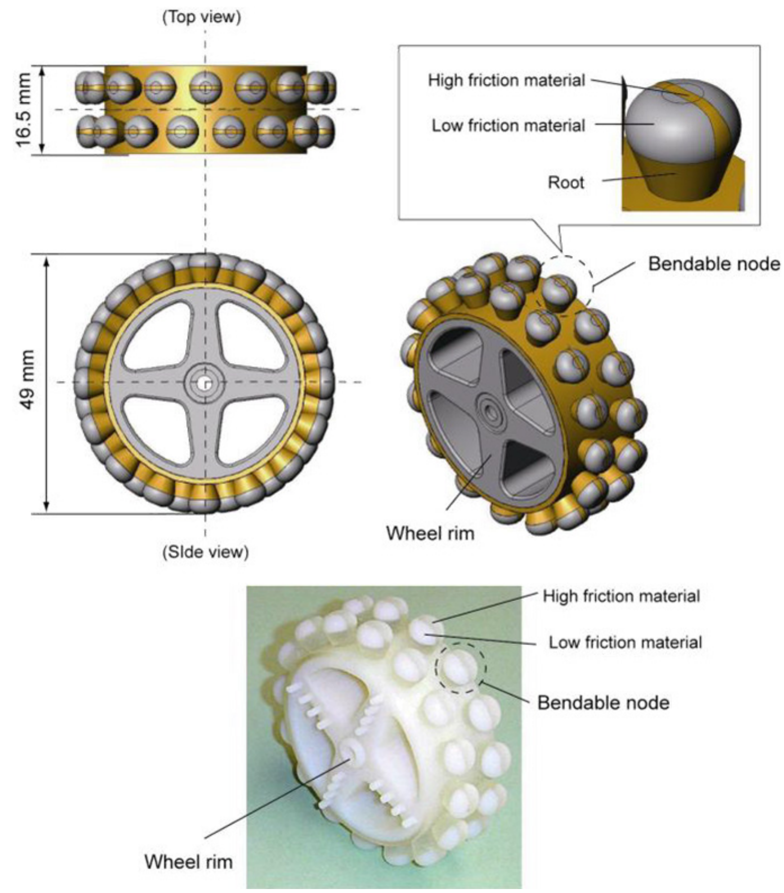

FIGURE 4
CAD model and prototype of the multi-material anisotropic friction wheel for omnidirectional vehicle.

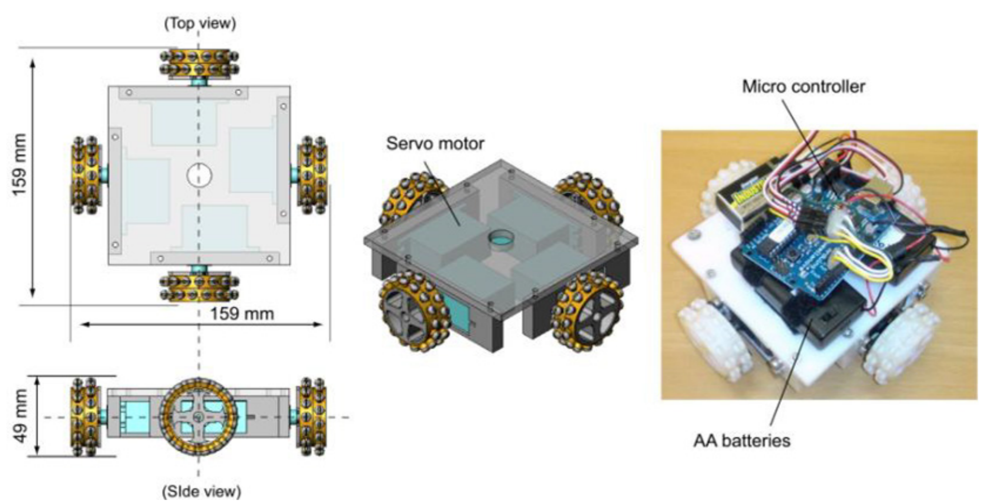

FIGURE 5
Prototype of the omnidirectional mobile with proposed wheel.

E. Saturated Particle Transport in Porous Media
Professor Patricia Culligan, Columbia University, Single Investigator Award

The goal of this work is to better understand the influence of flow direction and particle size distribution of particle transport in porous media. The researchers aim to model the behavior of subsurface contaminants, such as those present at Army installations including PCBs, fuels, solvents, herbicides/pesticides, heavy metals, munitions materials, and radioactive materials. To achieve this, a series of laboratory experiments were performed in which the concentrations of fluorescent particles of different sizes were measured as they moved through a saturated bed of glass beads (see FIGURE 6).

The real-time spatial resolution of concentrations of 1 μm, 3 μm, 6 μm, and 1-25 μm mixed fluorescent particles, as well as 1-um with 6-um particles present and 6 μm with 1 μm particles present, were measured under one-dimensional, steady state flow conditions through a saturated bed of 0.5 mm rough glass beads at a velocity of 1.7 m/d. Irreversible attachment rates (k_i) were lowest for downward flow ($3.78x10^{-5}$ s^{-1}) of 1 μm particles in contrast to upward ($6.00x10^{-5}$ s^{-1}) and horizontal ($5.49x10^{-5}$ s^{-1}) flow. Upward (k_i $0.92x10^{-3}$ s^{-1}) and downward ($1.00x10^{-3}$ s^{-1}) flow of mixed 1-25 μm particles were similar. Irreversible attachment rates (k_i) increased in conjunction with particle size (1-25 mixed>6>3>1 μm), although they decreased when 1 μm and 6 μm particles were combined. In all cases, the majority of particle retention occurred within the first 1 cm of the particle inlet boundary. This work highlights the influence of particle size distribution and flow direction on particle filtration. Future work will determine the real-time spatial resolution for 1 μm and 3 μm particles combined, repeat all experiments under vertical and horizontal flow conditions and undertake numerical modeling of the experiments.

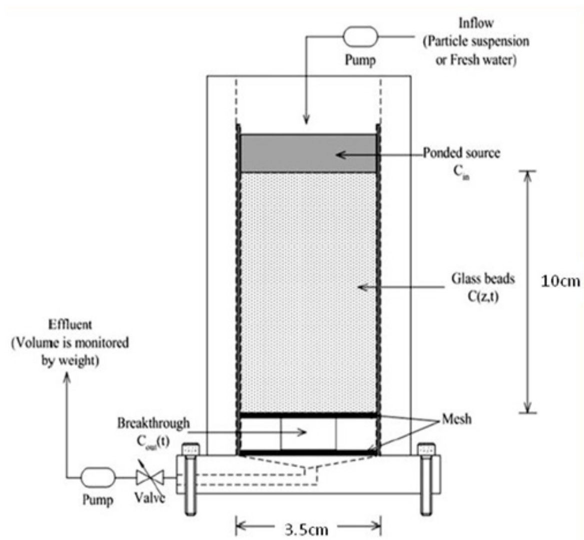

FIGURE 6
Schematic diagram of experimental box.

F. Predictive Mapping of Soil Thickness and Erosion Rates
Professor Jon Pelletier, University of Arizona, Single Investigator Award

Soil thickness and soil texture are important input parameters for hydrologic models. As the spatial distribution of soil thickness and texture are strongly variable at hillslope scales, modeling soil thickness and texture in the watershed scale is needed if the hydrologic and geomorphic processes that depend on soil thickness can be modeled accurately. Recent studies have demonstrated that numerical models that assume a long-term balance between soil production and soil erosion can accurately predict the spatial distribution of soil thickness in semiarid and relatively humid areas, where soil thickness varies gradually along hillslope profiles. However, these models have not been tested in arid regions, where soil thickness varies abruptly and where the influence of eolian accretion on soil thickness and on soil texture may be much more significant.

In this project, a numerical model for the prediction of soil thickness and dust content in an arid mountainous area of the Mojave Desert, characterized by thin soils (<1 m) and extreme variability in soil thickness at essentially all spatial scales, was developed and tested (see FIGURE 7). Soil production rates in the model are quantified using exponential and humped soil production functions, and soil erosion rates are quantified using the nonlinear depth- and slope-dependent transport function, assuming that only the upper soil horizons (A+B) can be transported. The research team calibrated the soil production and dust accretion rates in various plutonic lithologies (granite and diorite) using (i) field data of soil thickness and (ii) dust content of the soil estimated by analysis of immobile element concentrations. The model results were validated using measured data on soil thickness and the presence/absence of soil in an attempt to adequately represent the great spatial heterogeneity in soil thickness at the study sites. Good agreement was found between observed and predicted soil thickness and dust content in the soil. These results demonstrated that the prediction of soil thickness and fraction of eolian dust in the soil can at different sites across the landscape is possible.

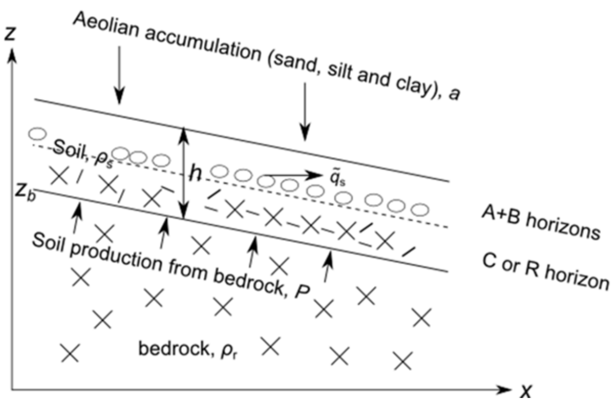

FIGURE 7
Schematic diagram of the main model components.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Improved Measurement System for Atmospheric Studies

Investigator: Professor Yannick Meillier, University of Colorado, Single Investigator and DURIP Awards
Recipient: ARL-CISD

Professor Meillier of the University of Colorado has made advances in developing a Tethered Lifting System (TLS) with sensors and high-wind blimps. The TLS consists of an aerodynamic blimp with a suspended line of multiple sensors to make measurements at either fixed altitudes or by profiling from the ground up to many kilometers altitude. Each of the multiple sensors consists of low-frequency temperature, velocity, pressure and humidity sensors, in addition to newly available low-noise high frequency hot-wire and cold-wire sensors for fine-scale measurements in the challenging low turbulence conditions of the night time boundary layer. Low-frequency information from the TLS is transmitted to a ground station for real-time input into measurement planning as well as hazard avoidance. The high wind blimp will permit observations for wind energy research and turbulence studies. The TLS has transitioned to ARL-CISD, where researchers in the Battlefield Environment Division will use the system to make atmospheric observations for input in turbulence models.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. High-Resolution Atmospheric Studies Using DataHawk

Professor Ben Balsley, University of Colorado, Single Investigator Award

The goal of this research is to provide data-collection support through a micro-autonomous vehicle that has the ability to make detailed observations of fine-scale temperature, humidity, wind speed, and turbulence fluctuations on scales of 1 second (temporally) and 1 meter (spatially) throughout the first few km of the atmosphere (see FIGURE 8). It is anticipated that in FY13, the research team will perfect the DataHawk's data sampling capabilities by developing additional sensor capabilities that enhances its value as a next-generation research tool for studying fine-scale atmospheric dynamics during the Materhorn Project. In addition, this serves as a testing platform of a low-cost method to acquire high-resolution spatial and temporal data that could affect future data acquisition significantly. Relative to a conventional radiosonde balloon system, the DataHawk can provide the following: (i) 10-100 times improved vertical-resolution needed for direct comparison with emerging high-resolution models of breaking atmospheric gravity waves and turbulence generation, (ii) unique information on atmospheric gravity wave structure (wave-front direction, slope, and width), and (iii) true vertical profiles in contrast to conventional systems, where the balloon is carried many km downwind by the wind. These flyers can be constructed for approximately $1000 and provide a low-cost means of obtaining *in situ* data for incorporation into atmospheric models. Several researchers have expressed interest in incorporating such devices into their field campaigns.

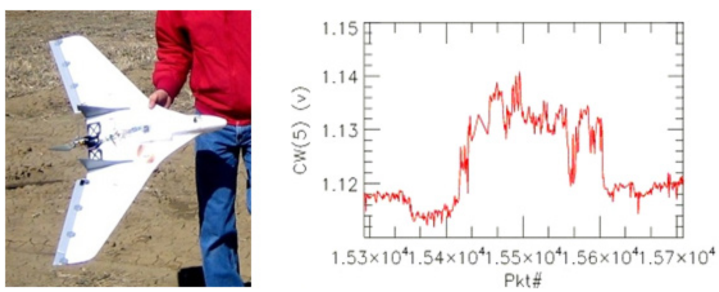

FIGURE 8

Micro-autonomous vehicle DataHawk. The DataHawk (left) is capable of providing real-time *in situ* measurements of the atmosphere. They can be launched on the ground or by balloon for high-altitude measurements. An example of an enhanced temperature upsurge (right) demonstrates its measurement capabilities.

B. Increasing Conversion Efficiency of Biomass into n-caproate with Reactor Microbiomes

Professor Largus Angenent, Cornell University, Single Investigator Award

The objective of this research is to achieve a mechanistic understanding of the complex reactor micro-biomes (open cultures of microbial consortia) that can chain elongate short-chain carboxylates form the carboxylate platform to produce n-caproate. The approach is to understand how hydrogen partial pressures can influence the production efficiencies of n-caproate at mesophilic temperatures. For an optimized bioprocess it is advantageous to maximize the carboxylate elongation with n-butyrate rather than with acetate to increase the ratio of the organic feedstock stream vs. the miscible ethanol stream. In this way, one can use a maximum amount of organic feedstock that was left over from ethanol fermentation. It is anticipated that in FY13, the research team will determine whether changes in the hydrogen partial pressures will alter the microbiome composition at mesophilic temperatures.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Kurt Preston
Division Chief
Program Manager, Habitation Science
Program Manager (Acting), Terrestrial Sciences

Dr. Gorden Videen
Program Manager (Acting), Atmospheric Science

Dr. Julia Barzyk
Contract Support, Terrestrial Sciences

B. Directorate Scientists

Dr. Thomas Doligalski
Director, Engineering Sciences Directorate

Mr. George Stavrakakis
Contract Support

C. Administrative Staff

Ms. Pamela Robinson
Administrative Support Assistant

CHAPTER 7: LIFE SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2012* is to provide information on the programs and basic research efforts supported by ARO in FY12, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Life Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY12.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Life Sciences Division supports research to advance the Army and Nation's knowledge and understanding of the fundamental properties, principles, and processes governing DNA, RNA, proteins, organelles, molecular and genetic systems, prokaryotic cells, eukaryotic cells, unicellular organisms, multicellular organisms, multi-species interactions, individual humans, and groups of humans. More specifically, the Division aims to promote basic research to elucidate the fundamental physiology underlying perception, cognition, neuro-motor output and non-invasive methods of monitoring cognitive states and processes during normal activity; basic research to understand antimicrobial resistance mechanisms; microbial community interactions including biofilm formation, cell-to-cell communications, population dynamics and host-pathogen/symbiont interactions; studies of organisms that are not culturable; studies of organisms at the single cell or mixed population (*e.g.*, metagenomic) level; studies of organisms that have adapted to grow or survive in extreme environments; identification and characterization of gene function, gene regulation, genetic interactions, gene pathways, gene expression patterns, mitochondrial regulation and biogenesis, nuclear and mitochondrial DNA replication, mutagenesis, oxidative stress, DNA repair, and regeneration; studies in structural biology, protein and nucleic acid structure-function relationships, molecular recognition, signal transduction, cell-cell communication, enzymology, cellular metabolism, and synthetic biology; and research to understand human behavior across different temporal, spatial and social scales. The results of these research efforts will lay a foundation for future scientific breakthroughs and will enable new technologies and opportunities to maintain the technological and military superiority of the U.S. Army.

2. Potential Applications. In addition to advancing worldwide knowledge and understanding of biological processes, the research managed by the Life Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the discoveries uncovered by ARO in the life sciences may provide new technologies for protecting the Soldier, for optimizing warfighter mental and physical performance capabilities, for creating new biomaterials, and for advances in synthetic biology for energy production, intelligence, and bioengineering.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Life Sciences Division coordinates and leverages efforts within its Program Areas with many other agencies, including the Defense Threat Reduction Agency (DTRA), the Defense Advanced Research Projects Agency (DARPA), the Joint Improvised Explosive Device Defeat Organization (JIEDDO), the Army Natick Soldier Research Development and Engineering Center (NSRDEC), the U.S. Army Corps of Engineers (USACE), the Army Research Institute (ARI), the Army Medical Research and Materiel Command (MRMC), the Center for Disease Control (CDC), the National Institutes of Health (NIH), the Intelligence Advanced Research Projects Agency (IARPA), the Department of Homeland Security (DHS), the Army Criminal Investigation Laboratory (ACIL), the Federal Bureau of Investigation (FBI), the Office of Naval Research (ONR), and the Air Force Office of Scientific

Research (AFOSR). In addition, the Division frequently coordinates with other ARO and ARL Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the ARO Chemical Sciences Division include promoting research to understand abiotic/biotic interfaces. The Life Sciences Division coordinates efforts with the Materials Science Division to pursue the design and development of new biomaterials. The Life Sciences Division also coordinates extensively with the Mathematical Sciences Division to develop new programs in bioforensics. In addition the Division coordinates with the Materials Science and the Mechanical Sciences Divisions to understand the effects of blast on synapses. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

To meet the long-term program goals described in the previous section, the Life Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY12, the Division managed research efforts within these six Program Areas: (i) Genetics, (ii) Neurosciences, (iii) Biochemistry, (iv) Microbiology, (v) Cultural and Behavioral Science, and (vi) Institutional and Organizational Science. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Genetics. The scientific goals of this Program Area are to identify and characterize the mechanisms and factors that influence DNA stability and mutagenesis, gene expression, and genetic regulatory pathways in prokaryotes, eukaryotes, and eukaryotic organelles. This program also seeks to understand genetic instability at a population level. The program supports basic research on mitochondrial regulation and biogenesis, oxidative phosphorylation, oxidative stress, and the interactions and communication between the mitochondria and the nucleus. The Genetics Program also supports basic research to develop an empirical understanding of general mechanisms by which genomic, transcriptomic, and proteomic components respond to alterations in the population-genetic environment. A third area of emphasis is the identification, characterization, and modulation of genetic pathways and molecular cascades that determine whether responses to stress or trauma are productive or counterproductive. Finally, the program supports high-risk, high payoff basic research that has the potential to create new Army capabilities, to optimize warfighter mental and physical performance capabilities, and to reduce the effect of PTSD, suicide, stress, and pathogens on warfighter readiness and Army capabilities.

2. Neurosciences. This objective of this Program Area is to support non-medically oriented research to elucidate the fundamental physiology underlying perception, cognition, neuro-motor output and non-invasive methods of monitoring cognitive states and processes during normal activity. The research areas include the perceptual and/or psycho-physiological implications of mind-machine interfaces ranging from optimizing auditory, visual and/or somatosensory display and control systems based on physiological or psychological states through modeling of individual cognitive dynamics and decision making. This Program Area is divided into two major research thrusts: (i) Neuroergonomics, and (ii) Neuromorphics. Within these thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goals. Research in the Neuroergonomics thrust aims to understand how the human brain functions in relation to sensory, cognitive and motor processes during its performance in real-world tasks in order to develop. Research in the Neuromorphics thrust is focused on understanding how individual neurons, circuits, and overall architectures create desirable computations, affect how information is represented, influence robustness to damage, incorporate learning and development, and facilitate evolutionary change. Cell culture and social insect models are being used to develop better understanding of living neural networks and swarm intelligence for eventual application in Army systems.

While these research efforts focus on high-risk, high pay-off concepts and potential long-term applications, current research may ultimately enable the development of neural biofeedback mechanisms to sharpen and differentiate brain states for possible direct brain-machine communication and determine how closely humans can approach hemispheric sleep as seen in some migrating birds and in dolphins.

3. Biochemistry. The goal of this Program Area is to elucidate the mechanisms and forces underlying the function and structure of biological molecules. Research in this program may enable the design and development of novel materials, molecular sensors and nanoscale machines that exploit the exceptional capabilities of biomolecules. This Program Area supports two research Thrusts: (i) Biomolecular Specificity, and (ii) Biomolecular Assembly and Organization. Within these Thrusts, innovative research efforts are identified and supported in pursuit of the vision of this program. Efforts in the Biomolecular Specificity Thrust aim to identify the determinants of the specificity of molecular recognition and to modulate and control this specificity through protein engineering and synthetic biology approaches. Research in the Biomolecular Assembly and Organization Thrust aims to explore the fundamental principles governing biological self-assembly, to understand and control the interactions and forces operating at the interface between biological molecules and abiological materials, and to identify innovative approaches to support biological activity outside of the cellular environment.

Research supported by this program promotes potential long-term applications for the Army that include biosensing platforms that incorporate the exquisite specificity of biomolecular recognition, nanoscale biomechanical devices powered by motor proteins, novel biotic/abiotic materials endowed with the unique functionality of biomolecules, drug delivery systems targeted by the activity and specificity of biomolecules, electronic and optical templates patterned at the nanoscale through biomolecular self-assembly, and novel power and energy systems that utilize biomolecular reaction cascades.

4. Microbiology. This Program Area focuses on understanding microbial physiology, genetics, ecology and evolution. Microbes are distributed throughout nature and are, in fact, essential for all life; however, microbes can also cause problems ranging from catalyzing materiel degradation to life-threatening infections. Therefore understanding how these organisms thrive and adapt to various environmental niches and how they adapt to new environments, is of great importance. This Program Area is divided into two research Thrusts: (i) Microbial Adaptation and Survival, and (ii) Systems and Synthetic Microbiology. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goals. Included in this program are studies to understand antimicrobial resistance mechanisms; microbial community interactions; microbial evolution, cell-to-cell communications, population dynamics and host-pathogen/symbiont interactions; studies of organisms that are not culturable; studies of organisms at the single cell level or in mixed populations (*e.g.*, metagenomic); and studies of organisms that have adapted to grow or survive in extreme environments. Also included is research on biochemical and physiological mechanisms underlying biodegradation processes in normal, extreme, and engineered environments; studies of microbiological mechanisms with potential for contributing to the remediation of sites contaminated with toxic waste; and the development and exploitation of microbial systems for unique biotechnological applications and bioengineering processes.

While these research efforts focus on high-risk, high pay-off concepts, potential long-term applications for the Army include strategies for harnessing microbes to produce novel materials, protect materiel, and efficiently produce desirable commodities. Fundamental research that may lead to innovative strategies for controlling bacterial infections and preventing or treating infectious diseases is also considered.

5. Cultural and Behavioral Science. The goal of this Program Area is to gain a better theoretical understanding of human behavior through the development of mathematical, computational, statistical, simulation and other models that provide fundamental insights into factors contributing to human socio-cultural dynamics (see FIGURE 1). This Program Area is divided into two research Thrusts: (i) Predicting Human Behavior, and (ii) Complex Human Social Systems. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. The program supports scientific research that focuses on the basic theoretical foundations of human behavior at various levels (individual actors to whole societies) and across various temporal and spatial scales. This includes, but is not limited to, research on the evolution and dynamics of social systems and organizations, human adaptation and response to both natural and human induced perturbations (*e.g.*, global climate change, mass migration, war, attempts at democratization), interactions between human and natural systems, the role of culture and cognition in accounting for variations in human behavior, human decision-making under risk and uncertainty, the search for organizing principles in social networks, and the emergent and latent properties of dynamic social systems and networks. The research involves a wide range of approaches, including computational modeling, mathematical modeling, agent-based simulations, econometric modeling and statistical modeling, to name a few. The program also recognizes the fact that the building and validation of models in the social sciences is often limited by the availability of adequate and appropriate sources of primary data. Thus some of the supported research includes the collection of primary data for the development and testing of models. Finally the program also supports research in the development of methodologies (*e.g.*, measurement, data collection, statistical methods, and research designs) that have the potential to help advance our scientific understanding of human behavior.

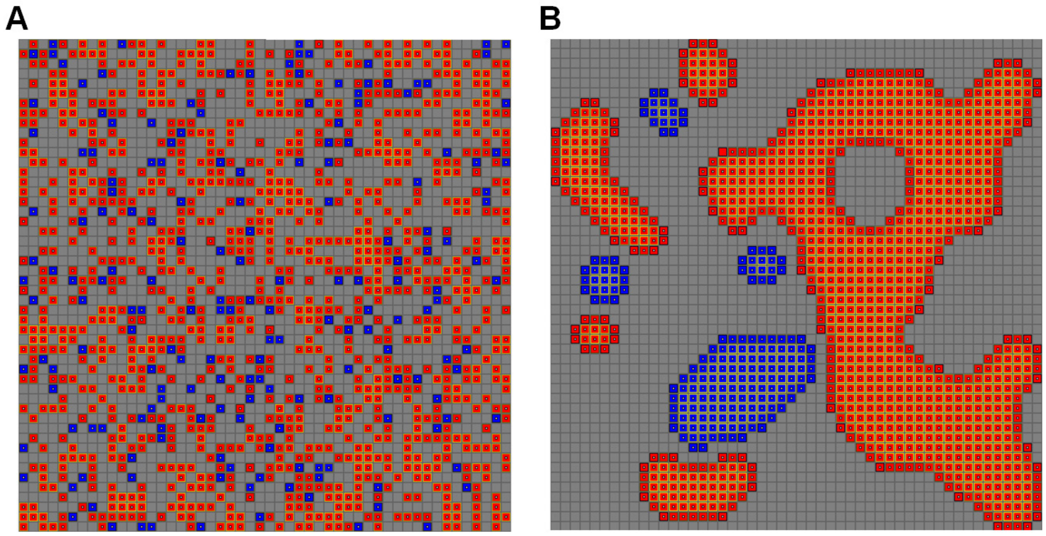

FIGURE 1

Simulation of socio-cultural dynamics. The figure illustrates the results of a cultural agent-based model with two cultures, simulating the evolution of subgroup formations under (**A**) moderately-positive attitudes towards in-group members and (**B**) negative attitudes towards out-group members.

Research focuses on high-risk approaches involving highly complex scientific problems in the social sciences. Despite these risks, the research has the potential to make significant contributions to the Army through applications that will, for example, improve decision-making at various levels (policy, combat operations), create real-time computer based cultural situational awareness systems for tactical decision-making, increase the predictability of adversarial intent, and produce integrated data and modeling in situ for rapid socio-cultural assessment in conflict zones and in humanitarian efforts.

6. Institutional and Organizational Science. The objective of this Program Area is to understand the emergence, maintenance, and evolution of human organizations and institutions, including but not limited to societies, states, religions, markets, economic systems, legal systems, bureaucracies, political parties, social movements, and formal and informal networks. Currently, subject matter expertise, which varies in quality and is subjective and unreliable, is the main tool of policy and decision makers in this area. Social scientific analysis, when applied, is applied *post-hoc* once crises are over to provide important insights and lessons learned, but are not employed to anticipate crises or evaluate social change in real time. This is to a large degree because current methods for collecting and analyzing data are too time consuming and costly to employ until an area of operation and specific research question are identified. Two specific goals of this Program Area are to (i) identify general theory, abstracted from the details of particular social contexts, to be used universally across the globe to anticipate crises or change, and (ii) make data collection and analysis less costly and sufficiently efficient to make feasible the consistent monitoring of events around the globe. Research projects in this Program Area can include a broad range of approaches including empirical approaches that require primary data collection, such as random control trials, quasi experiments, field experiments, surveys, comparative and observational studies, as well as the use of secondary data sources, such as archival data or news reports, and also formal, mathematical or computational approaches. Of special interest is research on the reciprocal effect of individuals on institutions and institutions on people: how do institutions shape attitudes and opportunities and constrain behavior and how do the choices and actions of people and groups, impact and change institutions.

The development of a systematic and efficient approach to collect and analyze data to describe fundamental social processes and detect changes in institutional structures can provide military decision makers with the means to understand and anticipate the decisions and activities that impact U.S. interests and national security.

C. Research Investment

The total funds managed by the ARO Life Sciences Division for FY12 were $82.1 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY12 ARO Core (BH57) program funding allotment for this Division was $6.3 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $14.8 million to projects managed by the Division. The Division also managed $1.5 million of Defense Threat Reduction Agency (DTRA) programs, $32.5 million of Defense Advanced Research Projects Agency (DARPA) programs, and $5.6 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $3.7 million for contracts. The Institute for Collaborative Biotechnologies received $15.1 million. Finally, $2.6 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY12 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research projects. Research projects are developed by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts.

The following subsections summarize projects awarded in FY12 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY12, the Division awarded 22 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to investigate the mechanisms of regenerative responses in mammals, that can be induced *in situ*, by using a negative pressure wound therapy device to generate a regeneration permissive environment, to delineate the mechanism of manganese superoxide dismutase dependent mitochondrial potential loss and triggering of anti-apoptotic pathways, to determine how several independent mutations selected in a single gene during evolution provide a selective phenotypic advantage to the organism, and to understand the structural determinants of target binding in an α/ß barrel protein. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Christopher Allan, University of Washington; *Exogenous Blastema Delivery*
- Professor Scott Banta, Columbia University; *Extremely Thermostable Alpha/Beta Barrel Scaffold*
- Professor Marcelo Bonini, University of Illinois - Chicago; *Role of Manganese Superoxide Dismutase Peroxidase Activity in Cellular Resistance Against Apoptosis*
- Professor David Breslauer, Refactored Materials, Inc.; *Mechanisms of Silk Fiber Metallization*
- Professor Renwick Dobson, University of Canterbury; *The Adaptive Evolution of an Enzyme*
- Professor Jerry Eichler, Ben-Gurion University of the Negev; *Post-translational Modification of Extremophilic Proteins: N-glycosylation in Archaea*
- Professor Steven Finkel, University of Southern California; *Physiological Signatures of Adaptive Evolutionary Events: A Role for the Growth Advantage in Stationary Phase Phenotype*
- Professor Shalene Jha, University of Texas at Austin; *Conservation Genetics*
- Professor David Kaplan, Tufts University; *Living Membranes*
- Professor David Kisailus, University of California - Riverside; *Organic Matrix Templating and Function in an Ultrahard Biological Composite*
- Professor Claire Kremen, University of California - Berkeley; *Pollinator Conservation*
- Professor Huan Liu, Arizona State University; *Assessing Trustworthiness in Social Media*
- Professor Michael Lynch, Indiana University at Bloomington; *Evolutionary Responses of Bacteria to Long-term Culture*

- Professor Jin Montclare, Polytechnic Institute of New York University; *Bottom-up Assembly of Protein Fibers*
- Professor Hai Rao, University of Texas Health Sciences Center - San Antonio; *Prion PrP's Path for Destruction*
- Professor David Ress, University of Texas at Austin; *Computational Modeling of Individual Brains*
- Professor Eric Schon, Columbia University Medical Center; *Increased ER-Mitochondrial Communication in the Pathogenesis of Alzheimer Disease*
- Professor Joel Snyder, University of Nevada - Las Vegas; *Perceptual and Neural Mechanisms of Auditory Change Detection*
- Professor Ilias Tagkopoulos, University of California - Davis; *Dynamics and Evolution of Associative Memory in Bacterial Populations*
- Professor Xinwei Wang, Iowa State University of Science and Technology; *Ultra-high Thermal Conductivity of Spider Silk: Protein Function Study with Controlled Structure Change and Comparison*
- Professor Stanley Wasserman, Indiana University - Bloomington; *Network Analysis: Effects of Sampling and Measurement Error on Models and Statistics*
- Professor Peng Yin, Harvard Medical School; *Self-Assembly of Complex 3D DNA Nanostructures from Modular Components*

2. Short Term Innovative Research (STIR) Program. In FY12, the Division awarded nine new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to explore the potential of coupled peptide mimetics and peptide nucleic acids and effects on bacterial growth, to develop a refined model of cognitive inattentional blindness, and to synthesize and characterize a new class of composite fibers composed of self-assembling peptide nanotubes embedded within aliphatic polyesters. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Paul Atchley, University of Kansas; *Dynamic Multitasking and Attention Endurance*
- Professor Haluk Beyenal, Washington State University; *Depth Resolved Nanospray Desorption Electrospray Ionization Mass Spectrometry in Biofilms*
- Professor John Evans, New York University; *Biomolecular Principles of Puncture Resistance and Crack Propagation*
- Professor Judith Gelernter, Carnegie Mellon University; *Situational Awareness and Inattentional Blindness*
- Professor Neel Joshi, Harvard Medical School; *Peptide Nanotube Reinforced Polymers*
- Professor Neville Kallenbach, New York University; *Antimicrobial Peptide-PNA Conjugates Selectively Targeting Bacterial Genes*
- Professor Claire Kremen, University of California - Berkeley; *Native Pollinators and Food Security*
- Professor Gerwin Schalk, Wadsworth Center, New York State Department of Health; *Methods for Functional Connectivity Analyses*
- Professor Minoru Shinohara, Georgia Technical University; *Exercise-induced Alteration in Brain Activity During Motor Performance Under Cognitive Stress*

3. Young Investigator Program (YIP). No new starts were initiated in FY12.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY12 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Center for Discrete Mathematics and Theoretical Computer Science Workshop on the Science of Expert Opinion*; New Brunswick, NJ; 24-25 October 2011
- *Sensory Transduction in Microorganisms Gordon Research Conference*; Ventura, CA; 15-20 January 2012
- *Biointerface Science Gordon Research Conference*; Les Diablerets, Switzerland; 20-25 May 2012
- *20th Bacterial Cell Surfaces Gordon Research Conference*; West Dover, VT; 24-29 June 2012

- *US-European Workshop on Structural Regeneration and Remodeling*; Venice, Italy; 28-29 June 2012
- *Silk: New Threads of Discovery Workshop*; Talloires, France; 20-23 July 2012
- *Drug Resistance Gordon Research Conference*; Easton, MA; 29 July - 3 August 2012
- *244th American Chemical Society National Meeting,* Abiotic/Biotic Interfaces Symposium; Philadelphia, PA; 19-23 August 2012

5. Special Programs. In FY12, ARO Core Research Program funds provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded nine new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Characterizing Interfaces between Living and Non-living Structures. This MURI began in FY06 and was awarded to a team led by Professor Paul Cederna at the University of Michigan. The goal of this research is to understand the neurological and physiological connections required for the normal function of appendages.

The long-term goal of this research is to uncover the materials and methods required to establish functional and structural connections between living limb segments and nonliving devices. The MURI team is exploring the interface between living and non-living structures, including bone, skin, muscle and nerve. Setting prosthetic materials research on a firm theoretical foundation, based in physiological interfaces and principles, will enable the current art of anatomical and physiological compensation to be on a scientific rather than an empirical foundation. The research team has already developed a method for directly connecting to peripheral nerves using a soft, electrically conductive scaffold that can be filled with muscle cells to act as targets for propagating axons (see FIGURE 2).

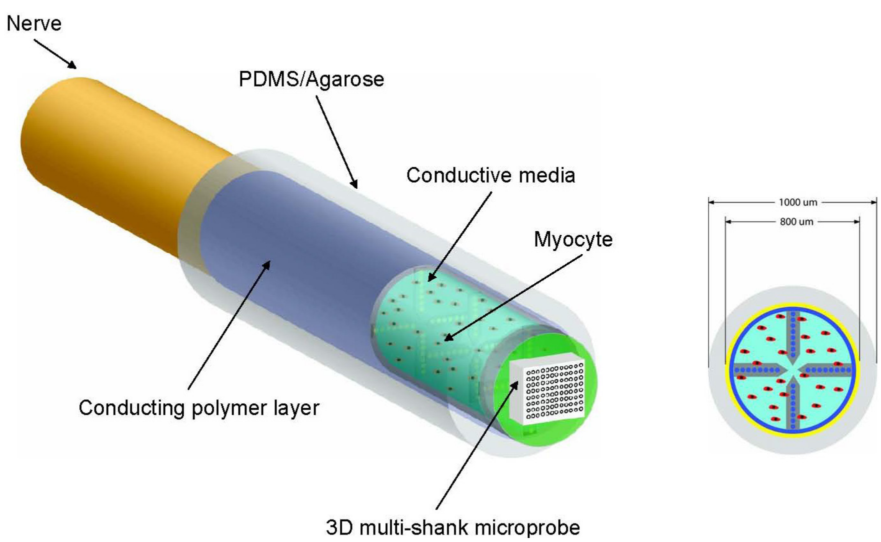

FIGURE 2

Artificial neuromuscular implants (ANMI). Proposed signal interface between a living nerve and an electronic recording system using conductive polymers and cultured muscles cells (myocytes).

As a result of these accomplishments, the research has led to a spin-off project currently being considered for separate funding in order to advance the state of knowledge to the point of clinical trials. The ability to design and build intelligent, adaptive, active devices using such engineered biological/non-biological interfaces could ultimately permit a complete return to duty for military personnel with no diminution of ability. In addition, it may ultimately enable the augmentation of limited function to normal or even enhanced performance.

2. Exploring Brain-to-muscle Neural Signaling. This MURI began in FY08 and was awarded to a team led by Professor Thomas D'Zmura at the University of California, Irvine. The objective of this research is to investigate brain signals and the corresponding muscle responses. This MURI is co-managed by the Computing Sciences Division and explores similar, but complementary concepts as the Computing Sciences Division MURI led by Professor Gerwin Schalk (see CHAPTER 4: COMPUTING SCIENCES DIVISION).

The team is using electroencephalographic (EEG) readings of the brain, which measure electrical activity along the scalp produced by the firing of brain neurons, to determine whether thought (*i.e.,* unspoken words) can be decoded. The MURI leverages breakthroughs in neuroscience and cognitive science uncovered in recent years. These breakthroughs, when coupled with technological advances in both hardware and software, have significantly advanced research that may ultimately lead to brain-computer interfaces (BCIs) that can decode the activity in brain networks. This potential long-term application is nearly analogous to the development of speech recognition software; however rather than having sound as the input, the inputs will be EEG signals. This concerted research effort will also attempt to develop a computational model that could decode intended mental speech and decode the direction of the attentional orientation of an individual based solely upon recorded activity from the surface of the scalp.

Preliminary results from the research teams have revealed that the EEG can be used to detect imagined speech rhythm and the pattern of stress in auditory imagery generated by imagined speech. Results from studies of attentional direction have suggested that covert spatial attention engages multimodal parietal areas as well as premotor and frontal areas are activated as part of motor planning for physical orienting (see FIGURE 3). EEG signals generated during lateralized covert attention strongly resemble those used in conventional BCIs to signal left and right through lateralized motor imagery.

Additional results using magnetoencephalography (MEG; a non-invasive technique used to measure magnetic fields generated by the small intracellular electrical currents in neurons) suggest that imagined movements are similar to imagined speech in that an internal forward model generates a somatosensory prediction produced during motor output planning. BCI software under development uses time-, frequency- and time-frequency-domain features of EEG signals to drive navigation and other behaviors in a 3D virtual environment and to drive a tube resonance model for speech synthesis. The evolution of this research beyond the MURI could lead to direct mental control of engineered systems by thought alone, ranging from automobiles to construction equipment to computers.

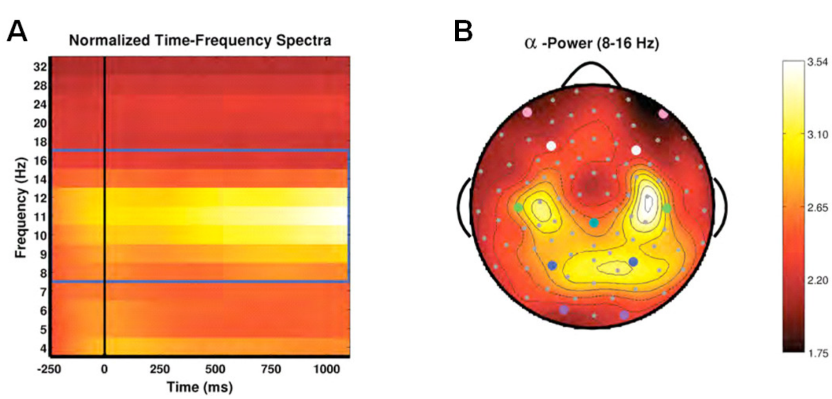

FIGURE 3

Covert spatial attention engages multimodal parietal areas as well as premotor and frontal areas.
(**A**) Alpha-band power increases just prior to the 500 msec mark at which stimuli to be attended first appear. Increased power extends through 1,100 msec, the latest time at which stimuli to be attended appear. (**B**) The topographic distribution of alpha power, averaged across time, displays the parietal and fronto-central components characteristic of attentional networks revealed by functional magnetic resonance imaging (fMRI) studies of visual attention.

3. Dynamic Models of the Effect of Culture on Collaboration and Negotiation. This MURI began in FY09 and was awarded to a team led by Professor Michele Gelfand at the University of Maryland, College Park. The objective of this MURI is to understand the effects of culture on collaborative and negotiation processes. Cross-cultural collaboration and negotiation are increasingly becoming an essential element of military combat and humanitarian operations (see FIGURE 4).

FIGURE 4

Inter-cultural negotiations. Understanding and applying culturally-appropriate interactions and negotiation tactics will significantly impact the success of these processes.

The goal of the MURI is to carry out a systematic examination of culture, negotiation and collaboration, with a particular focus on the Middle East. The first objective of the project is to develop a comprehensive understanding of core cultural values, norms, and attitudes within the Middle East. The second objective is to examine dynamic effects of culture on psychological and social processes in negotiation. The third objective is to examine dynamic effects of culture on collaboration processes, and the final objective is to examine how dynamical modeling and agent based modeling can help understand culture and negotiations and collaborations. The MURI initiated numerous efforts that span multiple methodologies (qualitative, experimental, survey, archival, computational) within each of these objectives.

4. Exploring Signaling Network Interactions Controlling Mouse and Salamander Limb Regeneration. This MURI began in FY09 and was awarded to a team led by Professor Ken Muneoka at Tulane University. The objective of this research is to identify and characterize signaling network interactions that control mouse and salamander limb regeneration.

The ultimate goal of this MURI is to establish the molecular-genetic foundation necessary for limb regeneration. The Mexican salamander is being used as a model organism (see FIGURE 5). The investigators are using a comprehensive approach to document all gene transcripts that are modified during limb regeneration in this model organism. The researchers will use this data to develop a complete regeneration specific microarray chip that can be used to gather data from mathematical modeling of temporal changes in cellular transcriptomes associated with regeneration, in particular, the reprogramming of fibroblasts. The team will model regeneration in the mouse digit tip that is mediated by blastema formation. The modeling is expected to identify specific nodes during the injury response that control whether a wound heals via scar tissue or via reprogramming to form a blastema and eventually regeneration. In the long term, the results of this research could potentially be used to initiate regenerative therapeutics to be tested on amputated limbs in a rodent model.

FIGURE 5

The axolotyl (Mexican salamander). This organism is capable of regenerating most of its body parts, and is being used as a model system for regeneration studies.

5. Mechanisms of Bacterial Spore Germination. This MURI began in FY09 and was awarded to a team led by Professor Peter Setlow at the University of Connecticut Health Science Center. The objective of this research is to decipher the biological mechanisms that underlie heterogeneity of bacterial spore germination with an emphasis on the slow germinating population

Most bacterial spores readily and quickly germinate after being exposed to appropriate growth conditions, a small percentage do not. Within the population, individual spores may germinate days, weeks, or even months, with serious implications. In food processing, the presence of slowly germinating spores results in a need for harsh processing conditions, such as high pressure and temperature, leading to a loss of food quality and appeal. Medically, delayed germination can result in disease appearance after antibiotic therapy has been discontinued. This research team is using a combination of "wet lab" experiments and computational modeling to understand the fundamental mechanisms of spore germination. This research may ultimately lead to strategies for preventing bacterial spore germination that could be used in food processing and medically-relevant therapeutic technologies, and for the enhancement of spore germination to be used in new methods of biofuel production.

6. Modeling Cultural Factors in Collaboration and Negotiation. This MURI began in FY09 and was awarded to a team led by Professor Katia Sycara at Carnegie Melon University. The objective of this MURI is to understand how cultural values, such as the highly-prized "sacred values," can shape the collaboration and negotiation process.

The team has made interesting discoveries in these studies, including the observation of certain values called "sacred values" that are considered as essential to the identity of a given social group, thereby leading members of the group to respond defensively when these values are seen to be challenged or threatened. One example of sacred values includes the observation that the Iranian nuclear program is treated as sacred by some Iranians, leading to a greater disapproval of deals that involve monetary incentives. In addition the team is exploring how humiliation may contribute to regulating relationships within Muslim countries. Humiliation seems to result in clashing behavioral tendencies that offer no regulatory strategies. Participants in the study motivated to change the status quo underestimated the extent to which the out-group moralized the domains of harm, care, fairness and justice. Further, participants motivated to maintain the status quo accurately identified that the out-group moralized harm, care, fairness and justice to the same extent that they themselves did. The investigators will replicate these studies in India and Israel/Palestine in the coming year.

7. Blast Induced Thresholds for Neuronal Networks. This MURI began in FY10 and was awarded to a team led by Professor David Meaney at the University of Pennsylvania. This research is jointly managed with the ARO Mechanical Sciences Division. The objective of this MURI is to understand the effects of a primary blast wave and how it can cause persistent damage to the nervous system and the brain at the meso- and micro-scale.

The research team will build and validate a model of the human brain/skull subject to blast loading and use this model to scale blast field conditions into cell culture and animal models. The project will develop multiscale blast thresholds for alteration of synapses, neuronal connectivity, and neural circuits (*in vitro* and *in vivo*) and will examine if these thresholds change for tissue and/or circuits in the blast penumbra. Finally, the researchers will determine the blast conditions necessary to cause persisting change in neural circuitry components (up to two weeks) and will correlate alterations in circuits to neurobehavioral changes following blast. This research should provide a basis for shifting defensive armor design efforts from defeating the threat based on material deformation, damage, and rupture, to mitigating the effects based on biological relevance. In addition the research may lead to medical applications for treating neurotrauma and in regenerative medicine.

8. Prokaryotic Genomic Instability. This MURI began in FY10 and was awarded to a team led by Professor Patricia Foster at Indiana University. The objective of this research is to identify and extract the mathematical signatures of prokaryotic activity in DNA.

The investigators are characterizing fundamental parameters in the microbial mutation process in a superior model system, including both cell-mechanistic and evolutionary components. The research is a comprehensive effort with strong experimental and computational components. The team will determine the contribution of DNA repair pathways, cellular stress, and growth conditions on the mutation rate and mutational spectrum of *E. coli* using whole genome sequencing over the course of strain evolution. The team is extending this analysis to a panel of twenty additional eubacterial species. To understand the forces that define short-term and long-term evolutionary mutation patterns, a new class of population-genetic models will also be developed. The investigators will include mutant strains with known deficiencies in genome maintenance. Parallel analyses in such strains will produce larger data sets that define, by comparison to wild type strains, the contribution of each repair pathway to the overall mutational spectrum. Mutational changes characteristic to specific environmental conditions/stresses/genotoxicants can be analyzed in the context of the mutational signatures of individual repair pathway throughout the genome. Overall, the proposed research presents an unprecedented opportunity to uncover patterns of mutational variation among prokaryotes. The approach is unique in that the investigators are using a comprehensive whole-genome, systems-biology approach to characterize and understand DNA instability at a whole-genome level, across a comprehensive range of prokaryotes.

9. Translating Biochemical Pathways to Non-Cellular Environment. This MURI began in FY12 and was awarded to a team led by Professor Hao Yan at Arizona State University. This MURI is exploring how biochemical pathways could potentially function in a non-cellular environment.

Cells provide a precisely organized environment to promote maximum efficiency of biochemical reaction pathways, with individual enzymatic components organized via multisubunit complexes, targeted localization in membranes, or specific interactions with scaffold proteins. The eventual translation of these complex pathways to engineered systems will require the ability to control and organize the individual components outside of the natural cellular environment. Although biological molecules have been successfully attached to inorganic materials, this process often requires chemical modification of the molecule and can restrict its conformational freedom. An alternative approach to maintain biological activity outside of the cell, while preserving conformational freedom, is to encapsulate enzymes within specialized materials or structures. Unfortunately, surface patterning of current encapsulating agents has not achieved the precision required to replicate the organizational capabilities of the cell.

The objective of this research is to develop the scientific foundations needed to design, assemble, and analyze biochemical pathways translated to a non-cellular environment using 3D DNA nanostructures. The MURI team is using DNA nanostructures to direct the assembly of selected biochemical pathways in non-cellular environments. The focus of this effort is to develop the scientific foundations needed to translate multi-enzyme biochemical reaction pathways from the cellular environment to non-biological materials. The ability to translate biochemical reaction pathways to non-cellular environments is critical for the successful implementation of these pathways in DoD-relevant technologies including responsive material systems, solar cells, sensor technologies, and biomanufacturing processes.

10. Evolution of Cultural Norms and Dynamics of Socio-Political Change. This MURI began in FY12 and was awarded to a team led by Professor Ali Jadbabaie at the University of Pennsylvania. This MURI is exploring the cultural and behavioral effects on societal stability.

Recent events involving the diffusion of socio-political change across a broad range of North African and Middle Eastern countries emphasize the critically important role of social, economic and cultural forces that ultimately affect the evolution of socio-political processes and outcomes. These examples clearly demonstrate that radically different outcomes and chances for conditions of state stability result from the different institutional frameworks within these countries. It is well established in the social sciences that change in or evolution of institutions depends on the behavior patterns or culture of the people involved in them, while these behavior patterns depend in part on the institutional framework in which they are embedded. This dynamic interdependence of culture and institutional change means that the modeling of societal stability requires the coupling of individual modeling approaches describing such issues as trust and cooperation with models describing institutional dynamics.

The objective of this MURI is to develop fundamental theoretical and modeling approaches to describe the complex interrelation of culture and institutions as they affect societal stability. The research team is extending the cultural approaches from application to individuals, families, and villages, to address stability of the larger social group. The models developed in this MURI may ultimately provide guidance in data collection and analysis of data on local populations that can provide planners with models to anticipate the second or third-order ramifications of actions that impact local populations.

11. Simultaneous Multi-synaptic Imaging of the Interneuron. This MURI began in FY12 and was awarded to a team led by Professor Rafael Yuste at Columbia University. The research team is exploring how individual neurons act as computational elements.

Interneurons are highly networked cells with multiple inputs and outputs. It has been to date impossible to record all the inputs and outputs from even a single living interneuron with synaptic levels of resolution in a living brain. While there is information on the morphological, physiological, and molecular properties of interneurons as a class and on their general synaptic connections, there is still little direct information on the functional roles of individual interneurons in cortical computations, and especially not on how each synapse relates to all the others within a single cell. Coupled with tagging via fluorescent molecules and/or chromophores and genomic modifications to control co-expression, electro-optical imaging may provide a solution, due to its ability to achieve subwavelength resolution across a relatively wide field of view.

The objective of this research is to explain and quantitatively model the entire set of neurotransmitter flows across each and every individual synapse in a single living interneuron, with experimental preparations ranging from cell culture systems through model neural systems. The research team will use genetically-engineered mice expressing specific labels in specific interneurons, high-throughput electron microscopy, and super-resolution imaging techniques to reveal the connectivity and the location of the synapses. This research may ultimately provide models that predict the information transitions and transformations that underlie cognition at the smallest scale where such activity could take place. These models could revolutionize the understanding of how human brains instantiate thought, and may lead to applications such as neural prostheses.

C. Small Business Innovation Research (SBIR) – New Starts

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY12, the Division managed two new-start Phase II SBIR contracts, in addition to active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications, such as demonstrating the feasibility of safely reducing or eliminating the perception of pain through the use of peripheral nervous system ultrasonic modulation of neurons.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY12, the Division managed 13 new-start STTR contracts, in addition to active projects continuing from prior years. Among these new starts, three Phase I new start contracts are exploring the development of high throughput methods for forensic palynology. Three Phase I STTRs were initiated to push the forefront of bioelectronics, and a Phase I STTR was initiated to develop a virtual laboratory for research into collective behavior and inter-group conflicts. A phase II STTR was initiated for high-capacity and cost-effect manufacture of chloroperoxidases. A Phase II STTR new start project aims to develop an automated system for training small animals to find explosives. Three Phase I STTRs were initiated to develop new tools to extract useful data from social media. Lastly, a Phase II STTR was initiated to bridge fundamental discoveries with potential applications through the development of a therapeutic that is effective against multi-drug resistant and biofilm-embedded bacteria.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY12, the Division managed three new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY12.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY12, the Life Sciences Division managed six new DURIP projects totaling $1.1 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including efforts to develop an advanced single-molecule imaging and spectroscopy system in support of research on bacterial spore germination and inactivation, and to study the natural adhesive properties of ivy nanoparticles.

H. University Affiliated Research Center (UARC): Institute for Collaborative Biotechnologies (ICB)

The ICB is managed by ARO on behalf of the Army and is located at the University of California, Santa Barbara (UCSB), in partnership with the Massachusetts Institute of Technology (MIT), the California Institute of Technology (Caltech) and industry. The scientific objective of the ICB is to investigate the fundamental mechanisms underlying the high performance and efficiency of biological systems and to translate these principles to engineered systems for Army needs. Through research and strategic collaborations and alliances with Army laboratories, Research, Development and Engineering Centers (RDECs), and industrial partners, the ICB provides the Army with a single conduit for developing, assessing and adapting new products and biotechnologies for revolutionary advances in the fields of biologically-inspired detection, materials synthesis, energy generation and storage, energy-dispersive materials, information processing, network analysis and neuroscience. A total of $15.1 million was allocated to the ICB in FY12, which was the fourth year of a $70 million contract that was renewed in FY09 for a five-year period. Of these FY12 funds, $11.3 million was allocated for 6.1 basic research and $3.8 million was allocated for five 6.2 projects, including two new projects.

In FY12, the ICB supported 74 faculty, 105 graduate students, and 60 postdoctoral fellows across 15 departments at UCSB, Caltech and MIT. The research falls into five Thrusts: (i) Biomolecular Sensors, (ii) Bio-Inspired Materials and Lightweight Portable Energy, (iii) Biotechnological Tools for Discovery (iv) Bio-Inspired Network Science, and (v) Cognitive Neuroscience. Detailed descriptions of each core research Thrust and corresponding projects are available at the ICB program website (*http://www.icb.ucsb.edu/research*). A U.S. Army Technical Assessment Board and an Executive Steering Board annually review the ICB research portfolio, assessing the project goals and accomplishments and set goals for the coming year.

I. DARPA Revolutionizing Prosthetics Program

The primary goal of this program is to develop the basic neuroscience and engineering needed to enable the realization of advanced prosthetic devices that function with the same motor capacity as the biological limb, including sufficient sensory feedback to the wearer. Research covers the entire field of human physiology and Soldier survival following trauma. The ARO Life Sciences and Materials Science Divisions currently co-manage projects within this program aimed at optimizing the programming and hardware for an upper limb prosthetic for home use as well as projects examining the detection of traumatic brain injury that could complicate prosthetic integration, laser treatment of intracranial hemorrhage, and the use of muscle signals in addition to brain signals for better prosthetic control. The results of this research may ultimately provide full anatomic and functional restoration from injuries to enable injured Soldiers and civilians to return to work.

J. DARPA Soldier Centric Imaging via Computational Cameras Program

The Soldier Centric Imaging via Computational Cameras (SCENICC) will fully exploit the computational imaging paradigm and associated emerging technologies to yield ultra-low size, weight, and power (SWaP) persistent/multi-functional soldier-scale Intelligence, Surveillance and Reconnaissance (ISR) systems that greatly enhance warfighter awareness, capability, security, and survivability. The ARO Life Sciences and Electronics Divisions co-manage this program, aimed at optimizing programming and hardware to enhance imaging by leveraging computational approaches and novel optical designs to lower required pixel counts for enhanced levels of performance in 360 degree situational awareness.

K. DARPA Reliable peripheral Interfaces (RPI) Program

The goal of this program is to develop reliable in-vivo peripheral motor-signal recording and sensory-signal stimulating interfaces. This program involves the design, fabrication, testing, and analysis of new materials and technologies to demonstrate substantial improvements in reliability and quantity of peripheral motor-signal information. Ultimately DARPA desires to develop clinically viable technologies, enabling wounded service members to control state-of-the-art prosthetic limbs. Specifically for the ARO managed portions of this program, one effort uses surface recorded electromyogram activity from residual muscles to inform controller software and hardware via activity pattern matching what the prosthetic user's movement intent is and to enable execution of that by the robotic limb. A second effort is designed to develop a sensory feedback interface from the prosthetic fingers to the user's skin to enable intuitive touch feedback during use.

L. DARPA Enabling Stress Resistance Program

The goal of this program, co-managed by the Life Sciences Division and DARPA, is to create a comprehensive, quantitative description of the impact of stress on the brain. This effort seeks to leverage cutting-edge technologies and recent advances in molecular neurobiology, neuroimaging and molecular pathway modeling as applied to animal models of acute and chronic stress. The objective of the effort is a proactive approach to stress mitigation, starting with development of a comprehensive understanding of the complex effects of multiple stressors on the brain. The program has the ultimate goal of the development and implementation of cognitive, behavioral, and/or pharmacological interventions that will prevent the deleterious effects of stress on the brain. The investigators will pursue their objectives through the creation of research teams to thoroughly investigate the multiple physiological pathways and molecular mechanisms involved in the brain's response to acute and chronic stress as well as physical, social, cognitive and affective stressors.

M. USACIL DoD Forensic Research and Development Program

The goal of this program, co-managed by the Life Sciences Division and USACIL, is to advance the Defense Forensic Enterprise in the areas of DNA analysis, latent prints, firearms and toolmarks, trace evidence, explosive detection and drug chemistry. In the first year of this research program, two projects were selected for funding. The first is focused on statistical analysis of firearms and aims to develop a system to allow for examiner-independent evaluation of impressions generated by the discharge of a firearm using Integrated Ballistics Identification System (IBIS) data. In the expeditionary environment, the proposed system will provide a useful measure of match statistics, reducing time and potentially the need for a verification step, allowing a single examiner to make decisions on firearm comparisons. The second project aims to identify body fluid-specific gene transcripts and incorporate them into an RNA-based body fluid multiplex identification system. The proposed system will enhance forensic capabilities of USACIL and civilian law enforcement by conclusively identifying all forensically relevant biological fluids in a given sample. The proposed system will also be seamlessly compatible with current DNA typing technology by enabling co-extraction of both DNA and RNA from the same forensic sample.

N. DARPA Phytoremediation of Atmospheric Methane Project

The Life Sciences Division currently co-manages a DARPA project in phytoremediation. Phytoremediation involves the treatment of environmental problems (*i.e.*, bioremediation) using plants to mitigate the problem without the need to remove the contaminant material and dispose of it elsewhere. This joint project is aimed at assessing whether transgenic plants expressing the bacterial genes for soluble methane monooxygenase can metabolize atmospheric methane to methanol. The project will achieve its goals by developing vectors for expression of the essential subunits of soluble methane monooxygenase genes in plant nuclear and plastid genomes, transforming these vectors into plants, and assessing methane monooxygenase gene expression using colorimetric oxidation and real-time polymerase chain reaction (RT-PCR) assays. The transformed plants will also be tested for methane oxidation directly using closed vessels and gas chromatographic analysis of headspace. Global warming will have a profound impact on future defense operations (*e.g.*, in the Arctic) and has the potential for large scale humanitarian disruption. Methane accounts for 20% of human-caused heat retention in the atmosphere. Therefore, an effective and inexpensive method to remove methane from the atmosphere would be a valuable tool with which to combat global warming.

O. DARPA Eukaryotic Synthetic Biology Program

ARO co-manages the DARPA Eukaryotic Synthetic Biology Program. The goal of this program is to develop specific orthogonal synthetic and modular genetic regulatory elements that can be used in mammalian cells. The research seeks to develop synthetic regulatory elements for in vivo biomedical applications including the detection and/or treatment of disease. Research challenges in this program include the discovery, characterization, evolution or design and demonstration of orthogonal genetic regulatory elements, construct stability and functionality in vivo, and synthesis, amplification and delivery of novel circuits to mammalian cells. In part through this program, synthetic modules must be designed to not have non-specific and unintended interactions with other cellular components.

P. Minerva Research Initiative (MRI) Topic: Chinese Military and Technology Research and Archive Programs

The objective of this MRI topic is to explore the social, cultural, and political characteristics and implications of trends and developments in the Chinese military as well as in supporting technological and industrial sectors. The Chinese publish a wealth of unclassified information about technological and scientific developments; however, much of this material is difficult for scholars outside of China to locate or access and most of it is not generally known beyond a small circle of researchers. The breadth and depth of material, and the scope of topics, offers insights into China regarding everything from industry and agriculture, to technology development and scientific research, to politics and military issues. Exploring these information resources can enable a better understanding of China, its future, and its aspirations in our evolving world. This topic calls for scholarly efforts to gather these materials, translate them where necessary, interpret them and make them available to a wider audience by creating an open source platform to facilitate, pool and network the knowledge and understanding of subject matter experts in Government and academia. A further objective is the creation of a physical or virtual archive or depository that will include automated tool suites for researcher access to the depository, to include electronic or web-based systems for search and retrieval, translation, automated semantic annotation and organization, collaboration, and scholarly production of text and multimedia sources, searchable in both English and Chinese. Research into the dynamics and trends in Chinese military and technology will provide valuable insights into the workings of an important and influential power. This research will be a valuable resource for developing expertise among academics and interested researchers, as an aid to policymakers, and ultimately to help the American people better understand China and its future role in our evolving world. The BAA for this MRI topic was released in FY08. Project selection and funding began in FY09. There was one active project pursuing research under this topic in FY12.

Q. Minerva Research Initiative (MRI) Topic: Iraqi Perspectives Project

The objective of this MRI topic is to explore the political, social, and cultural workings and changes within Iraq during the years Saddam Hussein was in power. Some examples of appropriate research might be studies of leadership dynamics; social psychological studies of national identity and political unity; and Iraqi perceptions of international relations and systems. In particular, emphasis is given to studies by experts capable of analyzing source material in the original languages, to studies that exploit materials that have not been previously translated, and to innovative multi-disciplinary projects that bring insights from the humanities and social sciences and relevant disciplines. In the course of Operation Iraqi Freedom, a vast number of documents and other media came into the possession of the Department of Defense. The materials have already been transferred to electronic media and organized. Yet these comprise only a small part of the growing declassified archive and its potential, combined with the open literature. This continuing collection offers a unique opportunity for multidisciplinary scholarship combined with research in methods and technologies for assisting scholarship in automated analysis, organization, retrieval, translation, and collaboration. A broad understanding of the culture of interest is a fundamental requirement for this topic area. This exploration and scholarship in Iraqi perspectives will offer insights into the dynamics of how such authoritarian regimes retain power and legitimacy, how their social and cultural contexts may influence perceptions and decision making, and how they acted internationally. These insights will allow scholars and policymakers important tools for understanding future challenges. The BAA for this MRI topic was released in FY08. Project selection and funding began in FY09. There was one active project pursuing research under this topic in FY12.

R. Minerva Research Initiative (MRI) Topic: Studies of Terrorist Organization and Ideologies

The objective of this MRI topic is to examine the relationship between transnational terrorist ideologies and intergroup conflicts. Areas of particular interest include: the interaction between political dynamics on the ground and terrorist goals and ideologies; the role of new media technologies in terrorist recruitment, radicalization, and de-radicalization; the spread of ideologies across culturally diverse populations; and the role of non-rational decision making (e.g., values, morals, trust, belief and emotions) in the collective behavior and how best to represent non-rational decisions in computational models of collective and group behavior. This research, if successful, will provide better understand the dynamics of terrorist organizations, their underlying motivations and ideologies, how they organize, how they recruit and retain members, and how they evolve and adapt in the face of new challenges. In addition to overall network characterization, there is an urgent need to be able to locate the points of influence and characterize the processes necessary to influence populations that harbor terrorist organizations in diverse cultures as well as individuals who identify with terrorist group figures of note. A better understanding of neuro-cognitive systems responsible for the processing of socio-cultural and other environmental cues is crucial both to research and to a whole range of practical situations. The BAA for this MRI topic was released in FY08. Project selection and funding began in FY09. There was one active project pursuing research under this topic in FY12.

S. Minerva Research Initiative (MRI) Topic: Science, Technology and Military Transformation in China and Developing States

The objective of this MRI topic is to explore the social, cultural, and political characteristics and implications of trends and developments in growing military powers such as China as well as in supporting technological and industrial sectors as they relate both to security policy and strategy and to the broader evolution of society. This research team utilizes a wealth of unclassified information, not generally known beyond a small circle of researchers, about military, technological and scientific developments that is published by the Chinese but difficult for scholars outside of China to locate or access. The breadth and depth of material, and the scope of topics, offers insights into Chinese industry and agriculture, technological development and scientific research, and politics and military issues. Access to this data will facilitate research into trends in military and technology development and promise to provide valuable insights into the workings of an important and influential power. The coding of this data into a comprehensive relational database that will be made available to Chinese scholars beyond this project combined with the projects continued focus on building a community of researchers collectively engaged in understanding these aspects of modern Chinese development will inform a wide range of decisions relevant to national security and economic policy, from diplomacy to science and technology planning to military resource allocation. The BAA for this MRI topic was released in FY11. Project selection and funding began in FY12. There were three active projects pursuing research under this topic in FY12.

T. Minerva Research Initiative (MRI) Topic: Security Implications of Energy, Climate Change, and Environmental Stress

The objective of this MRI topic is to establish new theories and models of societal resilience and collapse in response to external pressures related to energy, ecosystem, environmental stressors, and resource uncertainty and change. Until recently, most studies of energy and climate change have focused on natural processes, economic impacts, and policy implications. In the last few years, social scientists began to explore the intersection among these factors by asking how changes in energy technology and the environment alter risk perception and human behavior, and affect the availability and distribution of essential resources (e.g., water, grains) and geomorphologic changes (*e.g.*, desertification). Affected societies experiencing these shifts must work to mitigate competition over increasingly scarce resources, which can contribute to the emergence of political and social unrest. In addition, worldwide increases in demand for nonrenewable energy and other resources have the potential to limit the ability of societies to sustain current economic and social standards of living. This MRI supports research that will contribute to fundamental understanding of the implications of energy, climate change, and environmental stress from a global security perspective. This research will likely aid DoD decision-making and policy efforts in terms of the development of improved methods for identifying and anticipating potential hot zones of unrest, instability and conflict and help in strategic thinking about resource allocation for defense efforts and humanitarian aid. The BAA for this MRI topic was released in FY11. There were two active projects pursuing research under this topic in FY12.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Life Sciences Division.

A. Engineering Synthetic Ribosomes

Professor Michael Jewett, Northwestern University, Single Investigator Award

The ribosome is a molecular machine that assembles biological polymers (proteins) in a sequence-defined manner with atomic-scale resolution. It has been impossible to date to produce finely-tailored non-biological sequence-defined polymers (*i.e.*, materials of defined atomic sequence, exact mono-disperse length, and programmed stereochemistry). However, discovering methods for synthesizing polymers at this resolution could be considered to be the "Holy Grail" of polymer synthesis.

Professor Michael Jewett's research group at Northwestern University is using methods in synthetic biology to harness the extraordinary synthetic capability of the ribosome to assemble polymers containing non-biological building blocks (see FIGURE 6). Expanding the repertoire of ribosome substrates is a challenging task because the requirement of cell viability severely constrains the mutations that can be made to the ribosome. In practice, these constraints make the natural ribosome un-evolvable and so far, there is not a generalized method for modifying the catalytic active site of the ribosome to incorporate substrates beyond those found in nature. The keystone of this effort is an innovative ribosome engineering platform being designed by Professor Jewett that will be used to select and evolve synthetic ribosomes that are programmed to efficiently synthesize sequence-defined polymers containing multiple types of non-natural monomers. In addition to synthetic ribosomes, this effort will also require the creation of non-natural building blocks and a code that directs the ribosome to polymerize these monomers in a specific sequence.

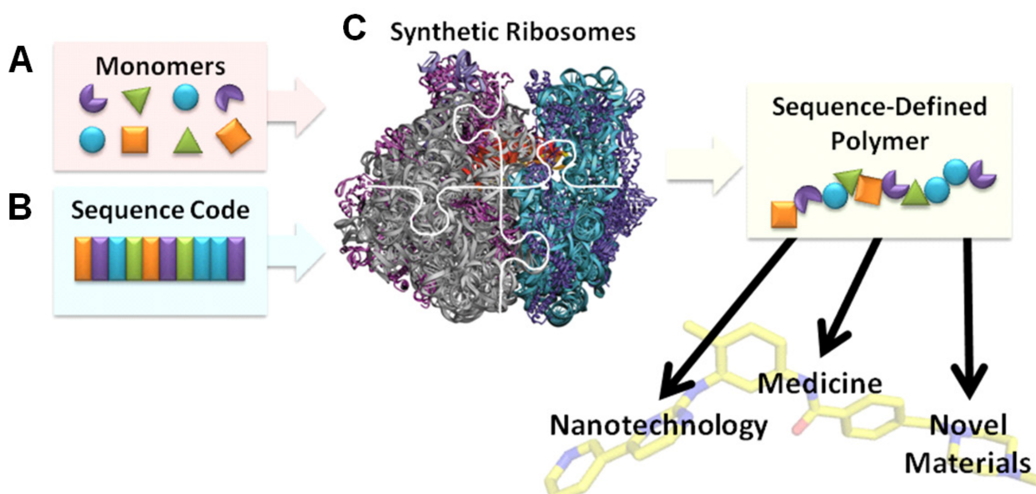

FIGURE 6

Engineering Ribosomes to Assemble Non-Biological Polymers. Synthetic ribosomes will overcome long-standing technological barriers to allow genetically encoded evolution of non-natural peptide therapeutics and hybrid materials, leading to breakthroughs in nanotechnology, medicine and novel materials. This approach will require the creation of (**A**) non-natural building blocks and (**B**) a sequence code that directs the insertion of these monomers by (**C**) synthetic ribosomes that are programmed to efficiently synthesize sequence-defined polymers containing multiple types of non-natural monomers.

In FY12, the research team synthesized and purified an artificial ribozyme, named Flexizyme, which will be used to create the non-natural building blocks to be incorporated into polymer chains. The team also developed a simple and efficient method to purify active ribosomal subunits. The traditional approach used for ribosomal purification is time consuming and results in low yields of active molecules, which has caused the availability of active ribosomes to be the limiting factor in experimental design. Building on a recently described ribosomal purification method using affinity tags, the research team developed a method to independently isolate non-tagged versions of the large and small subunits of the ribosome. To isolate the small subunit, the team purified the ribosomal complex based on affinity tags added to the large subunit and then separated the two subunits. To isolate the large subunit, the team moved the affinity tags to the small subunit and used the same approach. This simple and rapid purification process resulted in increased purity, activity and yield of the subunits. The team has also made significant progress toward optimization of reaction conditions to maximize the activity of assembled ribosomes. Using Optimal Mixture Design experiments, the team had determined that a 3:1 ratio of small:large subunits and 8 mM magnesium results in maximal activity. The team is now poised to begin modifying the ribosomal subunits and assembling synthetic ribosomes that are programmed to accept non-natural building blocks as substrates.

By exploiting the biosynthetic potential of the ribosome to produce non-natural sequence-defined polymers in non-cellular environments, this effort aims to far surpass the compositional control previously achieved by chemical approaches. Because atomic-scale resolution should give the greatest possible control over macroscopic behavior of the resultant polymer, this technology could be applied to tailor the functions of non-biological sequence-defined polymers for specific applications, such as the synthesis of robust hybrid materials endowed with tunable properties including responsiveness, shape memory, and self-healing. Such materials may ultimately find utility in applications for advanced personal protective gear, wound-healing materials, sophisticated electronics, and nanofabrication.

B. Prokaryotic DNA Stability
Professor Patricia Foster, Indiana University, MURI Award

The objective of this multi-investigator effort is to characterize fundamental parameters in the microbial mutation process in a superior model system, including both cell-mechanistic and evolutionary components. To date the investigators have identified and analyzed thousands of spontaneous, unselected independent mutations in four different prokaryotic species, with 100-fold sequencing depth. Previous efforts to define spontaneous mutation rates have generally been limited to single gene reporter assays. Recently, the Foster laboratory found that the mutation rates extrapolated from reporter assays are inaccurate; the real genomic mutation rate in *E. coli* is three-fold lower than previously thought. In addition, the investigators determined that (i) the loss of a functional mismatch repair system shifted the spectrum of base pair substitutions from GC to AT transitions to AT to GC transitions, (ii) transitions have a strong DNA strand bias with AT transitions more likely to occur when the adenosine is on the lagging strand and GC transitions are more likely to occur when the guanine is on the leading strand, (iii) transitions are more likely to occur with a 3' cytosine, (iv) dam methylation sites are hotspots for A to T transversions, (v) dcm methylation sites are hotspots for G to C transitions, and (vi) the mutation rate per nucleotide is inversely proportional to the average effective population size.

These results have profound implications for understanding how mutations occur, and also reveal that mismatch repair is a major determinant of the nucleotide balance in genomes. This first genomic analysis of mutational spectra also revealed that there is a genome scale topology to mutation rates; however, the structural cause of this topology remains unclear. This research has also revealed surprising differences in long term survival patterns of *E. coli* grown on different types of media.

C. Fundamental Studies on Lensfree Microscopy and Tomography
Professor Aydogan Ozcan, University of California - Los Angeles, YIP Award

Recent revolutionary advances in digital technologies include the development of relatively inexpensive 2D solid state detector arrays that, compared to previously available arrays, have significantly larger areas with smaller pixels, better dynamic ranges, frame rates, and noise performance, as well as development of much faster, cheaper and more powerful digital processors and memories. The objective of this project is to combine these technological advances with imaging theory and numerical algorithm advances to develop fundamentally new lens-free on-chip microscopy and tomography modalities.

Professor Ozcan's laboratory, with funding through an ARO YIP award, ONR, DARPA, and other agencies, recently discovered a fundamental new way to image microorganisms using visible or ultraviolet light. This new method, called holographic microscopy may ultimately provide a cost-effective, handheld, lightweight, and rapid diagnostic system to enhance battlefield medicine capabilities.

Holographic microscopy has overcome many fundamental and practical barriers of conventional optical microscopy. Current optical microscopes are expensive, cumbersome to transport, and require frequent technical maintenance. For example, accidently jarring a microscope will typically require time-intensive realignment by a specialist. In contrast, holographic microscopy simply requires a sensor, software, computing power, and a display, and will enable imaging devices that are inexpensive, compact, and virtually maintenance-free (see FIGURE 7). This technology should allow imaging solutions at significantly lower cost (tens of dollars per device vs. thousands for each optical microscope), improved ruggedness (no moving parts or optics), reduced weight (grams rather than kilograms), and smaller size relative to optical microscopes.

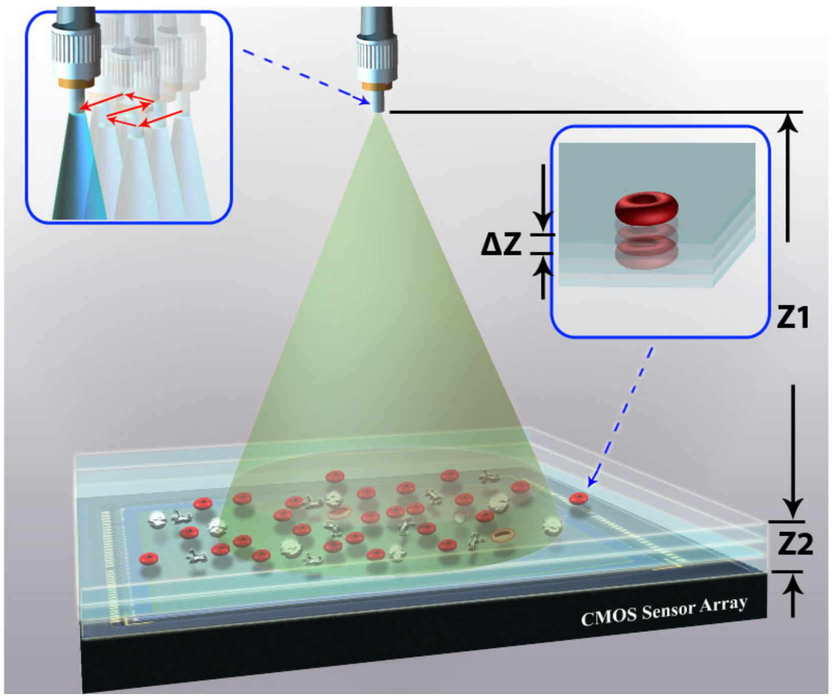

FIGURE 7

Schematic diagram of the lensfree holographic imaging method. The entire active area of the sensor-array becomes the imaging field of view (e.g., ~24 mm^2) for this lensfree on-chip microscopic imaging method.[1]

In FY12, the research team demonstrated submicron (<1 µm) resolution using their holography method, which is comparable to that achieved by oil-immersion optical microscopes, over fields-of-view (FOV) that are over one thousand times greater than optical microscopes, and at depths-of-field (DOF) >4 millimeters, compared to DOF of a few µm at similar resolution for optical microscopes (see FIGURE 8). In addition to significant improvements in static microscopy enabled by these advances, by increasing the FOV and DOF it is now possible to obtain visual tomography of microscopic particles. This fundamental research has not yet identified performance barriers of digital holography, but the group has already achieved <1 µm x <1 µm x <3 µm resolution over an imaging volume of ~40 cubic millimeters, and continue to push the limits of the system. The experimental methods and results from this research are described in more detail in the Ozcan Laboratory's recent publications.[1,2,3]

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[1] Greenbaum A and Ozcan A. (2012). Maskless imaging of dense samples using pixel super-resolution based multi-height lensfree on-chip microscopy. *Optics Express*. 20:3129–43.

[2] Mudanyali O, Dimitrov S, Sikora U, et al. (2012). Integrated rapid-diagnostic-test reader platform on a cellphone. *Lab Chip*. 12:2678-86.

[3] Mavandadi S, Dimitrov S, Feng S, et al. (2012). Distributed Medical Image Analysis and Diagnosis through Crowd-Sourced Games: A Malaria Case Study. *PLoS ONE*. 7:e37245.

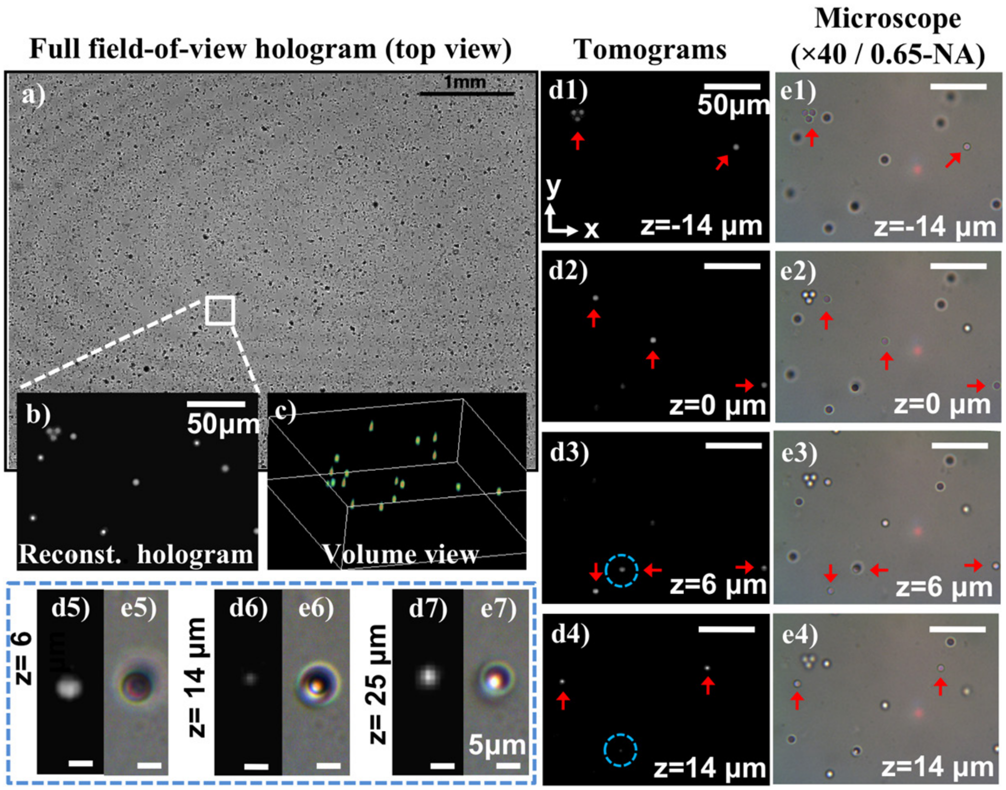

FIGURE 8

Sub-micron resolution over large FOV and DOV. (A) Full FOV (area: 24 mm^2) vertical projection hologram of a sample comprising randomly distributed micro-beads having 5 μm diameter. (B) Digital reconstruction of a small region of interest within the vertical hologram, where all the beads in the chamber are imaged owing to the long depth-of-focus of digital inline holography. (C) 3D view of the sample volume obtained by tomographic reconstruction. (D1-D4) Slice images for a small region of interest to be compared against the microscope images in (E1-E4). Red arrows point to the beads that are in-focus at the corresponding depth. (D5-D7) Demonstrates sectioning of axially overlapping beads, which can be validated by the sectional images in (E5-E7) obtained by a conventional brightfield microscope (40×, 0.65-NA).

Given its compact, inexpensive, and rugged capabilities, this technology may ultimately lead to many capabilities relevant to the Army and civilians. Holographic microscopy may revolutionize point-of-care diagnostics, as tests that are currently restricted to hospitals or clinics could be readily conducted on the battlefield and in the remotest areas of the world. Other potential applications of the technology might include detection of micro-fractures in materiel such as helicopter rotor blades, or detection of microbes on surfaces. (See also the related Technology Transfer example in Section IV-B.)

D. Dissecting the Behavior of Bacterial Biofilms with Non-Canonical Amino Acids

Professor David Tirrell, California Institute of Technology, Institute for Collaborative Biotechnologies

Professor David Tirrell has recently demonstrated the first state-selective labeling of bacterial proteins in response to oxidative stress and the ability to spatially resolve the labeled proteins from pathogenic Pseudomonas aeruginosa in biofilms. This selective labeling method will benefit medical research efforts both within DoD and basic research programs within academic laboratories that are seeking to understand how phenotypic heterogeneity in bacterial biofilms contributes to antibiotic resistance and chronic infections. Professor Tirrell devised a novel method to selectively label and enrich cell proteins using a bio-orthogonal, non-canonical amino acid tagging (BONCAT) strategy that allowed him to study changes in the proteome of specific subpopulations of bacterial pathogens in biofilms, where proteins synthesized in predetermined physiological states can be identified. This method provided the research team insight into the mechanisms of biofilm pathogenesis, which in turn promises to facilitate the identification of new targets for antibiotic treatment.

To label bacterial proteins in response to oxidative stress, Professor Tirrell noted that transcriptional activity from a specified promoter can provide a useful marker for the physiological state of a bacterial cell. Using a methionine surrogate, azidonorleucine (Anl), as a metabolic label and an engineered methionyl-tRNA synthetase (NLL-MetRS), the researchers induced the bacteria to synthesize tagged proteins that incorporated Anl (see FIGURE 9). This method allowed the researchers to complete a state-selective analysis of the proteome, where proteins synthesized in predetermined physiological states can be identified depending on whether or not genes encoding NLL-MetRS are expressed. Using this method, Professor Tirrell then assessed the response of *E. coli* to superoxide or nitric oxide: NLL-MetRS expression was placed under the control of a transcription factor (SoxR) whose activity is sensitive to the level of oxidation in the cell (see FIGURE 10). The experimental methods and results from this research are described in more detail in the researcher team's recent publication.[4]

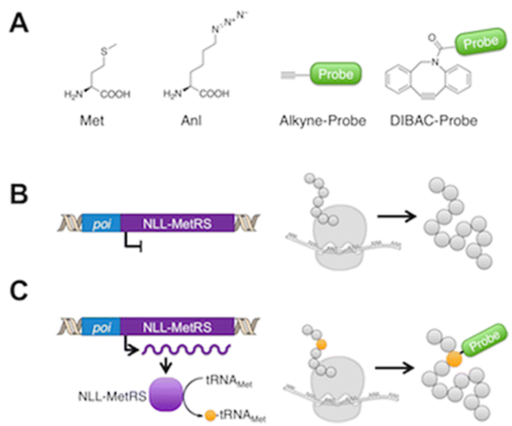

FIGURE 9

Promoter-directed proteomic labeling with Anl. (A) Structures of the amino acids and a simplified representations of the probes used; (B) NLL-MetRS expression is placed under control of a promoter of interest (*poi*). When transcriptional activity of the *poi* is low the NLL-MetRS is not expressed and proteins are not tagged. (C) When transcription of the *poi* is high the NLL-MetRS is expressed and newly synthesized proteins are tagged.

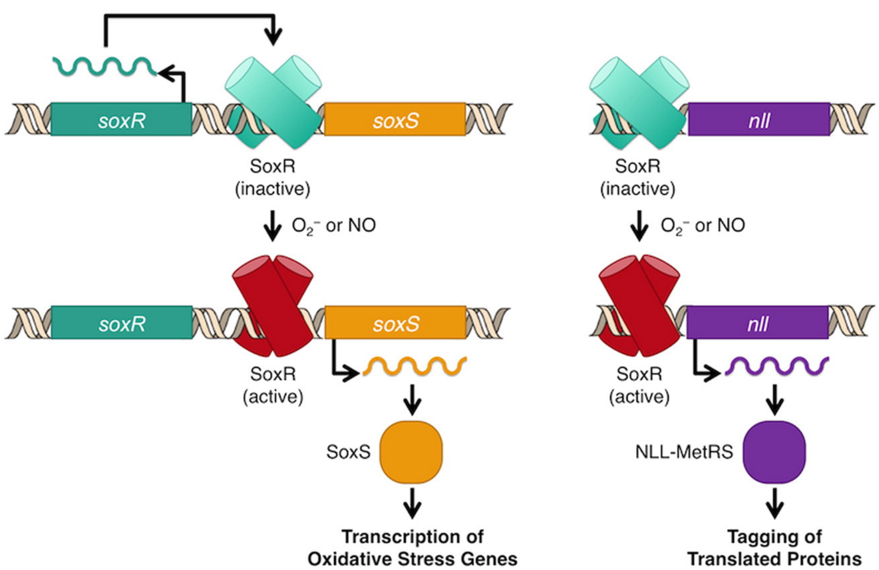

FIGURE 10

Proteomic labeling with Anl under conditions of oxidative stress. The NLL-MetRS is under the control of the SoxRS regulon and is activated by superoxide or nitric oxide. Using this construct, the research team demonstrated rapid tagged protein production that is sensitive to the level of oxidative stress, providing an unambiguous measure of the physiological state of the bacteria.

[4] Ngo JT, Babin BM, Champion JA, et al. (2012). State-Selective Metabolic Labeling of Cellular Proteins. *ACS Chem. Biol.* 7:1326-30.

Having developed a method to probe the physiological state of *E. coli*, the Tirrell laboratory subsequently evaluated the ability of endogenous genetic mechanisms to restrict NLL-MetRS expression and protein labeling to cell states of interest in biofilms of the pathogen *Pseudomonas aeruginosa* (see FIGURE 11). For these experiments, constructs were introduced in *Psuedomonas* that restricted NLL-MetRS expression to a slow-growing, antimicrobial-resistant subpopulation of cells within a biofilm, labeled with Anl and then detected after reacting with a fluorescent alkyne probe. As Anl incorporation was restricted to the desired subpopulation of bacteria within the biofilm, this constituted the first demonstration of global, spatially-controlled protein synthesis in microbial biofilms, and provides a potential means to understand the impact of the phenotypic heterogeneity of complex cellular systems in microbial biofilms.

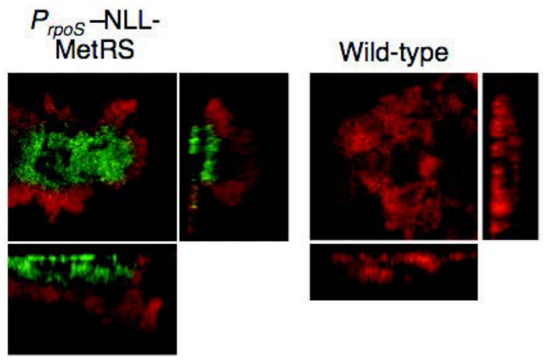

FIGURE 11

Spatially patterned protein labeling in *P. aeruginosa*. Biofilms grown in flowcells from strains of *P. aeruginosa* that were either wild type (right) or engineered to express NLL-MetRS under control of an endogenous promoter (left). The biofilms were subsequently treated with Anl and fixed. A fluorescent molecule probe, SYTO red, binds to DNA and indicates the extent of the biofilm structure (red color). Another fluorescent molecule probe, an alkynyl-functionalized rhodamine green, reacts with azide-containing proteins to indicate Anl labeling (green color). Note that the large central images show confocal slices of the biofilms parallel to the glass substrate, while the flanking images show vertical cross-sections.

E. Neurosensory Optimization of Information Transfer

Dr. Leonard Trejo, Pacific Development and Technology LLC, Single Investigator Award

The goals of this project are to characterize brain activity signatures of performance and fatigue induced by sleep deprivation within the context of a task that measures multiple aspects of attention and cognitive control. More specifically, the research team is developing ecologically-valid measures of hemispheric attention using an extended version of the Lateralized Attention Network Test (LANT), develop dynamic physiological models of the networks of the LANT, and to develop new electroencephalography (EEG) protocols to modulate and optimize in real-time the interactions between the hemispheric attention networks. This enhanced LANT system uses electroencephalography (EEG; measurement of brain electrical activity) and electrooculography (EOG; a measurement of eye movements) signatures of personality, performance, cognitive workload, and fatigue in order to test whether optimized hemispheric input and selective hemispheric activation with EEG neurofeedback can be used as a training aid and/or as an operational tool to prevent performance degradation or mission failure due to fatigue and/or information overload, by directing attentional loads to different brain hemispheres.

In FY12, the research team discovered that LANT results from volunteers completing various attention tasks revealed daily rhythms in each hemisphere, 180º out of phase, and demand-driven redistribution of hemispheric labor with a selective specialization of the right hemisphere for processing social and emotional personality and mood variables (gaze cues, watching movies alone). Further, EEG-biofeedback training could selectively and quickly modulate a specific network in one hemisphere. This research on gaze-contingent displays may ultimately be useful in designing and optimizing soldier-crewstation interfaces such that alerts or targets of interest are re-represented and directed to the brain hemisphere most suited for the required cognitive processing, taking into account the aptitude, personality, cognitive status, and mood of the operator.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Analysis of the Impact of Growth Conditions on CRISPR Evolution

Investigator: Professor Jill Banfield, University of California - Berkeley, Single Investigator Award
Recipient: Center for Disease Control (CDC); Federal Drug Administration (FDA)

Clustered regularly interspaced short palindromic repeats (CRISPR) are hypervariable genomic loci that are widely distributed in bacteria and archaea. Spacers between the repeats provide acquired immunity against foreign genetic elements, including bacteriophage and viruses of archaea. The objective of this project is to understand how CRISPR sequences evolve in both a natural environment (acidophilic biofilms in mine drainage) and a closed *in vitro* system (see FIGURE 12). Recently, the research team discovered that (i) maintenance of a CRISPR-active host:phage in pure culture over long time periods (few months) is impractical, (ii) deep sampling of the CRISPR spacer inventory provided a very sensitive way to detect the past (or current) presence of low abundance (contaminant) phage in the environment of the host that might differentiate cultures from different laboratories, (iii) loss of old end (early acquired) spacers occurs slowly, and the oldest spacers often persist over year(s) time scales, (iv) CRISPR spacer acquisition patterns are not random: a sampling motif is required, and potential spacers are not equally represented in the loci, with patterns pointing to very strong selection for highly effective spacers, and (v) metagenomic analyses can provide direct information about environmental complexity. The experimental methods and results from this research are described in more detail in the researcher team's recent publications.[5-6]

These results have transitioned to the CDC for further study in potential applications such as the identification and tracking of disease outbreaks. The results of this research project also transitioned to the FDA where scientists expect to incorporate these results into new systems to improve the security and safety of the U.S. food supply.

FIGURE 12

Natural environment of acidophilic bacterial. Acid mine drainage sites are used for CRISPR analysis as the extreme acidity and high levels of toxic metals reduces the complexity of the prokaryotic population by several orders of magnitude. In addition, samples spanning the last two decades are available. Bacterial populations are relevant to these superfund sites as the prokaryotes can increase the toxicity of the mining drainage.

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[5] Young JC, Dill BD, Pan C, et al. (2012). Phage-Induced Expression of CRISPR-Associated Proteins is Revealed by Shotgun Proteomics in Streptococcus thermophilus. *PLoS ONE*. 7:e38007.

[6] Weinberger AD, Sun CL, Plucinski MM, et al. (2012). Persisting Viral Sequences Shape Microbial CRISPR-based Immunity. *PLoS CompBiol*. 8:e1002475.

B. Fundamental Studies of Lens-free Microscopy and Tomography
Investigator: Professor Aydogan Ozcan, University of California - Los Angeles, YIP Award
Recipients: Defense Threat Reduction Agency (DTRA); Edgewood Chemical and Biological Center (ECBC); Private Industry

The objective of the project leading to this transition was to conduct studies on lens-free, holographic microscopy and tomography by systematically probing the potential and limitations of the system for analysis of biological systems. Professor Ozcan's laboratory, with funding through an ARO YIP award, ONR, DARPA, and other agencies, recently discovered a new way to image microorganisms using visible or ultraviolet light. In FY12, by exploring fundamentally-new design architectures based on imaging theory and by developing new numerical algorithms, the research team increased resolution from about 2 µm to <1 µm which provided sufficient resolution to visualize individual bacteria. There are many potential applications for using this high-resolution approach with the inherently broad field-of-view and deep depth-of-field of holographic microscopy, such as pathogen detection and scanning structural components for microscopic cracks. This research recently transitioned to DTRA, ECBC, and private industry, for additional research to develop cell-phone-based wide-field fluorescent imaging for multiplexed pathogen detection (see FIGURE 13).

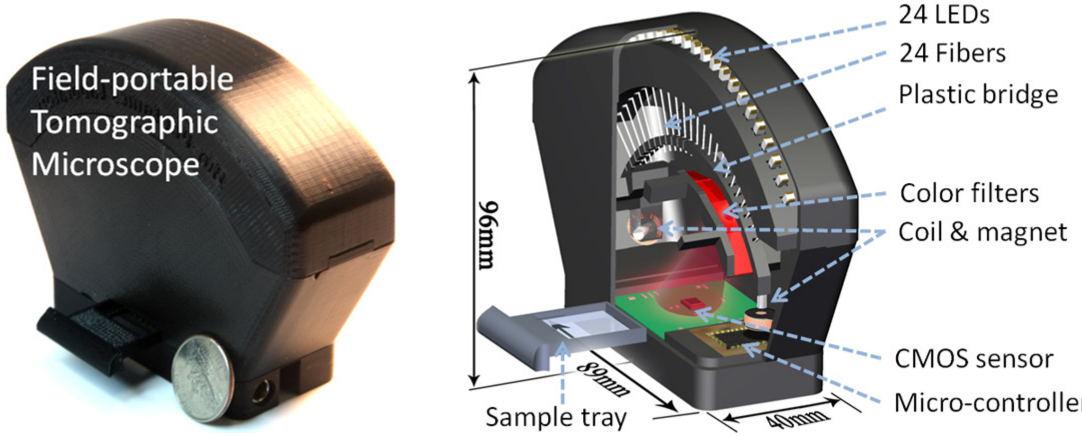

FIGURE 13

Photograph (left) and schematic diagram (right) of the field-portable lensfree tomographic microscope. The Ozcan group has demonstrated that their holographic imaging method can be sufficiently miniaturized for eventual integration into field-portable devices. The miniaturized tomographic microscope weighs only ~110 grams and is designed for low-resource settings. Individual LEDs coupled to multimode optical fibers provide multiple angles of illumination. Optical fibers are electromagnetically actuated to implement source-shifting based pixel super-resolution at each illumination angle. This device enables 3-dimensional imaging of microscopic particles, a never-before-available capability.[7]

C. Discovery of Optical Scanning Method and Investigation of Use in Identifying Counterfeit Electronics
Investigator: ChromoLogic LLC, SBIR Contract
Recipient: Picatinny Arsenal; Aviation and Missile Research, Development and Engineering Center (AMRDEC); Private Industry

The goal of this SBIR project is to explore the properties of DNA to determine if the information-rich natural polymer could be used in a new bar-coding system that would provide enhanced security relative to conventional tracking methods. To recognize the relevance and importance of this research, one must consider the 2011-2012 investigation by the Senate Armed Services Committee (SASC) that found overwhelming evidence that international counterfeiters are taking old, sub-standard electronic components and altering them to appear as new, brand-name parts that are then integrated into DoD munitions, aircraft, sensors, and other electronic devices. SASC chairman, Sen. Carl Levin, stated that the "flood of counterfeit parts, overwhelmingly from China, threatens national security, the safety of our troops and American jobs." Although the SASC uncovered sources of many of these counterfeit parts, an ongoing challenge is to consistently and reliably identify these

[7] Isikman, Bishara, and Ozcan. (2011). Partially coherent Lensfree tomographic microscopy. *Appl Opt*. 50:H253-64.

forgeries and prevent their integration into DoD and Army materiel. The SASC released a report in May 2012 emphasizing this challenge by documenting "failures by defense contractors and DoD to report counterfeit parts and gaps in DoD's knowledge of the scope and impact of such parts on defense systems." This investigation led to an amendment, signed by President Obama, to stop the integration of counterfeit electronic parts into DoD systems and to address weaknesses in the supply chain.

This SBIR project began as result of an SBIR topic conceived by scientists from ARL-ARO and the Natick Soldier Research, Development and Engineering Center (NSRDEC) in 2007. The California-based performer, ChromoLogic, LLC, has developed a tag with a biomimetic barcode that can be aligned in the proper order and decoded by an optical reader, akin to how the sequence of a DNA molecule can be read. This biomimetic tag and reader system has robust information-storage capabilities that are unambiguous and readily authenticated, with no reagent or material exchange between the tag and reader. This technology will provide a capability that complements ongoing research led by ECBC, which focuses on embedding DNA in printed barcodes which can be transferred to a reference test ticket to verify authentic military materiel.

As is often true for high-risk, high-payoff research, this ARO-funded project led to an unexpected discovery that may have an even greater impact than was initially thought, and has led to a novel technology that will help address many of the challenges noted in the SASC report. The research team discovered that the optical scanning technology developed to decode the biomimetic tag is capable of mapping the intrinsic surface of electronic components, providing a type of fingerprint to distinguish authentic or counterfeit circuits. Given that counterfeit electronic components are forged chiefly by altering their surface layers, this discovery provides a powerful method for screening integrated circuits based on their intrinsic surface patterns, which can be scanned in as little as one second. ChromoLogic has developed this surface-scanning technology into the DTEK system, which provides quantitative optical inspection of integrated circuits (see FIGURE 14).

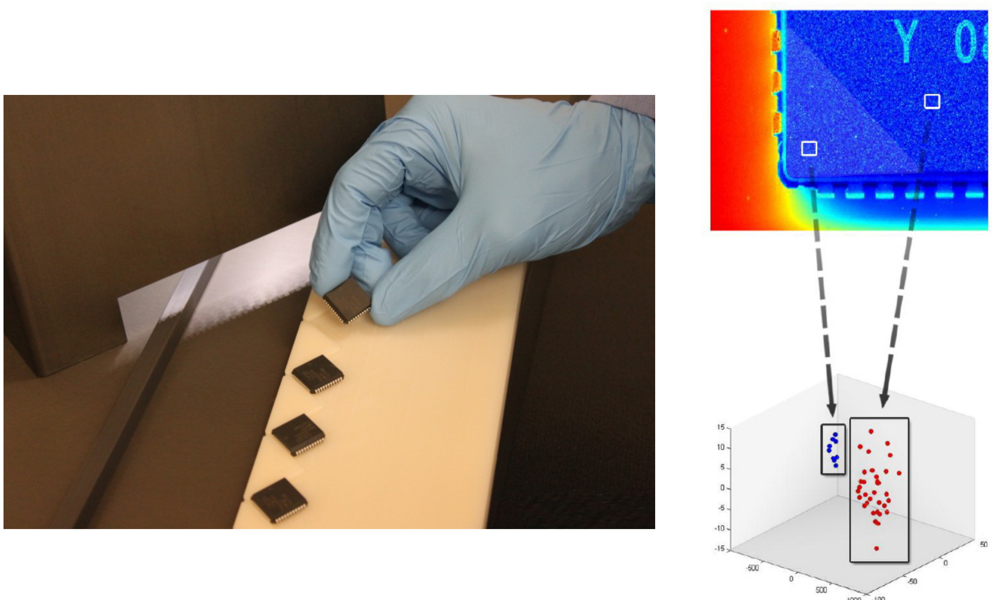

FIGURE 14

The DTEK bio-inspired surface-scanning technology. The DTEK optically analyzes the surface of an electronic component and outputs unambiguous quantitative information about the surface for use in comparative analysis. *[ChromoLogic/Covisus]*

The DTEK system recently began evaluation through multiple electronics manufacturers, and the technology has already been adopted by NASA-JPL and Boeing. The DTEK optical scanning technology is also capable of identifying and tracking materiel in the absence of external tags or barcodes. ChromoLogic began working with Picatinny Arsenal and AMRDEC to develop and test a hand-held scanner that can be used for covert tracking and management of high-value Army commodities. The DTEK system, used as part of a comprehensive counterfeit-mitigation process, may ultimately reduce the influx of forgeries into Army materiel and improve the reliability of mission-essential equipment used by the Soldier.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Dynamics and Evolution of Associative Memory in Bacterial Populations

Professor Ilias Tagkopoulos, University of California - Davis, Single Investigator Award

Associative memory occurs when an organism associates two events such as observed with the Pavlovian response, and has traditionally been viewed as a characteristic of complex organisms. Evidence has been accumulating, however, that simple organisms such as bacteria, are able to internalize and relate environmental cues over evolutionary timescales. Moreover, it has been shown that these history-dependent behaviors are not just a manifestation of necessary physical and chemical couplings, since they exhibit significant plasticity under environmental variation. Professor Tagkopoulos is investigating the ability of bacteria to store associations between environmental signals and events. It is anticipated that in FY13, the research team will characterize the dynamics of associative memory formation in bacterial populations and begin developing a predictive model for bacterial associative memory dynamics and evolution. The research team will conduct learning experiments to determine the mechanistic basis of associative memory in bacteria. An understanding of associative memory should provide insight into microbial physiological processes that influence microbial survival and is likely to be relevant to medical or industrial applications.

B. Translating Biochemical Pathways to Non-Cellular Environments

Professor Hao Yan, Arizona State University, MURI Award

Cells provide a precisely organized environment to promote maximum efficiency of biochemical reaction pathways, with individual enzymatic components organized via multisubunit complexes, targeted localization in membranes, or specific interactions with scaffold proteins. The eventual translation of these complex pathways to engineered systems will require the ability to control and organize the individual components outside of the natural cellular environment. A new MURI program led by Professor Hao Yan at Arizona State University is developing the scientific foundations needed to design, assemble, and analyze a biochemical pathway in a non-cellular environment using DNA nanostructures to organize the individual pathway components.

Over the course of the program, the multidisciplinary research team will employ a comprehensive approach including design, modeling, assembly and characterization to control the organization of both multi-enzyme reaction pathways and photosynthetic systems using DNA nanostructures as scaffolds. It is anticipated that in FY13, a multi-enzyme pathway will be organized on a DNA nanostructure to identify the inter-enzyme distances and spatial arrangements that are necessary for maximal pathway activity (see FIGURE 15 A-B), and the formation of the assembled structures will be verified using atomic force microscopy and transmission electron microscopy. In addition, the directed diffusion of reaction intermediates between enzymes will be explored using a structural protein bridge and an engineered swing arm (see FIGURE 15 C-D), and successful transfer of intermediates will be verified using steady-state and single molecule fluorescence measurements. The results will be used to construct more complex, bioelectroactive enzyme pathways that in future years may be interfaced with external conductive materials to create new capabilities in photo-energy generation and energy storage.

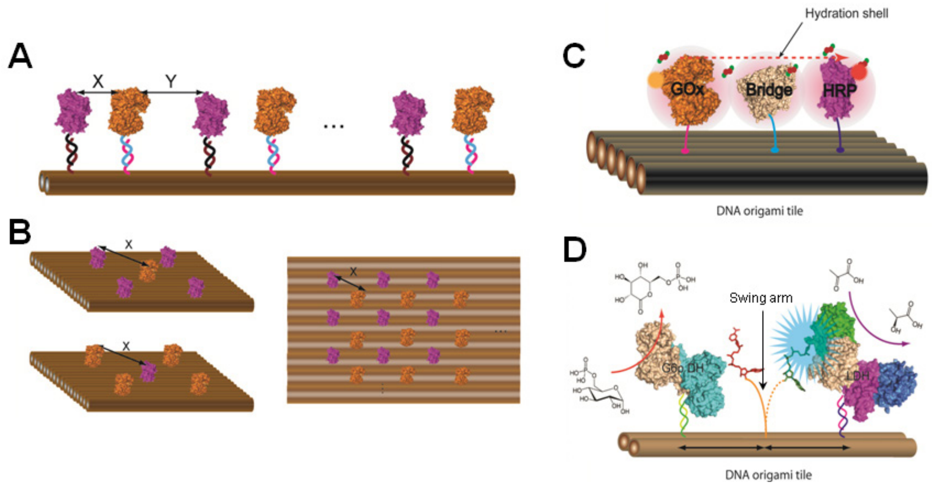

FIGURE 15

Organizing and Controlling Biochemical Pathways Outside of the Cellular Environment. The MURI team will explore the impact of inter-enzyme distances on reaction pathway activity in (**A**) 1D and (**B**) 2D architectures. The program will also explore synthetic approaches to direct the transfer of reaction intermediates between enzymes, including (**C**) a structural protein bridge that provides a hydration shell to prevent diffusion of intermediates in 3D space and (**D**) an engineered swing arm that can transfer a reaction intermediate directly between two enzymes.

C. Rugged Automated Training System (RATS)

Barron Associates Inc. and Coherent Technical Services Inc., Single Investigator Award; STTR Contract; DARPA Award

There is an increasing trend towards the use of non-metal based mines, necessitating the use of direct detection of explosive vapors instead of the simpler metal detectors. Direct detection of vaporized explosive compounds is accomplished either by explosive vapor detector equipment or with animals. Although not rigorously quantified, it is apparent that trained animals are capable of detecting explosives at levels lower than abiotic systems such as gas chromatography / mass spectrometry. The DoD currently relies on dogs for animal-based explosive detection; however, a Dutch organization has demonstrated that rats can be used to reliably find mines. Rodents have multiple advantages over dogs for the detection of explosives: (i) rodents are more acceptable to use than dogs in some cultures, (ii) humans do not typically have the emotional attachment to rodents as to dogs, (iii) rodents do not have the emotional attachment to humans that dogs do; therefore, rodents will work for anyone and not just a selected trainer, (iv) rodents are smaller, enabling transport in a backpack and allowing searches in smaller spaces, (v) rodents can climb trees, (vi) rodents need less food, less space, less medical care, and less logistical support than a dog.

Although it is not the intent of these efforts to replace military working dogs with military working rats, it is desirable to develop a rodent capability to complement existing dog capabilities. In addition to detecting mines, trained rodents could also be used to find humans or bodies after natural disasters such as earthquakes, and can be used to search in caves, sewers, walls, and other spaces too difficult for dogs to access. Rats are also more conducive to operating in stealth mode than dogs; they are common sights in many environments and they are quiet (see FIGURE 16). Through joint research with demining engineers at West Point and Fort Leonard Wood, it is anticipated that in FY13 the RATS scientists and engineers will make significant progress towards developing and validating a machine that will reliably train small animals to detect explosives or other compounds of interest, and can provide an objective unbiased measurement of each animal's sensitivity and accuracy.

FIGURE 16

African giant pouched rat in training to detect mines in Tanzania. ARO-funded researchers in collaboration with USMA and Fort Leonard Wood are designing and validating a system to reliably train small animals for mine detection.

D. Ultrasound Neuromodulation
Neurotrek, Inc., SBIR Contract

Managing pain acute traumas is generally accomplished with narcotics, which is greatly problematic in battle scenarios as these compounds severely affect cognitive abilities. Many studies have established the beneficial effects of neurostimulation for managing pain. The goal of this research project is to develop a software platform, optimize the ultrasound parameters for human pain modulation, perform safety testing in phantom and animal models, and finally to develop a prototype that can modulate pain using ultrasound neuromodulation. It is anticipated that in FY13 this research will provide optimized parameters for future testing of human pain management using neuromodulation. A peripheral ultrasound neuromodulation may offer several advantages versus narcotics and current methods of neurostimulation. This technology has the potential to be highly portable as a battlefield analgesic and has the advantage of leaving the soldiers cognitive abilities intact.

E. Ethnographic Assessment and Data Management Integration
Charles River Analytics, Inc., STTR Contract

The collection and analysis of socio-cultural data is becoming increasingly important for the conduct of effective military operations. The production of more scientifically-valid models of human behavior has become increasingly dependent on the available forms of socio-cultural data. The ability to rapidly collect social and cultural data in field settings is challenging under most circumstances, and in conflict, denied, or high-risk areas these challenges become even more pronounced. The goal of this project is to develop a data management toolkit that provides integrated, extensible analysis tools powered by proven cultural anthropology data collection and analysis techniques, comprehensive data collection tools using state-of-the-art mobile devices, and standards-based server-side data management capabilities. It is anticipated that in FY13, this STTR contract will successfully design and implement a software tool using algorithms incorporating ethnographic methods for the rapid collection of cultural, social, and economic data based on structured and semi-structured interviews, qualitative text sources, or unobtrusive observations. The software development and validation will be completed in Phase II of the STTR contract. This research may ultimately provide an enhanced ability to mine, collect, analyze and manage social and cultural data, which will ultimately enable better decision-making at various levels (e.g., policy, combat operations).

VI. Scientific and Administrative Staff

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CHAPTER 8: MATERIALS SCIENCE DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2012* is to provide information on the programs and basic research efforts supported by ARO in FY12, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Materials Science Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY12.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Materials Science Division seeks to realize unprecedented materials properties by embracing long-term, high risk, high-payoff opportunities for the U.S. Army, with special emphasis on four Program Areas: Materials by Design, Mechanical Behavior of Materials, Physical Properties of Materials, and Synthesis and Processing of Materials. The objective of research supported by the Materials Science Division is to discover the fundamental relationships that link chemical composition, microstructure, and processing history with the resultant material properties and behavior. These research areas involve understanding fundamental processes and structures found in nature, as well as developing new materials, material processes, and properties that promise to significantly improve the performance, increase the reliability, or reduce the cost of future Army systems. Fundamental research that lays the foundation for the design and manufacture of multicomponent systems such as composites, hierarchical materials and "smart materials" is of particular interest. Other important areas of interest include new approaches for materials processing, new composite formulations, and surface treatments that minimize environmental impacts, and novel composite concepts, including multifunctional and hierarchical materials. Finally, there is general interest by the Division in research programs to identify and fund basic research in the area of manufacturing science, which will address fundamental issues related to the reliability and cost (including environmental) associated with the production and long-term operation of Army systems.

2. Potential Applications. In addition to advancing and exploiting worldwide knowledge and understanding of new materials to achieve unprecedented properties, research managed by the Materials Science Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter and battlesystems. In the long term, the basic research discoveries made by ARO-supported materials research is expected to provide a broad base of disruptive and paradigm-shifting capabilities to address Army needs. Advanced materials will improve mobility, armaments, communications, personnel protection, and logistics support in the future. New materials will target previously identified Army needs for stronger, lightweight, durable, reliable, and less expensive materials and will provide the basis for future Army systems and devices. Breakthroughs will come as the fundamental understanding necessary to achieve multi-scale design of materials, control and engineering of defects, and integration of materials are developed.

3. Coordination with Other Divisions and Agencies. To realize the vision of the Materials Science Division and maximize transition and leveraging of new materials discoveries worldwide, the Division collaborates with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the Defense Advanced Research Projects Agency (DARPA), and across federal-funding agencies (*e.g.*, Nanoscale Science and Engineering Technology subcommittee, Reliance 21 Community of Interest for Materials and Processes), and in international forums (*e.g.*, the Technical Cooperation Program). The Materials Science Division is also very active in pursuing other ARO Divisions to co-fund research, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. In particular, ongoing collaborations exist with the ARO Chemical Sciences, Electronics, Life Sciences, Mechanical Sciences, Mathematical Sciences, and Physics Divisions.

B. Program Areas

To meet the long-term program goals described in the previous section, the Materials Science Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY12, the Division managed research efforts within these four Program Areas: (i) Materials Design, (ii) Mechanical Behavior of Materials, (iii) Physical Properties of Materials, and (iv) Synthesis and Processing of Materials. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Materials Design. The goal of the Materials Design Program Area is to enable the bottom-up design and fabrication of highly complex multifunctional materials with new and unprecedented properties (*e.g.*, negative index composites with optical cloaking properties or new classes of smart materials that can alter their behavior in response to environmental stimuli). In pursuit of this goal, this Program Area supports research that falls into three broad Thrusts: (i) Foundations for Future Directed Self-assembly of Materials, (ii) New Analytical Techniques for Characterizing Materials at the Nanoscale, and (iii) Understanding Complex Behavior that Emerges in Highly-coupled Systems (*i.e.*, studying frustration effects in magnetic systems, or better understanding field coupling effects in multiferroics). It is envisioned that the confluence of these Thrusts will culminate in the development of a new generation of engineered materials with new and unique capabilities. To realize this goal the program recognizes that the experimental program will require a strong complementary theoretical underpinning that addresses modeling of the relevant phenomenology, identification of robust pathways for directed self-assembly, and prediction/optimization of the final material properties.

Research supported under this Program Area is expected to provide materials that enable future disruptive capabilities and applications in communications, sensors, electronics, and logistics support. In addition, these efforts may enhance self assembly to affect property changes over time that introduce new properties, optimize performance, enhance reliability, and reduce cost and time to development.

2. Mechanical Behavior of Materials. This Program Area seeks to establish the fundamental relationships between the structure of materials and their mechanical properties as influenced by composition, processing, environment, and loading conditions. The program emphasizes research to develop innovative new materials with unprecedented mechanical and other complementary properties. Critical to these efforts is the need for new materials science theory that will enable robust predictive computational tools for the analysis and design of materials subjected to a wide range of specific loading conditions, particularly theory that departs from standard computer algorithms and is not dependent upon tremendous computational facilities. The primary research Thrusts of this Program Area are: (i) High Strain-rate Phenomena and (ii) Materials Enhancement Theory. The High Strain-rate Phenomena is focused on research to design new characterization methods and tools to elucidate the deformation behavior of materials exposed to high-strain rate and dynamic loading conditions, establish a detailed understanding of the physical mechanisms that govern this deformation, and realize novel mechanisms of energy absorption and dissipation. Materials Enhancement Theory focuses on developing a robust understanding of the interrelationships between materials processes and compositions and the range of properties that can be attained by them, particularly in terms of developing new materials theory capable of predicting such processing-property relationships and identifying novel mechanisms for enhancing specific toughness, engineering and synthesizing new materials containing unique and specifically designed chemical and biological functionalities and activities while maintaining, and preferably enhancing, requisite mechanical properties.

Research supported under this Program Area is anticipated to realize new materials that enable revolutionary capabilities in Soldier and systems protection, lightweight structural materials, predictive materials design theory, sensors, fuel cell membranes, and Soldier sustainment.

3. Physical Properties of Materials. This Program Area seeks to develop an understanding of the fundamental mechanisms responsible for the various physical properties (electronic, magnetic, optical, and thermal) of materials/composites through support of basic research that ultimately leads to development of future Army devices. General areas of research include modeling, innovative processing methods of materials with unprecedented physical properties, and novel characterization techniques for the determination of these physical properties. Three main Thrusts of this program are: (i) Defect Engineering of Advanced Materials, (ii) Materials for Thermal Management, and (iii) Novel 2D Free-standing Crystalline Materials. Defect Engineering of Advanced Materials involves studies of semiconductors, ferroelectrics, superconductors, and others, and structures such as bulk materials, thin-films, and interfaces in advanced materials (*e.g.*, oxides, nitrides, carbon-based materials). Materials for Thermal Management involves studies of novel thermal interface materials for thermal management of advanced electronics, carbon based materials, alloys, composites, as well as novel thermal property characterization methods. Novel 2D Free-standing Crystalline Materials includes fundamental research efforts with the goal of investigating the physical properties of novel free-standing crystalline 2D and composites of 2D/3D/1D materials (*e.g.*, oxides, nitrides), and characterizing unique properties/phenomenon in free-standing 2D crystalline materials.

These research Thrusts are expected to provide new materials that will address vital Army needs such as sensing, flexible displays, advanced electro-optical technologies, electronic materials/devices, advanced RF technologies, as well as power and energy (*e.g.*, micro, Soldier and portable power).

4. Synthesis and Processing of Materials. This Program Area focuses on the use of innovative approaches for processing high performance structural materials reliably and at lower costs. Emphasis is placed on the design and fabrication of new materials with specific microstructure, constitution, and properties. Research interests include experimental and theoretical modeling studies to understand the influence of fundamental parameters on phase formation, micro structural evolution, and the resulting properties, in order to predict and control materials structures at all scales ranging from atomic dimensions to macroscopic levels. The specific research Thrusts within this Program Area are: (i) Metastable Materials and Structures and (ii) Novel Processing Strategies. Metastable Materials and Structures focuses on (a) developing superior and affordable alloys, fibers, and composites with amorphous, ultra-fine grain, or otherwise highly controlled and meta-stable structures, (b) using *ab initio* theoretical approaches to design target electronic structures for functional moieties, and (c) synthesizing materials that exhibit these units to produce novel properties. Novel Processing Strategies supports research with the goals of (a) establishing and utilizing advanced and innovative processing approaches such as field enhanced processing, soft lithography, self-assembly, and bio-inspired and biomimetics, and (b) developing unique high strength alloys, metal matrix composites, and ceramic and polymeric composites, particularly those that offer enhanced repair or self-healing capabilities.

These research Thrusts are expected to generate new materials that will provide revolutionary solutions to Army needs in the areas of: lightweight alloys and composites for vehicle structures, lightweight armaments, airframes, and bridging; advanced ceramics for improved armor; improved materials and processes for joining of components; high density metals for kinetic energy penetrators; fabrics and polymeric body armor; thermal and acoustical insulating foams; materials for gun tubes; and directed energy weapons.

C. Research Investment

The total funds managed by the ARO Materials Science Division for FY12 were $38.0 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY12 ARO Core (BH57) program funding allotment for this Division was $6.4 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $10.1 million to projects managed by the Division. The Division also managed $16.6 million of Defense Advanced Research Projects Agency (DARPA) programs, and $0.1 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.3 million for contracts. Finally, $3.5 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY12 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research projects. Research projects are developed by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts.

The following subsections summarize projects awarded in FY12 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY12, the Division awarded 32 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as determining physical properties through novel characterization techniques, development of new generations of engineered materials, and modeling to predict and control materials structures at scales ranging from atomic dimensions to macroscopic levels. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Sean Agnew, University of Virginia; *Dynamic Failure Mitigation Through Microstructure Control: Application to Aluminum and Magnesium Alloys*
- Professor Michel Barsoum, Drexel University; *Nanocrystalline MAX/Mg Composites with Exceptional Properties*
- Professor Laurent Bellaiche, University of Arkansas; *Searching For Novel Phenomena in Two-Dimensional Ferroelectrics and Multiferroics*
- Professor Raffi Budakian, University of Illinois - Urbana; *Nanometer-Scale Force-Detected Nuclear Magnetic Resonance Imaging*
- Professor David Cahill, University of Illinois - Urbana; *Extraordinary Spin-Wave Thermal Conductivity in Low-Dimensional Copper Oxides*
- Professor Srinivasan Chandrasekar, Purdue University; *Synthesis and Processing of Materials: Enhancing Deformation Processing Capability of Structural HCP Metals*
- Professor Joshua Goldberger, Ohio State University; *Germanium Graphane Analogues*
- Professor Peter Hammel, Ohio State University; *Nanoscale Resolution Magnetic Resonance Studies of Spin Dynamics and Defect Properties in Diamond Nanostructures*
- Professor Heinrich Jaeger, University of Chicago; *Jamming/Unjamming Dynamics in Granular Materials*
- Professor Valery Levitas, Iowa State University of Science and Technology; *Strain-Induced Phase Transformations in Ceramics under High Pressure*
- Professor John Lewandowski, Case Western Reserve University; *Size, Scale and Confinement Effects on Metallic Glasses*

- Professor Matthew Libera, Stevens Institute of Technology; *Hierarchical Self Assembly of Multifunctional Biointeractive Surfaces*
- Professor J. Ping Liu, University of Texas - Arlington; *Exchange-coupled Hybrid Nanocomposite Magnets*
- Professor John Marohn, Cornell University; *Nanoscale Magnetic Resonance Imaging and Characterization of Organic Electronic Materials*
- Professor Joanna Millunchick, University of Michigan - Ann Arbor; *Point Defect Reduction in Far Infrared Materials via Surface Engineering*
- Professor Andreas Mortensen, Swiss Federal Institute of Technology; *Exploring the Role of Hydrostatic Pressure on Yield, Deformation and Fracture of Infiltrated Ceramic Particle Reinforced Metals*
- Professor Nathan Newman, Arizona State University; *Defect Engineering for Ultra-low Loss Microwave Dielectrics*
- Professor Christopher Palmstrom, University of California - Santa Barbara; *Epitaxial Semiconducting Heusler Alloy Heterostructures*
- Professor Wounjhang Park, University of Colorado - Boulder; *Self-Assembly of Reconfigurable By-Design Optical Materials with Molecular-Level Control*
- Professor John Perepezko, University of Wisconsin - Madison; *Deformation Driven Alloying and Transformation*
- Professor Yu Qiao, University of California - San Diego; *Mitigating Stress Waves by Using Nanofoams and Nanohoneycombs*
- Professor Julian Rimoli, Georgia Tech Research Corporation; *Guiding of High Amplitude Stress Waves Through Stress-Induced Domain Switching in Multiphase Materials*
- Professor Timothy Rupert, University of California - Irvine; *Tailoring Grain Boundary Chemistry for Failure Resistant Nanostructured Metals*
- Professor Darrell Schlom, Cornell University; *Synthesis of Defect-Mitigating Tunable Dielectric Materials with Atomic-Layer Control*
- Professor Henry Sodano, University of Florida - Gainesville; *Photoresponsive Polymers for Autonomous Structural Materials with Controlled Toughening and Healing*
- Professor Gopalan Srinivasan, Oakland University; *Self-Assembled Multiferroic Nanostructures and Studies on Magnetoelectric Interactions*
- Professor Izabela Szlufarska, University of Wisconsin - Madison; *Microstructural Evolution Model for Design of Ultra-Mild-Wear Coatings*
- Professor Klaus van Benthem, University of California - Davis; *Determination of the influence of electric fields upon the densification of ionic ceramics*
- Professor Charles Winter, Wayne State University; *New Chemical Precursors for the Growth of Ferroelectric and Mid-Valent Metal Oxide Films*
- Professor Qiming Zhang, Pennsylvania State University; *Understanding the Scientific Basis of Electrocaloric Effect In Defects Modified Ferroelectric Polymers*
- Professor Yuntian Zhu, North Carolina State University; *Probing Deformation Mechanisms of Nanostructured Mg Alloys for Unprecedented Strength and Good Ductility*

2. Short Term Innovative Research (STIR) Program. In FY12, the Division awarded 11 new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies of self-adaptive 3D lattices for stress wave mitigation and energy absorption, characterize of materials for physical properties such as excitonic absorption and emission in the presence of external magnetic fields, and the effect of pre-stressing of constituent materials along microstructural morphologies on the composites overall load bearing performance. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor L. Catherine Brinson, Northwestern University Evanston Campus; *Architectured Porous Shape Memory Alloys and Composites - Novel Processing and Characterization*

- Professor Mo Li, Georgia Tech Research Corporation; *Residual Stress and Its Effects on Mechanical Properties and Performance of HCP Nanocrystalline Mg and Alloys*
- Professor Linyou Cao, North Carolina State University; *Synthesis and Magneto-optical Characterizations of of 2D Lead Chalcogenide PbX (X=S, Se, Te) Nanosheets*
- Professor Mark Horstemeyer, Mississippi State University; *Toward New Magnesium Alloy Design - Theoretical and Experimental Studies of the Influence of Alloying Elements on Deformation Twinning*
- Professor Anastasia Muliana, Texas Engineering Experiment Station; *The Effect of Pre-stresses and Microstructural Morphology on the Overall Mechanical Properties of Composites*
- Professor Gregory Olson, Northwestern University Evanston Campus; *Ductilization of High-Strength Magnesium Alloys*
- Professor Yoosuf Picard, Carnegie Mellon University; *In-situ Characterization of Defects Controlling Memristive Behavior*
- Professor Surajit Sen, State University of New York (SUNY) at Buffalo; *On the Possibility of Novel, Thin, Light-Weight, Shock Absorptive and Heat Resistant Materials*
- Professor Lih-Sheng Turng, University of Wisconsin - Madison; *A Novel Supercritical Fluid-assisted Fabrication Technique For Producing Transparent Nanocomposites*
- Professor Mingzhong Wu, Colorado State University - Ft. Collins; *Growth of Low-Damping Yttrium Iron Garnet Nano Films by Magnetron Sputtering*
- Professor Hongbin Yu, Arizona State University; *Probing Electrostatic Potential Profile in ZincBlende/Wurtzite Quantum Structures in Semiconducting Nanowires Using Electron Holography*

3. Young Investigator Program (YIP).

No new starts were initiated in FY12.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY12 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *2011 Materials Research Society Fall Meeting;* Boston, MA, 28 November - 2 December 2011
- *Armor Ceramics Symposium 2012 - ACerS 36th International Conference on Advanced Ceramics and Composites;* Daytona Beach, FL, 22-27 January 2012
- *Biological Materials Science Symposium;* Orlando, FL, 11-15 March 2012
- *Phase Transformations and Deformation in Magnesium Alloys Symposium Mechanical Behavior at Nanoscale I Symposium Ultrafine Grained Materials VII Symposium;* Orlando, FL, 11-15 March 2012
- *2012 Materials Research Society (MRS) Spring Meeting;* San Francisco, CA, 9-13 April 2012
- *Research Developments and Stimulating Technical Exchanges at the International Field Emission Society 2012 Conference;* Tuscaloosa, AL, 21-25 May 2012
- *9th International Conference on Magnesium Alloys and their Applications;* Vancouver, Canada, 8-12 July 2012
- *2012 International Conference on 3D Materials Science;* Seven Springs, PA, 8-12 July 2012
- *Workshop on Two Dimensional Materials Beyond Graphene;* Columbus, OH, 7-8 August 2012
- *2012 Defects in Semiconductors Gordon Research Conference*; Biddeford, ME; 12-17 August 2012
- *Harnessing the Materials Genome Conference;* Vail, CO, 30 September - 5 October 2012

5. Special Programs. In FY12, ARO Core Research Program funds provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded two new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

C. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Materials Science Division; therefore, all of the Division's active MURIs are described in this section.

1. Characterizing Ionic Liquids in Electro-active Devices (ILED). This MURI began in FY07 and was granted to a team led by Professor Timothy Long at the Virginia Polytechnic Institute and State University (Virginia Tech). The goal of this MURI is to use ionic liquids both as a reaction medium for synthesizing polymers, as an active component incorporated into the final polymer structure, and to fabricate and characterize new actuator devices with dramatically improved performance. This program is co-managed with the ARO Chemical Sciences Division.

Electroactive materials are materials that exhibit a physical response, usually a change in shape, under activation by an electrical potential. These materials are useful in a number of applications including MEMS, stimuli-responsive structures, energy harvesting, micro-sensors, chem-bio protection, and portable power. The main technological limitations of these materials, which limit their usefulness, are their relatively slow response time and low actuation authority (the maximum force they can apply). The focus of the research is on molecular design, synthetic methodology, nanoscale morphological control, property measurements, modeling, and characterization of device performance. The specific research areas of this project include the study of (i) free radical, step growth, and condensation, (ii) polymer structure characterization using atomic force microscopy (AFM), scanning transmission electron microscopy (STEM), small angle X-ray scattering (SAXS), dynamic mechanical analysis (DMA), transmission electron microscopy (TEM), and standard polymer characterization techniques, such as nuclear magnetic resonance and gel permeation chromatography, (iii) synthesis of zwitterionic monomers using step- and chain-growth polymerizations to form membranes and crosslinked networks, and (iv) synthesis and characterization of liquid crystalline monomers containing imidazolium sites.

2. Materials on the Brink: Unprecedented Transforming Materials. This MURI began in FY07 and was granted to a team led by Professor Kaushik Bhattacharya at the California Institute of Technology. The objective of this research is to develop a fundamental understanding and establish the engineering expertise needed to tailor the electrical, optical, or magnetic (EMO) properties of phase transforming materials through the design and implementation of highly reversible, phase-transformations.

This research is investigating different approaches to achieving highly reversible phase transformations, including such effects as engineered phase compatibility and frustration. The broad selection of material systems (perovskites and multi-ferroics, Heusler alloys, SMA, and oxy-acid proton conductors), and the design of the studies, will develop a fundamental understanding of the underlying physics that developers need to predict the occurrence of states and the range of behaviors that can be realized within engineered phase transforming materials. The specific goals of this project are to develop and characterize (i) perovskites for electrically tunable photonics and RF-to-optical converters, (ii) metal-ferroelectric multilayers for negative refractive index material applications (a negative surface-plasmon polariton was shown to provide NIM behavior in the visible part of the spectrum), light modulators, thermo-magnetic cooling, spintronics and magnetic field sensing, (iii) shape-memory alloys for large-strain actuators, and (iv) proton-conducting electrolytes for fuel cells. New strategies based on phase engineering of materials have been successfully realized in actuation systems (*e.g.*, in shape memory alloys and relaxor ferroelectrics). These same underlying principles may ultimately be transferable to the development of EM sensors, tunable phase shifters, adaptive optics, optical limiting and energy harvesting devices for use by the Army.

3. Spin-Mediated Coupling in Hybrid Magnetic, Organic, and Oxide Structures and Devices. This MURI began in FY08 and was granted to a team led by Professor Michael Flatte at the University of Iowa. The objectives of this research are to (i) improve the field's understanding of spin behavior in hybrid systems where magnetic semiconductors and/or organics are integrated with ferromagnetic metals and multiferroic oxides, and (ii) develop the engineering expertise needed to exploit spin-mediated processes to establish nanoscale control over spin transport, local magnetic order, and electrical/optical/magnetic properties of hybrid magnetic systems.

More specifically, the goals of this project are to (i) investigate, both experimentally and theoretically, spin behavior and magnetic field manipulation in hybrid magnetic systems, (ii) develop a fundamental understanding of the physics involved in spin current generation and control, spin momentum transfer, and magnetic field manipulation, (iii) establish techniques for controlling dynamic spin phenomena in nanoscale systems, including both isolated nanomagnets and nanomagnetic arrays, and (iv) design and fabricate device structures that utilize spin polarization currents and momentum transfer as a means of attaining new functionality and capabilities. The research may lead to novel electronic devices that include: circularly polarized light emitting diodes, lasers and detectors, nanoscale microwave and millimeter wave oscillators for signal processing and chip-to-chip communications, reconfigurable circuitry, smart sensors for IED detection, and spin-based logic processing (including quantum computing) for data manipulation and computing.

4. Design of Adaptive Load Mitigating Materials Using Nonlinear Stress Wave Tailoring. This MURI began in FY09 and was granted to a team led by Professor John Lambros at the University of Illinois, Urbana. This research is focused on understanding and exploiting wave tailoring phenomena in highly nonlinear inhomogeneous granular media.

The effort builds on recent results demonstrating remarkable dynamic properties in such media, including tunability, energy trapping and wave redirection, primarily because of the highly nonlinear forces that are generated during contact of the granular crystals. Specific granular microstructures will be designed to fully exploit the nonlinear contact effect. Additionally, novel phase transforming ceramics will be fabricated that enhance the granular materials properties by, for example, preferentially strengthening or weakening the material to control local energy dissipation. The specific goals of this research are to (i) incorporate a granular medium in the material system in order to introduce nonlinearity in the material microstructure through local contact between material “elements”, thereby furnishing an adaptive and nonlinear targeted energy transfer (TET) capability, (ii) provide additional adaptively coupled with enhanced energy absorption by developing new phase transforming ceramics, (iii) arrange these and other elements in a material system that is either layered (2D), or integrated with a 3D microstructural architecture, and (iv) utilize geopolymers (polymer-like ceramics) to create interfaces that join constituents and also act as “traditional” wave arrestors or reflectors. The comprehensive understanding of propagation and mitigation of high-pressure stress-waves in complex media will guide the future design and demonstration of new materials optimized for high-strain-rate ballistic performance, particularly armor materials. The research is expected to ultimately enable lightweight military hardware with dramatically enhanced survivability, in addition to new paradigms for insensitive munitions.

5. Innovative Design and Processing of Multi-functional Adaptive Structural Materials. This MURI began in FY09 and was granted to a team led by Professor Ilhan Aksay at Princeton University. The objective of this research is to develop innovative processing techniques for the design and modeling of hierarchically porous adaptive structures that are optimized for strength and transport and that support multiple functions ranging from biosensing and catalysis to self healing.

The effort focuses on sensing stress variations on the struts of cellular or porous structures and responding with mass deposition at those sites to negate the weakening effect of the increased stress. More specifically, the goals of this research effort are to (i) understand the dispersion and percolation characteristics of FGS in the solutions, (ii) understand the mechanisms of conduction with FGS-filled coatings, (iii) optimize the multifunctionality of the composites with respect to mechanical properties (*e.g.*, stiffness, strength, thermal stability, radiation resistance, and dimensional stability with water and solvents), (iv) maximize the conductivity of individual FGS by regulating its C/O ration through heat treatment, and (v) understand and minimize the effects of contact resistance between the sheets. This research effort may lead to significant innovations in the design and integration of adaptive materials, which would lead to substantial contributions to DoD missions. Specifically, the research is expected to produce novel systems with multiple functions that include catalysis, self-healing, heat transport, and energy production.

6. Reconfigurable Matter from Programmable Colloids. This MURI began in FY10 and was granted to a team led by Professor Sharon Glotzer at the University of Michigan - Ann Arbor. This MURI project is co-managed by the Materials Science and the Chemical Sciences Divisions. The goal of this program is to enable the design and synthesis of an entirely new class of self-assembled, reconfigurable colloidal material capable of producing materials with radically increased complexity and functionality. This will revolutionize the ability to build complexity and functionality into materials of the future. Opportunities for manipulating the assembly process include the utilization of shape, intermolecular interactions, induced conformation changes, functionalized adduct and site-specific binding groups, molecule-to-substrate interactions, and external fields. Pathways including both sequential assembly and selective disassembly processes are being investigated. Selective disassembly and reconfigurability are to be accomplished by judicious exposure to heat, pH or light. The research includes aspects of self-limiting growth of superclusters. The experimental program is complemented by a very strong theoretical component. Research thrusts include:

- Sequential staged self-assembly of nano-particles into complex and hierarchical architectures
- Development of theoretical tools and computational algorithms to model the self-assembly process, to identify stable self assembly pathways that lead to the targeted hierarchical structures, and finally to predict the final properties of the assembled material
- Future derivation of tailored properties and functions within highly complex or hierarchical materials

7. Stress-controlled Catalysis via Engineering Nanostructures. This MURI began in FY11 and was granted to a team lead by Professor William Curtin at Brown University. The objective of this research is to prove that macroscopic applied loading can be used to actively control and tune catalytic reactions through the use of innovative nanoscale material systems.

This research is based on the hypothesis that active control using cyclically-applied stress can alleviate the well-established "volcano" effect wherein a desired reaction is optimal only in a narrow operating window due to competing reactions, and thereby overcome what has been believed to be a fundamental limiting factor in design of catalytic systems. The scientific underpinning will be demonstrated by developing two general platforms that can sustain high mechanical loading while also accommodating a range of material systems and catalytic reactions. The main outcome of the project will be the unambiguous proof-of-principle that stress can be used to substantially modify and control chemical reactions, along with possible engineering paths, via both thin film and bulk metallic glass nanostructures for implementing stress control across a wide material space.

8. Atomic Layers of Nitrides, Oxides, and Sulfides (ALNOS). This MURI began in FY11 and was granted to a team lead by Professor Pulickel Ajayan at Rice University. The main objective of this MURI is to explore innovative top-down and bottom-up routes for the synthesis or isolation of high quality uni-lamellar sheets and ribbons of nitrides, oxides, and sulfides and to characterization these free standing 2D atomic layers to establish structure-property correlations in 2D layers.

The synthetic approaches of this research will span from simple mechanical/chemical exfoliation techniques to controlled chemical vapor deposition to create various 2D freestanding materials. Researchers will use computational tools based on density functional theory (DFT) methods to investigate binding energies, barriers and stabilities of different dopants and how they affect the band structure of the 2D host materials**.** 2D materials will be characterized for electrical conductivity/resistivity, Hall effect, carrier concentration, mobilities, ionic conductivity and thermal conductivity. If successful, this project could advance the basic science required to develop future DoD applications in chemical and biological sensors, opto-electronics, and power and energy.

D. Small Business Innovation Research (SBIR) – New Starts

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY12, the Division managed three new-start SBIR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of two Phase I contracts and one Phase II contract. These new-start contracts aim to bridge fundamental discoveries with potential applications, including the development of a process to manufacture thermally stable aluminum alloy with a nanoscale grain size and microstructural uniformity and the development of Equal Channel Angular Extrusion (ECAE) prototype tooling and processing technology for large scale (250-350 kg) billets of ultrafine/nano grained light alloys.

E. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY12, the Division managed four new-start Phase I STTR contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications, including the development of a scalable piezoMEMS manufacturing process using the atomic layer deposition (ALD) of lead zirconium titanate (PZT) films and demonstrating the feasibility of growing epitaxial, stochiometric AlGaN films with low dislocation density on bulk GaN substrates by HVPE (Hydride Vapor Phase Epitaxy) method.

F. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY12, the Division managed seven new REP awards. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

G. Presidential Early Career Award for Scientists and Engineers (PECASE)—New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The PECASE winners for each calendar year are announced by the White House in the last quarter of the fiscal year. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Strongly Coupled Multiferroic Materials – Hierarchical Organization at the Atomic and Nanoscales. The objective of this PECASE, led by Professor Craig Fennie at Cornell University, is to combine models, symmetry principles, and crystal chemistry to develop materials design rules that will facilitate the atomic-level design of multifunctional multiferroic materials with strong electric and magnetic cross-coupled responses.

This research program will utilize a combination of microscopic models, symmetry principles and crystal chemistry to develop material design rules (chemically and physically intuitive design rules) that facilitate the atomic level design of new multifunctional multiferroic materials possessing strong cross-coupled electric and magnetic responses. Once identified, the material implementation of these design rules will be explored using first-principles quantum computational techniques to screen for potential realizations of these rationalized design criteria. Two strategies, nanostructuring and interfacial strain engineering, will be utilized for inducing structural and symmetry changes into established materials systems. Once candidate material systems have been identified *ab initio*, then actual synthesis of the systems will be attempted in collaboration with experimental groups. The approach seeks to add to current multifunctional materials design methodologies a new material architecture component that superimposes onto what is now largely a compositionally driven design methodology. The approach will be demonstrated in complex oxide systems where atomic layer-by-layer growth techniques permit the growth of precise oxide structures. This research may enable these principles to be better applied to the design of materials, which will have broad impact on the development of multifunctional materials beyond multiferroics and impact future applications in communications, target acquisition and data computation.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY12, the Materials Science Division managed six new DURIP projects, totaling $1.1 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of electronic transport characterization of free-standing two dimensional materials and self assembly of colloidal matter.

I. DARPA Nanostructured Materials for Power (NMP) Program

The DARPA NMP program seeks to exploit advanced nano-structured materials for revolutionary improvements in power applications of DoD interest. The ability to decouple and independently control physical, chemical, electromagnetic, and thermal phenomena through nanoscale design, is being tapped to enable improvements in the energy product of permanent magnets and the efficiency of future thermoelectric devices. The Materials

Science Division currently co-manages projects within this program. The goals of these projects are ultimately to provide new nano-structured magnetic and thermoelectric materials with enhanced figures of merit for development of higher performance compact power sources in the future.

J. DARPA Bioinspired Photonics (BIP) Program

The goal of the DARPA BIP program is to harness innovative bioinspired synthetic organic and inorganic approaches to drive improved photonic material capabilities. Nature's hierarchical structures, scaling from micron to nanometer level, achieve remarkable optical functionality through complex scattering, reflection and absorption phenomena. The Bioinspired Photonics program draws inspiration from the best of nature's photonic structures to demonstrate tunable reflectors and volatile organic vapor sensors capable of operating in the visible and near infrared. The Materials Science Division currently co-manages projects within this program with the goal of identifying new approaches to the design and fabrication of future high performance photonic systems.

K. DARPA Low-Cost Light Weight Portable Photovoltaics (PoP) Program

The goal of the DARPA PoP program is to provide low-cost light-weight portable photovoltaics to DoD. The Materials Science Division currently co-manages projects within this program with the goal of exploring new materials solutions that can meet these goals.

L. DARPA Advanced Structural Fiber (ASF) Program

The goal of the ASF program is to develop and produce a fiber that offers at least a 50% increase in strength and stiffness. The ASF program is focused on exploiting recent breakthroughs in the understanding of materials synthesis at the atomic level, new materials characterization techniques, and advanced fiber manufacturing processes to scale up production fiber technologies that have already shown revolutionary lab-scale results. The Division currently co-manages projects within this program seeking to explore and optimize the most promising fiber compositions and processing strategies and to establish new paradigms for revolutionary fiber precursors.

M. DARPA Fracture Putty Program

The DARPA Fracture Putty program seeks to create a dynamic putty-like material which, when packed in/around a compound bone fracture, provides full load-bearing capabilities within days, creates an osteoconductive bone-like internal structure, and degrades over time to harmless by-products that can be reabsorbed as the normal bone regenerates. This new material could rapidly restore a patient to ambulatory function while normal healing ensues, with dramatically reduced rehabilitation time and elimination of infection and secondary fractures. The Division currently co-manages projects within this program attempting to achieve a convergence of materials science, mechanics, and orthopedics to enable new paradigms in bone stabilization, growth, and regeneration.

N. DARPA Plasma Sterilization of Wounds and Medical Devices Program

The DARPA Plasma Sterilization program is investigating the ability of a plasma (partially-ionized gas), to kill pathogenic bacteria on the surface of the skin, thereby leading to improved wound healing outcomes and reduction of secondary infections. Preliminary research has indicated that a non-thermal, atmospheric pressure plasma can drastically reduce the population of a wide range of pathogenic bacteria placed on skin surrogates in controlled experiments. By investigating how these results may safely translate to living skin, the program will build the foundation for a novel medical technology. The Materials Science Division co-manages a project within this program seeking to assess and enhance the mitigating effects of plasma on bacterial infections.

O. DARPA Revolutionizing Prosthetics Program

The DARPA Revolutionizing Prosthetics program will create, within this decade, a fully-functional (motor and sensory) upper limb that responds to direct neural control. This revolution will occur by capitalizing on previous

DARPA investments in neuroscience, robotics, sensors, power systems, and actuation. DARPA has delivered a prosthetic for pre-clinical trials that is far more advanced than any device currently available. This prosthetic enables many degrees of freedom for grasping and other hand functions, and will be rugged and resilient to environmental factors. This program now seeks to deliver a prosthetic for clinical trials that has function almost identical to a natural limb in terms of motor control and dexterity, sensory feedback (including proprioception), weight, and environmental resilience. The results of this program will allow upper limb amputees to have as normal a life as possible despite their severe injuries. The ARO Materials Science and Life Sciences Divisions currently co-manage a project within this program with the goal of optimizing materials and controlling architectures to realize maximum capabilities in upper-arm prostheses.

P. DARPA Structural Logic Program

The DARPA Structural Logic program seeks to enable structural systems that make up the basis for modern military platforms and buildings to adapt to varying loads and simultaneously exhibit both high stiffness and high damping. By demonstrating the ability to combine stiffness, damping, and adaptive dynamic range in a single structure, the Structural Logic program will enable the design of military platforms with the ability to continually change their properties to match the demands of a broad range of dynamic environments. The Division currently co-manages projects within this program seeking to realize novel design paradigms for passively adaptive structural systems that combine high stiffness, damping, and unprecedented adaptability.

Q. DARPA Maximum Mobility and Manipulation Program

The DARPA Maximum Mobility and Manipulation program seeks to create and demonstrate significant scientific and engineering advances in robotics that will create a significantly improved scientific framework for the rapid design and fabrication of robot systems and greatly enhance robot mobility and manipulation in natural environments. Additionally, the program seeks to significantly improve robot capabilities through fundamentally new approaches to the engineering of better design tools, fabrication methods, and control algorithms. The Maximum Mobility and Manipulation program covers scientific advancement across four tracks: design tools, fabrication methodologies, control methods, and technology demonstration prototypes. The Division currently co-manages projects within this program seeking to realize novel material design and fabrication paradigms for advanced sensing and actuation materials.

R. DARPA Microphysiological Systems Program

The DARPA Microphysiological Systems program seeks to develop a platform that uses engineered human tissue to mimic human physiological systems. The interactions that candidate drugs and vaccines have with these mimics will accurately predict the safety and effectiveness that the countermeasures would have if administered to humans. As a result, only safe and effective countermeasures will be fully developed for potential use in clinical trials while ineffective or toxic ones will be rejected early in the development process. The resulting platform should increase the quality and potentially the number of novel therapies that move through the pipeline and into clinical care. The Division currently co-manages projects within this program seeking to realize safe and effective countermeasures based upon novel characterization tools, molecular structures, and materials architectures.

S. High Energy Laser Research & Development for HEL-JTO

The High Energy Laser Research & Development Program seeks to support farsighted, high payoff scientific studies leading to advances in HEL science and technology science with the end goal of making HELs lightweight, affordable, supportable, and effective on the modern battlefield. The ARO Materials Science Division currently manages solid-state laser research of processes and technologies that provide enhancement to the manufacturability of current and innovative design of ceramic gain material.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Materials Science Division.

A. Experimental Validation of Removal of Stacking Fault Tetrahedra by Twin Boundaries

Professor Xinghang Zhang, Texas Engineering Experiment Station, Single Investigator Award

The objective of this effort is to understand fundamental mechanisms through which interfaces (grain boundary and interphase interfaces) in nanocrystalline and nanolayer metallic materials accumulate and promote annihilation of radiation induced point defects (*e.g.*, interstitials and vacancies). Researchers at the Texas Engineering Experiment Station recently demonstrated the removal of stacking fault tetrahedra (SFT) in nanotwinned silver samples at room temperature. More specifically, transmission electron microscopy revealed twin thickness dependent reduction of dislocation loop density, destruction of SFTs by twin boundaries and consequently drastic reduction of density of SFTs. This work constitutes the first experimental validation of these SFT removal mechanisms, which have been predicted by MD simulations. The research also revealed radiation induced migration of coherent and incoherent twin boundaries (ITBs). These findings provide important implications for the design of swelling resistant structural materials, and offer the basis for exploration of physics of radiation induced twin boundary migrations. Epitaxial Ag films with thickness of ~ 1 μm were synthesized on Si (111) substrate by using DC magnetron sputtering technique at room temperature. Specimens were irradiated with 1 MeV Kr^{++} ions up to a maximum fluence of 2×10^{14} ions/m^2 (corresponding to a maximum of 1 dpa) at room temperature at the IVEM-TANDEM facility at Argonne National Laboratory.

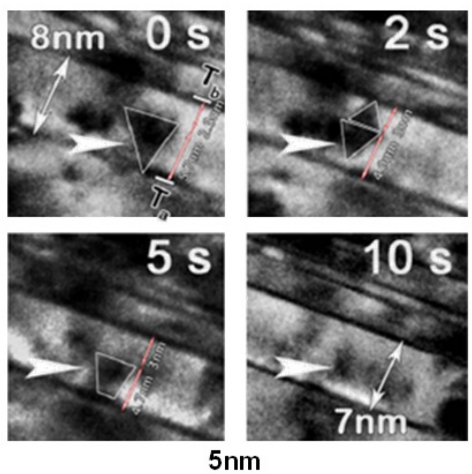

FIGURE 1

***In situ* observation of stacking fault tetrahedra (SFT) removal by interacting with coherent twin boundaries over a dose range of 0.075 - 0.081 dpa.** The apex of a 5 nm SFT is in contact with the twin boundary, T_a, at 0 s. The SFT split into two smaller SFTs joint from their bases at 2 s. By 5 s, the upper SFT adjacent to T_b vanishes and the lower SFT is truncated from its tip. At 10 s, the SFT has a core barely discernible and the twin spacing shrinks by 1 nm.

B. Novel Titanium Composites Via Freeze-Casting

Professor Surya Kalidindi, Drexel University, Single Investigator Award

The objective of this effort is to characterize the local anisotropic elastic-plastic properties of microscale constituents and interfaces at various hierarchical length scales in composite material systems. In contrast to freeze-cast ceramics and polymers, which have been studied in great detail, few freeze-cast metal scaffolds have been described, to date. Systematic studies of structure-processing correlations in freeze-cast Ti-6Al-4V scaffolds have demonstrated how processing parameters determine the scaffold architecture formed during the directional solidification of water-based metal slurries and the final architecture after sintering. Researchers at

Drexel University recently demonstrated new processing methods for producing Ti-6Al-4V freeze-cast samples that reduce particle sedimentation by 15% and volume shrinkage during sintering by 30%. The samples produced with these new protocols exhibited final porosities and pore sizes of 60-30% and 41-523 µm, respectively (see FIGURE 2). These methods are capable of producing samples with superb mechanical strength, stiffness, and toughness. In addition, protocols were developed to successfully infiltrate these porous samples with polymethyl-methacrylate (PMMA), creating a new Ti-6Al-4V-PMMA composite for lightweight, high-toughness applications. Future work will focus on varying the metal-polymer interface topology and chemistry to produce differences in bulk mechanical performance; nanoindentation stress-strain curves at the interface will provide new insights into the role of the interface in mechanical performance at multiple length scales.

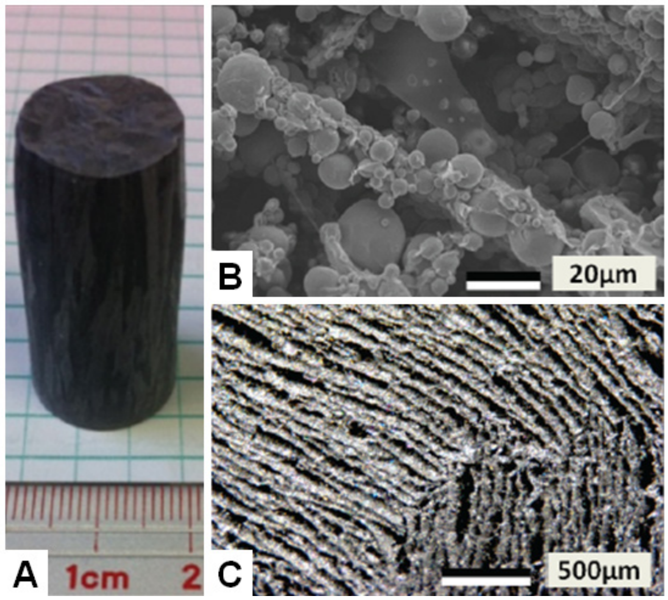

FIGURE 2

Optical and SEM images of Ti-6Al-4V scaffolds. The panels display the (A) typical scaffold size, (B) SEM image of the scaffold wall, and (C) an optical image of a horizontal cross-section.

C. Mesoscale Folding, Instability and Disruption of Laminar Flow in Metal Surfaces

Professor Srinivasan Chandrasekar, Purdue University, Single Investigator Award

Machining and grinding processes are ubiquitous in the manufacturing realm, however little has been studied on the surface phenomena of the processed materials. The objective of this SI project seeks to advance the deformation processing science of metals by employing a hybrid cutting-extrusion process—Large Strain Extrusion Machining (LSEM)—to conduct unique studies on the interactive effects of strain, strain rate, temperature and hydrostatic pressure over wide ranges. Critical to this process is the material deformation and flow ahead of the cutting tool and the resultant surface quality of the sheet material.

Professor Chandrasekar and colleagues recently reported the first-ever observation of non-laminar flow in a metal ahead of the cutting tool via in-situ velocity field analysis (see FIGURE 3) and a model is developed to explain this surprising phenomena. This turbulence phenomena is highly unexpected in solids (in contrast to liquids and gases) which typically fail by shear banding or cracking under such stress conditions. The observations of fluid-like behavior and turbulent vortices are determined to be caused by plastic instability caused by heterogeneous grains inducing mesoscale folding of the surface. These results can be thought to take place in any grinding, cutting or polishing operation, and the findings may lead to improvements in surface quality of machined/polished metals through better control of grain geometries and cutting angles of tooling.

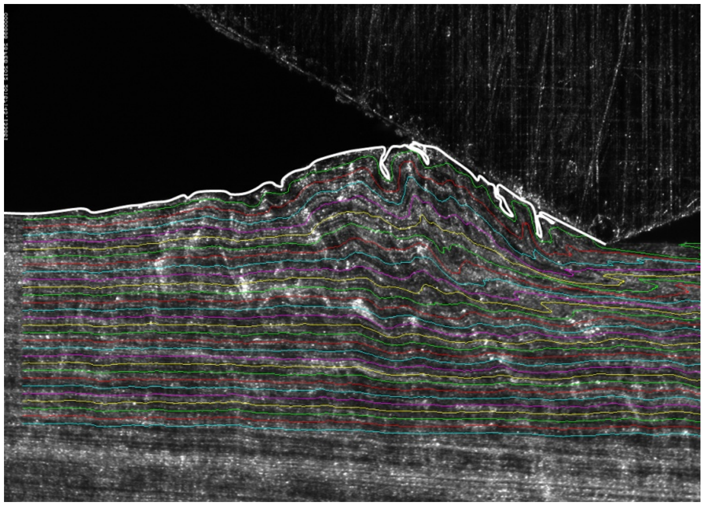

FIGURE 3

Complex, nonlaminar flow and fold formation in wedge-machined Cu. This frame is selected from an in situ high-speed image sequence to show fold development. The uppermost, thick white line is the manually identified surface showing the generation of non-laminar flow and folds. Superimposed, subsurface, colored lines are streak lines produced from velocity measurements.

D. Design of Stable Nanocrystalline Alloys

Professor Christopher Schuh, Massachusetts Institute of Technology, Single Investigator Award

Nanocrystalline metals and alloys have demonstrated strength properties significantly higher than their course grained counterparts, however, they are plagued by the long-standing tendency to undergo grain growth or phase transformation at temperatures needed for subsequent processing, thus losing their beneficial properties. The objective of this research is to predict elemental alloy segregation thermodynamics that provides for both thermal and phase stability in nanocrystalline metals at high homologous temperatures.

The investigator has demonstrated a successful theoretical framework and practical approach for predicting thermally stable binary alloys in systems with negative heat of mixing. The thermodynamic models that have been developed predict phenomena unexpected based on conventional thermodynamics. In this approach, each combination of parameters, the free energy of nanocrystalline structures was compared to that of the bulk regular solution. An example case for the nanocrystalline stability map is presented in FIGURE 4. Given a bulk stable case where the nanostructured phases fall above the common tangent line, the W-Ag system will prefer to phase separate at bulk scales as dictated by the bulk regular solution thermodynamics. Particular binary tungsten alloys were placed on the map after calculating the enthalpies of mixing and segregation; for W-Ti, the typical ranges of uncertainty of these calculations are shown in FIGURE 4. The successful prediction of stability in the W system demonstrates the successful application of the model, and forecasts the potential to design similar stability in multiple other alloy systems.

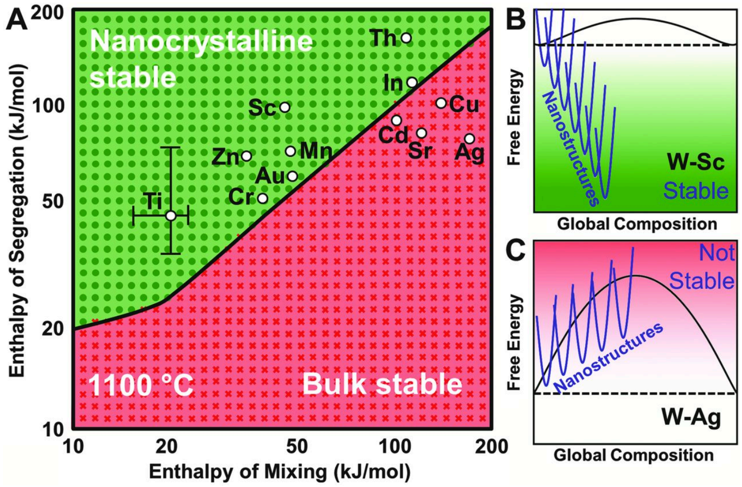

FIGURE 4

The nanostructure stability map for tungsten-based alloys at 1100°C. The map was calculated on the basis of variation of the enthalpy parameters. The panels illustrate (**A**) an example case for the nanocrystalline stability map, and (**B**) another stable region for a specific alloy of W-Sc. The free energy of the nanostructured phases is below that of the regular solution common tangent (dashed line). In (**C**), a bulk stable case is shown where the nanostructured phases fall above the common tangent line is shown; the W-Ag system will then prefer to phase separate at bulk scales as dictated by the bulk regular solution thermodynamics.

E. Synthesis and Properties of Mono- and Few-layer Hexagonal Boron Nitride (h-BN) Films

Professor Gopalan Srinivasan, Oakland University, Single Investigator Award

The objective of this project is to investigate nucleation and growth mechanisms of free standing monolayer or a few-layer 2D h-BN films on different substrates. The PI and his team have constructed a low pressure chemical vapor deposition (LPCVD) reactor and systematically explored different experimental conditions such as time-temperature profiles, pressure, flow rate, substrates, gas mixtures etc. to develop the necessary understanding of processing- structure-property relationships of 2D h-BN films. They found that in hot-wall LPCVD using diborane and ammonia as precursors, a certain control on the thickness (number of layers) of the h-BN film was possible through the growth time. The research team was able to synthesize single-crystal triangular-shaped and, single-layer h-BN domains of ~100 μm size (see FIGURE 5).

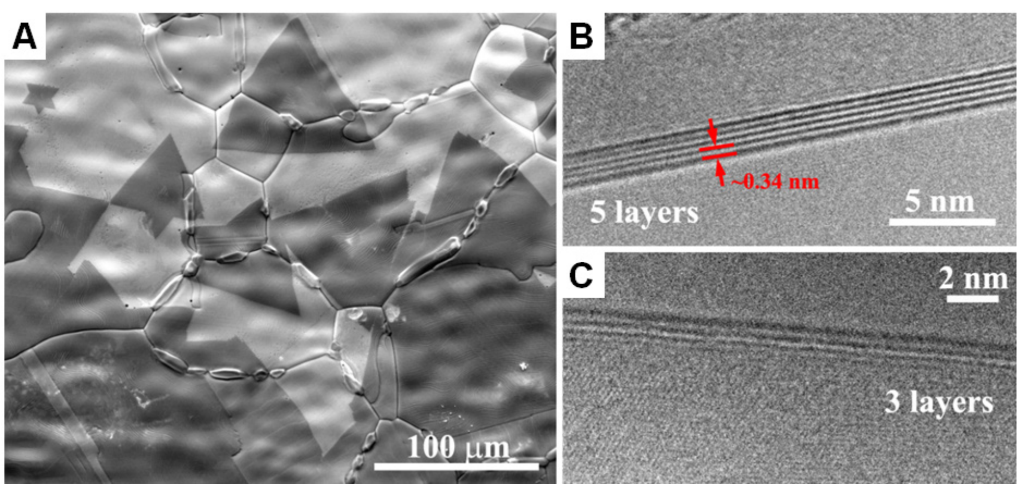

FIGURE 5

Single-crystal triangular-shaped and, single-layer h-BN domains of ~100 μm size. (**A**) Scanning electron microscope images showing submonolayer h-BN film on Ni, showing the triangular single-crystal domains as big as ~100 μm. Single-layer h-BN appears dark and the Ni (presumably Ni oxide) bright. (**B-C**) Transmission electron microscope images of a typical h-BN films with 5 and 3 layers, respectively.

The researchers also demonstrated direct synthesis of thin graphite/h-BN and few-layer graphene/h-BN 'stacked films'. This was achieved by first exposing Ni or Co substrates to a carbon source (*e.g.*, amorphous carbon, acetylene or methane gas, etc.) followed by the synthesis of h-BN films on the surface of the metal. The thin graphite or few-layer graphene is formed while cooling the metal by the segregation/precipitation of carbon at the h-BN/metal interface. The results obtained on a Ni foil by exposing to Acetylene, followed by the synthesis of h-BN using diborane and ammonia are shown in FIGURE 6A-C. A Raman spectrum from a h-BN/thin graphite stack film confirming the presence of these layers by using ^{13}C enriched methane as the carbon feedstock for the thin graphite formation is shown in FIGURE 6D. 2D h-BN films have high Army relevance to develop future high frequency, low power RF applications, flexible electronics, nano-electromechanical (NEMS) systems as well as deep UV light-emitting devices.

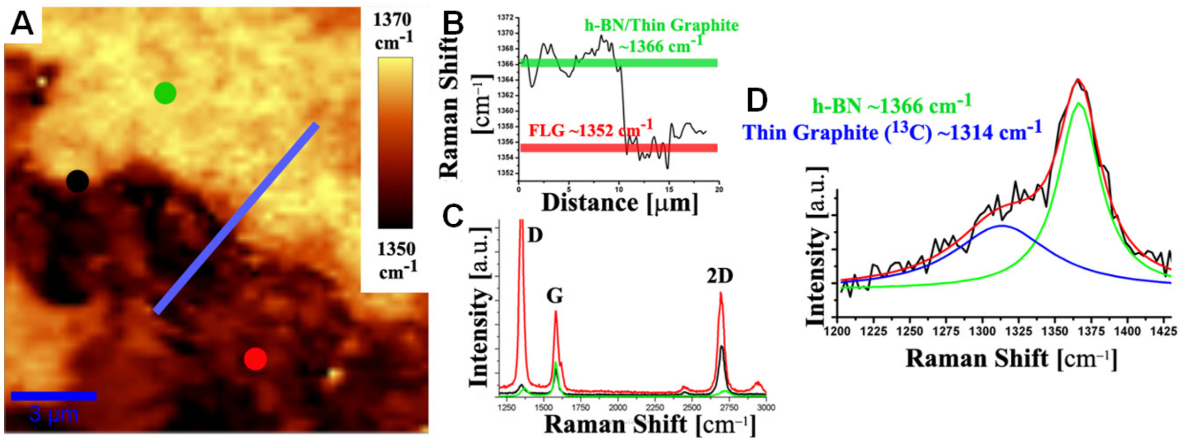

FIGURE 6

Exposure of Ni foil to acetylene followed by synthesis of h-BN using diborane and ammonia. (A) Mapping with the D-band and h-BN peaks (1300-1400 cm^{-1}). (B) Cross section along the light blue line in (A) showing an abrupt down-shift from ~1366 cm^{-1} to ~1350 cm^{-1}. (C) Raman spectra from the colored points in (A). (D) Raman spectra of a h-BN/thin graphite (by $^{13}CH_4$) showing the D-band (blue) at ~1314 cm^{-1} and the h-BN peak at ~1366 cm^{-1} (green).

F. Searching For Novel Phenomena in Two-Dimensional Ferroelectrics and Multiferroics

Professor Laurent Bellaiche, University of Arkansas, Single Investigator Award

The objective of this project is to investigate various static and dynamical properties of two-dimensional ferroelectrics and multiferroics, and to discover novel phenomena of large fundamental and technological importance in these ultrathin films. Ferroelectrics form an important class of materials that possess spontaneous electric dipoles below their Curie temperature and have been intensively investigated in their bulk forms because of their large piezoelectric and dielectric responses. Furthermore, multiferroics are attracting attention because they exhibit coupled long-range-ordered electric and magnetic degrees of freedom. Such magneto-electric coupling is promising to design new devices taking advantage of the control of magnetic properties by the application of an electric field. Moreover, the quest for efficient miniaturized devices and the search for novel phenomena have recently generated a vast amount of studies devoted to *two-dimensional* ferroelectrics and multiferroics. This research is highly relevant to national defense for communication devices operating in the GHz and THz regimes, phase arrays, night vision goggles, optical devices based on spontaneous optical activity, actuators, and transducers. This objective has been tackled via the development and use of different state-of-the-art *ab-initio* numerical tools.

In FY12, Professor Bellaiche's laboratory discovered the previously overlooked nanoscale (twinned) phases in the technologically-important $BiFeO_3$ and $EuTiO_3$ multiferroics (see FIGURE 7).[1] These phases possess complex oxygen octahedral tilting patterns that are coupled with unusual antiferroelectrity. These phases also provide a successful explanation for puzzling experimental data, such as X-ray spectra varying over a long-time period or a dramatic difference between short-range and average crystallographic structures.

[1] Prosandeev S, Wang D, Ren W, et al. (2013). Novel nanoscale twinned phases in perovskite oxides. *Adv. Funct. Mater.* 23:234–240.

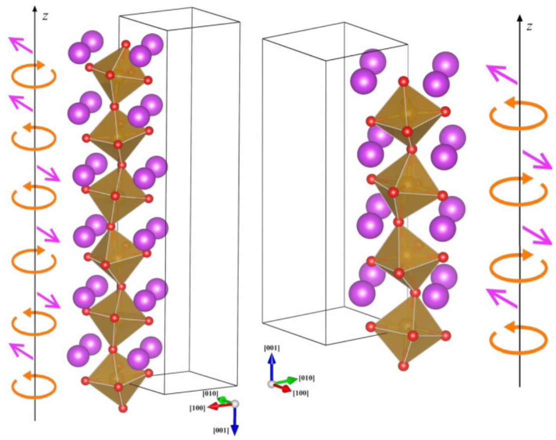

FIGURE 7

Schematic of the nanoscale twinned octahedral tilting structures found in $BiFeO_3$. The straight arrows represent the antiferroelectric displacements, while the curled arrows indicate if the displayed oxygen octahedra tilting is clockwise or counterclockwise.

G. Super-Resolution Optical Imaging

Professor Vasily Astratov, University of North Carolina - Charlotte, Single Investigator Award

The objective of this research program is to develop new high throughput techniques for selecting groups of supermonodispersive microspheres, self organizing these into closely spaced 3D arrays, and investigating the mechanisms of optical coupling and wave propagation in resonant optical circuits composed of arrays of these nearly identical microresonators. Researchers at UNC - Charlotte have shown that barium titanate glass microspheres with diameters in the range 2-125 µm and a high refractive index (n~1.9-2.1) can be used for super-resolution imaging of liquid-immersed nanostructures. Using micron-sized spheres with diameters on the order of several microns it was possible to discern features with far field resolutions on the order of $\lambda/7$, where λ is the illumination wavelength. Microspheres with larger diameters >50 µm were found to provide lower resolutions (~$\lambda/4$) but extraordinarily wider (>30 µm) super-resolution fields-of-view (see FIGURE 8). The relative simplicity of the research team's approach makes it very attractive as a means of extending existing imaging capabilities down to the nanoscale and therefore is expected to have direct application to biomedical, microfluidics and nanophotonics research.

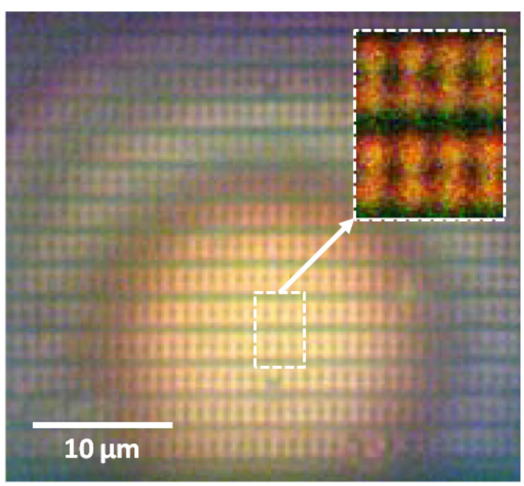

FIGURE 8

Au nanoparticles. The far field virtual images of an array of Au nanoparticles as viewed through a 125um glass sphere (n~1.9) immersed in isopropyl alcohol (index 1.37) using an illumination wavelength of 550 nm. The individual gold nanoparticles (120 nm diameter particles with separations of 150 nm and 200 nm) can be clearly resolved, showing a $\lambda/4$ spatial resolution.

H. Predictive Self-Assembly of Polyhedra into Complex Structures
Professor Sharon Glotzer, University of Michigan, MURI Award

The objective of this research is to develop the scientific foundations to create an entirely new class of self-assembled, reconfigurable colloidal materials with radically increased complexity and functionality. Researchers at the University of Michigan are investigating colloidal systems that share many of the same attributes possessed by simple life forms, including the ability to assemble and dissemble based on size and shape. The central goal for the group is to be able to predict the resulting structure based on the attributes of the building blocks. Recent work has helped to isolate the role that building-block shape plays in self-assembly of particles where only hard interactions are active. Professor Glotzer's group has investigated 145 convex polyhedra whose assembly arises solely from their anisotropic shape (see Figure 9). For this case, entropy maximization principles drive the preferential alignment of flat facets to maximize the number of configurations available to the system. The results indicate a remarkably high propensity for thermodynamic self-assembly and structural diversity. The research team discovered that simple measures of particle shape and local order in a fluid can be employed to predict the formation of broad classes of 3D assemblies which can broadly be classified as liquid crystals, plastic crystals, crystals, and disordered glasses. These published results provide general insights into the ordering behavior of molecules and the 3D crystallization of colloids, proteins and viruses.[2]

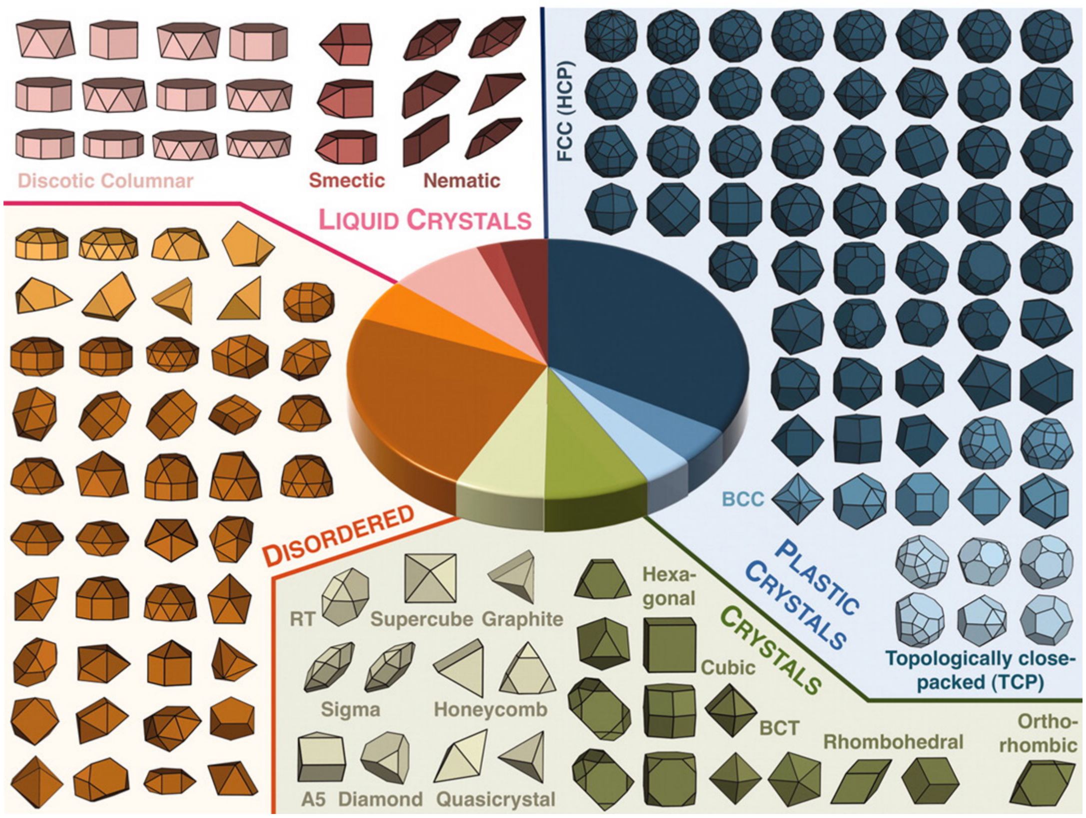

FIGURE 9
Colloidal systems. In colloidal self assembly, particle shape determines the long-range order of the system.[2]

[2] Damasceno PF, Engel M, and Glotzer SC. (2012). Predictive self-assembly of polyhedra into complex structures. *Science* 337:453-457.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Low-Cost Electrorheological Valves

Investigator: Professor Anette Hosoi, Massachusetts Institute of Technology, Single Investigator Award
Recipient: Vecna Technologies

The objective of the research effort that has led to this technology transfer is to explore and demonstrate small-scale actuation based on electro-active fluids. A prototype electrorheological (ER) valve was designed with four tubular channels in an H-bridge type configuration. The fluid is valved within the gap between concentrically nested thin-walled metal tubes, and then appropriately routed within the end-caps. The electronics both push and pull high voltage for fast frequency response, allowing pulse width modulation in the hundreds of Hz range and enabling fine proportional flow control of the ER valves. Given that ER valves can be integrated into the hydraulic lines as part of the fluid power distribution system, they can provide a significant savings in the sense of production cost, weight, and integration complexity of the system. Research on the development of ER valves has focused on ER fluid characterization, and design and fabrication of micro-structured channels. In particular, significant enhancements have been achieved via optimization of electrode roughness and aspect ratio of the channel cross-section. Vecna Technologies is developing new low-cost ER valve devices based on these results.

B. Large Strain Extrusion Machining of Metal Foils and Sheet

Investigator: Professors Kevin Trumble and Srinivasan Chandrasekar, Purdue University, Single Investigator Award
Recipient: Convolutus, Inc.

The objective of the originating research effort that led to this technology transfer is to advance the deformation processing science of hexagonal close packed (HCP) metals, such as Ti- and Mg-alloys, by employing a hybrid cutting-extrusion process—Large Strain Extrusion Machining (LSEM)—to conduct unique studies on the interactive effects of strain, strain rate, temperature and hydrostatic pressure over wide ranges. During conventional rolling, sheets are reduced in thickness using multiple, energy intensive steps, such as pre- and post-heating to avoid fracture during the multiple rolling steps. The recent scientific discoveries used to optimize the LSEM process have resulted in a single-stage, cost-effective and energy-efficient operation that converts round cast billets (ingots) into strips, while imposing sufficiently large strain to enhance the mechanical properties of the material (see FIGURE 10).

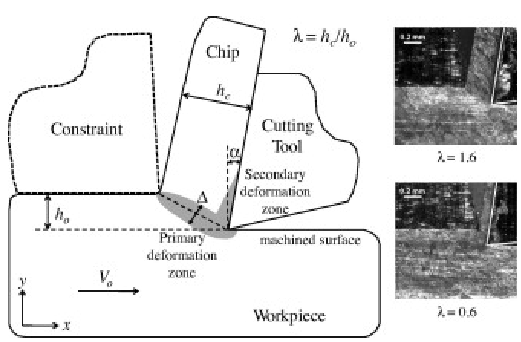

FIGURE 10
Plane-strain LSEM showing parameters. Inset shows images of process for two constraint levels.

This process is performed at room temperature, resulting in significant lower surface losses and reduced energy requirements. Edge cracking is also minimal due to the unique deformation characteristics of LSEM. These promising results have transitioned to Convolutus, Inc. which has received grants from the State of Indiana and Purdue University for continued development and implementation of the LSEM process.

C. Supported and Free-Standing 2D Semimetals

Investigator: Professor Deji Akinwande, University of Texas - Austin, YIP Award
Recipient: ARL Sensors and Electron Devices Directorate (ARL-SEDD)

The objectives of this project are to develop novel growth methods to synthesize semimetals down to a monolayer thickness and to characterize these materials to determine unique physical properties. Rare-earth arsenides (RE-A) are promising 2D nanomaterials that can be synthesized by molecular beam epitaxy (MBE) on standard III-V substrates. They are known to be semimetallic in the bulk phase owing to a small overlap of the conduction and valence bands quite similar to the case of graphite. A pressing question involves the prospects of a phase transition from semimetallic to semiconducting (SM-SC) character at the limit of one or a few monolayers (ML). This prospect is of fundamental importance because realization of these free-standing 2D films could in principle afford a wider variety of tunable single-crystal atomic sheets owing to the sensitivity of the interface dangling bonds compared to van der Waals (vdW) layered atomic sheets such as graphene and h-BN. The PI initiated a study on the wide spectrum of the RE-A including the endpoints of the family (LaAs, LuAs), and the prototypical ErAs. The investigator prepared MBE nanoparticle-seeded growth of high-quality ErAs (~3nm) that did not reveal anti-phase domains, which have traditionally plagued the growth of rock-salt crystals (see FIGURE 11A). Conductivity studies uncovered large size dependence with more than three orders of magnitude reduction for 3ML ErAs (see FIGURE 11B). Other effects such as surface scattering could also contribute to a size dependency. This work is focused on elucidating the physical properties of free-standing RE-A 2D films that can be employed as atomically thin functional designer materials for Army applications, which might go far beyond the functionality afforded by the vdW hexagonal layered crystals which do not have interface dangling bonds. This research has transitioned to ARL-SEDD, including research results regarding 2D materials synthesis, transfer, electronic/spectroscopic measurements of 2D materials. This transition will enable future collaborations that may lead to 2D nanomaterial applications for advanced warfighter electronics.

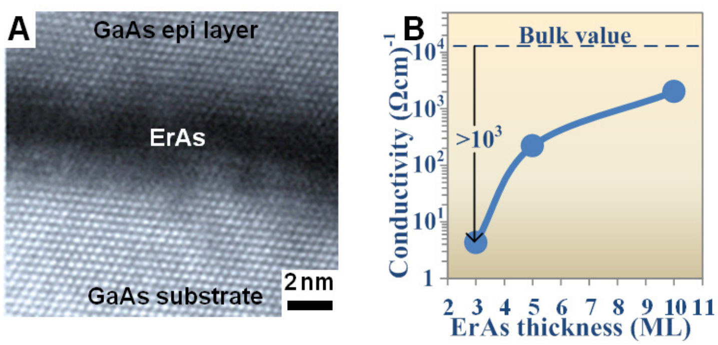

FIGURE 11

MBE nanoparticle-seeded growth of high-quality ErAs. The panels display (**A**) cross-sectional transmission electron microscope image of ErAS films, and (**B**) size effect in the conductivity of ErAs thin films.

D. Lightweight Polymer Optics

Investigator: Jim LeBlanc and Peter LaPolice, Fosta-Tek Optics, Inc, Congressional Program
Recipients: U.S. Army Armament Research, Development and Engineering Center (ARDEC)

Fosta-Tek Optics is developing laser dye loaded polymer optics as an alternative approach for laser protective filters. Dye saturation effects have historically made this approach unworkable; however, these investigators have overcome this barrier. FostaTek has shown that integrated optical elements can be manufactured to fully satisfy the stringent optical requirements set forth for the filters currently being employed in Army materiel. This research has transitioned to ARDEC for the development of prototype systems. The cost estimates indicate that the cost savings could be significant (20-50%) and that the dye approach also provides a solution for other future concerns (*e.g.*, glint reduction) that are not addressed by the current optics.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Elucidating the Jamming/Unjamming Transition

Professor Heinrich Jaeger, University of Chicago, Single Investigator Award

The project aims to explore the jamming/unjamming transition in particle-based systems under stress loading, and to map out the nonlinear dynamic system responses in the unjammed region. The proposed effort will utilize an integrated approach incorporating unique experimental capabilities and computer simulations on model systems to achieve this objective. The proposed research will study fully three-dimensional systems and concentrate on the effects of particle shape and interstitial fluids, since these factors directly affect the interactions among particles and therefore are critical for the delineation of different dynamic regimes. It is anticipated that in FY13, the research team will investigate the jamming/unjamming transition in particle-based systems under stress loading, and provide a first-ever understanding of the solidification process and an explanation of the large normal stresses generated by these suspensions under impact. More specifically, high-speed videography, embedded force sensing, and X-ray imaging will be used to capture the detailed dynamics of stress generation during impact. Additionally, a comprehensive model will be developed to predict dynamic solidification and its effect on the surrounding suspension that reproduces the observed behavior quantitatively.

B. Pressure and Temperature Effects on Plasticity of Metallic Glasses

Professor John Lewandowski, Case Western Research University, Single Investigator Award

The objective of this project is it develop a basic understanding of how concurrently imposed hydrostatic pressure and temperature effect the global plasticity of bulk metallic glasses, which typically suffer from low plasticity at ambient pressure and temperatures below the glass transition temperature. Zr-based and La-based metallic glasses will be tested in an extrusion apparatus capable of superimposing a hydrostatic pressure.

It is anticipated that the microstructural factors which determine viscous flow, pressure-induced structural relaxation and/or divitrification will be determined, and the subsequent knowledge will be used to determine regimes of temperature and pressure that maximize material flow while maximizing strength in a variety of bulk metallic glass systems. The ability to fabricate high-strength metallic glass components with complex shapes may result in a new classes of structural and armor material, and represents a major breakthrough in materials processing.

C. Synthesis of Defect-Mitigating Tunable Dielectric Materials with Atomic-Layer Control

Professor Darrell Schlom, Cornell University, Single Investigator Award

The goal of this project is to grow $(Ca,Sr, Ba)_{n+1}Ti_nO_{3n+1}$ tunable dielectric Ruddlesden-Popper (R-P) heterostructures with reduced defects and controlled strain. The MBE method will be used to grow these films with a good atomic layer growth control. In FY13, the investigators will explore the influence of buffer layers, elevated growth temperatures and ex-situ annealing etc. as means to improve the crystalline quality and figure of merit of $Sr_2(Ba,Sr)_{n-1}Ti_nO_{3n+1}$ films integrated with sapphire and Si substrates. Initially $BaTiO_3$ and then $Ba_xSr_{1-x}TiO_3$ will be inserted into a Ruddlesden-Popper structure by synthesizing $Sr_2Ba_{n-1}Ti_nO_{3n+1}$ phases on $REScO_3$ substrates. If successful, this project could lead into novel materials that can be used to make thin film devices (such as tunable filters, isolators, resonators, phase shifters etc.) with dielectric constants at GHz frequencies that can be tuned by applying quasi static fields.

D. Rare Earth Doped Quasi-2DEG at the Interface of $LaAlO_3/SrTiO_3$

Professor Yuri Suzuki, University of California - Berkeley, MURI Award

UC Berkeley researchers are investigating the magnetic doping of the two dimensional electron gas (2DEG) system that forms at $LaAlO_3/SrTiO_3$ interfaces. The doping of various rare earths (*e.g.*, Lu and Tm) into the $LaAlO_3$ layer is being pursued as a means of introducing localized magnetic moment as well as spin-orbit scattering centers into the system. Preliminary results indicate that the dopants are entering on the La sites and that the doped heterointerface exhibits metallic behavior very similar to that of the undoped system. This is consistent with current understanding that the metallicity of the $LaAlO_3/SrTiO_3$ system largely resides on the $SrTiO_3$ side of the interface. In FY13, a detailed investigation of long-range magnetic ordering and transport behavior in this system will be conducted over the next year to establish the feasibility of utilizing spin-polarized 2DEG systems in future spin-based electronic applications.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. David Stepp
Division Chief
Program Manager, Mechanical Behavior of Materials

Dr. John Prater
Program Manager, Materials Design

Dr. Chakrapani (Pani) Varanasi
Program Manager, Physical Properties of Materials

Dr. Suveen Mathaudhu
Program Manager, Synthesis and Processing of Materials

B. Directorate Scientists

Dr. Thomas Doligalski
Director, Engineering Sciences Directorate

Mr. George Stavrakakis
Contract Support

C. Administrative Staff

Ms. Pamela Robinson
Administrative Support Assistant

CHAPTER 9: MATHEMATICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2012* is to provide information on the programs and basic research efforts supported by ARO in FY12, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Mathematical Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY12.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mathematical Sciences Division supports research efforts to develop a foundational framework for the understanding and modeling of complex nonlinear systems, for stochastic networks and systems, for mechanistic models of adaptive biological systems and networks, and for a variety of partial differential equation (PDE) based phenomena in various media. These research areas focus on discovering nonlinear structures and metrics for modeling and studying complex systems, creating theory for the control of stochastic systems, spatial-temporal statistical inference, data classification and regression analysis, predicting and controlling biology through new hierarchical and adaptive models, enabling new capabilities through new bio-inspired techniques, creating new high-fidelity computational principles for sharp-interface flows, coefficient inverse problems, reduced-order methods, and computational linguistic models. These efforts will ensure the U.S. is on the research frontier in mathematical sciences, and will enable new advances in disciplines that depend on mathematics.

2. Potential Applications. In addition to advancing global knowledge and understanding of mathematical concepts, structures, and algorithms, the research efforts managed in the Mathematical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. Long term basic research discoveries regarding the modeling of complex systems may enable full (*i.e.*, not only physical) situational awareness through modeling of urban terrain and small-group social phenomena. Outcomes of basic research in probability and statistics may provide enhanced levels of information assurance, improved awareness of and defense against terrorist threats, next generation communication networks, and improved weapon design, testing, and evaluation. New discoveries in biomathematics may lead to protection against future biological and chemical warfare agents, improve wound-healing, lead to self-healing communication networks, enhance cognitive capabilities for the Soldier, and contain or prevent infectious disease. Advances from basic research in the area of numerical analysis may enable faster/better analysis, design, prediction, real-time decision making, and failure autopsy.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives and to maximize the impact of potential discoveries for the Army and the nation, the Mathematical Sciences Division frequently coordinates and leverages efforts within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), and the Air Force Office of Scientific Research (AFOSR). In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the Network Sciences Division pursue common interests in cognitive modeling, bio-network modeling and design, and new concepts in computational optimization. The Mathematical Sciences Division coordinates efforts with the ARO Computing Sciences Division to promote investigations of new architectures and algorithms for the future of heterogeneous computing and to pursue related interests in image recognition and information fusion. Research efforts also complement initiatives in the Life Sciences Division to model and understand the relationship between microbial growth conditions and composition, leading to advances in microbial forensics. The creation of new computational methods and models to better understand molecular structures and chemical reactions are an area of collaboration between the Chemical Sciences and Mathematical Sciences Divisions. The Mathematical Sciences Division also coordinates efforts with the Physics Division to pursue fundamental research in quantum control. The Division also interfaces with Program Areas in the Mechanical Sciences Division to explore the mechanics of fluids in flight and to better understand combustion. These interactions promote synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

To meet the long-term program goals described previously, the Mathematical Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY12, the Division managed research efforts within these four Program Areas: (i) Modeling of Complex Systems, (ii) Probability and Statistics, (iii) Biomathematics, and (iv) Numerical Analysis. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Modeling of Complex Systems. The goal of this Program Area is to develop quantitative models of complex, human-based or hybrid physics and human-based phenomena of interest to the Army by identifying unknown basic analytical principles and by using human goal-based metrics. Complete and consistent mathematical analytical frameworks for the modeling effort are the preferred context for the research, but research that does not take place in such frameworks is considered if the phenomena are so complex that such frameworks are not feasible. The identification of accurate metrics is part of the mathematical framework and is of great interest, as traditional metrics often do not measure the characteristics in which observers in general, and the Army in particular, are interested. For many complex phenomena, new metrics need to be developed at the same time as new models. This Program Area is divided into two research thrusts: (i) Geometric and Topological Modeling and (ii) Small-group Social and Sociolinguistic Modeling. In FY12, the Modeling of Complex Systems Program included legacy efforts in information fusion. New efforts in information fusion will be part of the Information Processing and Fusion Program in the ARO Computing Sciences Division.

This Program Area develops mathematical analysis for fully 3D (rather than 2.5D) geometric and topological modeling of large urban regions up to 100 km x 100 km, which is important for situational awareness, mission planning and training. It develops the quantitative, analytical models of small social groups and of sociolinguistic phenomena which are required for operations, training, simulation (computer generated forces) and mission planning.

2. Probability and Statistics. The goal of this Program Area is to create innovative theory and techniques in stochastic/statistical analysis and control. Basic research in probability and statistics will provide the scientific foundation for revolutionary capabilities in counter-terrorism, weapon systems development, and network-centric warfare. This Program Area is divided into two Thrust areas: (i) Stochastic Analysis and Control, and (ii) Statistical Analysis and Methods.

The goal of the Stochastic Analysis and Control Thrust is to create the theoretical foundation for modeling, analysis, and control of stochastic networks, stochastic infinite dimensional systems, and open quantum systems. Many Army research and development programs are directed toward modeling, analysis, and control of stochastic dynamical systems. Such problems generate a need for research in stochastic processes, random fields, and/or stochastic differential equations in finite or infinite dimensions. These systems often have non-Markovian behavior with memory for which the existing stochastic analytic and control techniques are not applicable. The research topics in this Thrust include, but are not limited to, the following: (i) analysis and control of stochastic delay and partial differential equations; (ii) complex and multi-scale networks; (iii) spatial-temporal event pattern analysis; (iv) quantum stochastics and quantum control; (v) stochastic pursuit-evasion differential games with multi-players; and (vi) other areas that require stochastic analytical tools.

The objective of the Statistical Analysis and Methods Thrust is to create innovative statistical theory and methods for network data analysis, spatial-temporal statistical inference, system reliability, and classification and regression analysis. The research in this Thrust supports the Army's need for real-time decision making under uncertainty and for the design, testing and evaluation of systems in development. The following research topics are of interest to the Army and are important for providing solutions to Army problems: (i) Analysis of very large or very small data sets, (ii) reliability and survivability, (iii) data, text, and image mining, (iv) statistical learning, (v) data streams, and (vi) Bayesian and non-parametric statistics, (vii) statistics of information geometry, and (viii) multivariate heavy tailed statistics.

Potential long-term applications for research carried out within this Program Area include optimized design and operation of robust and scalable next-generation mobile communication networks for future network-centric operations made possible through advances in stochastic network theory and techniques. Also, advances in stochastic fluid turbulence and stochastic control of aerodynamics can improve the maneuvering of helicopters in adverse conditions and enable optimal design of supersonic projectiles. In addition, new results in density estimation of social interactions/networks will help detect adversarial behaviors and advances in spatial-temporal event pattern recognition and will enable mathematical modeling and analysis of human hidden intention and will provide innovative approaches for counter-terrorism and information assurance. Finally, new discoveries in signature theory will significantly improve reliability of Army/DoD systems and experimental design theory, and will lead to accurate prediction and fast computation for complex weapons.

3. Biomathematics. The goal of this Program Area is to identify and mathematize the fundamental principles of biological structure, function, and development across biological systems and scales. The studies in this program may enable revolutionary advances in Soldier health, performance, and materiel, either directly or through bio-inspired methods. This program area is divided into three main research thrusts: (i) Computational Cell and Molecular Biology, (ii) Multiscale Modeling/Inverse Problems, and (iii) Fundamental Laws of Biology. Within these thrusts, basic, high-risk, high pay-off research efforts are identified and supported to achieve the program's long-term goals. Efforts in the Computational Cell and Molecular Biology thrust area seek to elucidate and model the fundamental principles by which biological elements such as genes, proteins, and cells are integrated and function as systems. Research in the Multiscale Modeling/Inverse Problems thrust area involves creating mechanistic mathematical models of biological systems at different temporal and/or spatial scales and synchronizing their connections from one level of organization to another, with the goal of achieving a deeper understanding of biological systems and eventually connecting top-down and bottom-up approaches. Research in the Fundamental Laws of Biology thrust area is high-risk research in Biomathematics at its most fundamental level, seeking to find and formulate in a mathematical way the basic, general principles underlying the field of biology, a feat that has been performed for other fields, such as physics, but is in its infancy with respect to biology.

While these research efforts focus on high-risk, high pay-off concepts, potential long-term applications for the Army include new and better treatments for biowarfare agent exposure, improved military policies on troop movements in the presence of infectious disease, optimized movements of groups of unmanned autonomous vehicles and communications systems, and improved understanding of cognition, pattern recognition, and artificial intelligence efforts. Research efforts in this Program Area could also lead to improved medical diagnoses, treatments for disease, limb regeneration, microbial forensics, detection of terrorist cells, and self-healing networks. Finally, efforts within this program may result in a revolutionized understanding of biology in general, which will at the very least allow future modeling efforts to be much more efficient and also undoubtedly have far-reaching effects for the Army in ways yet to be imagined.

4. Numerical Analysis. The goal of this Program Area is to develop a new mathematical understanding to ultimately enable faster and higher fidelity computational methods, and new methods that will enable modeling of future problems. The research conducted within this program will enable the algorithmic analysis of current and future classes of problems by identifying previously unknown basic computational principles, structures, and metrics, giving the Army improved capabilities and capabilities not yet imagined in areas such as high fidelity modeling, real-time decision and control, communications, and intelligence. This Program Area is divided into three research Thrusts: (i) Multiscale Methods, (ii) PDE-Based Methods, and (iii) Computational Linguistics. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goals. The goal of research in the Multiscale Methods Thrust is to achieve higher fidelity and more efficient modeling of multiscale phenomena in a variety of media, and to create general methods that make multiscale modeling accessible to general users. Efforts in the PDE-Based Methods Thrust focus on developing the mathematics required for higher fidelity and more efficient modeling of sharp-interface phenomena in a variety of media, to discover new methods for coefficient inverse problems that converge globally, and to create reduced order methods that will achieve sufficiently-accurate yet much more efficient PDE solutions. Efforts in the Computational Linguistics Thrust focus on creating a new understanding of natural language communication and translation through new concepts in structured modeling.

While these research efforts focus on high-risk, high payoff concepts, potential long-term applications for the Army include force protection concrete and improved armor, more stable but efficient designer munitions, high density, rapid electronics at low power, and nondestructive testing of materials. Program efforts could also lead to more capable and robust aerial delivery systems, more efficient rotor designs, systems to locate explosive materials, more efficient combustion designs, and real-time models for decision-making. Finally, efforts within this program may lead to natural language interactions between bots and humans in cooperative teams, new capabilities for on-the-ground translation between deployed U.S. forces and locals, especially in low-resource language regions, new and improved capabilities for automated translation, automatic summarization, and textual analysis within the strategic intelligence communities.

C. Research Investment

The total funds managed by the ARO Mathematical Science Division for FY12 were $20.3 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY12 ARO Core (BH57) program funding allotment for this Division was $4.7 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $13.7 million to projects managed by the Division. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $0.8 million for contracts. Finally, $1.1 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY12 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research projects. Research projects are developed by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts.

The following subsections summarize projects awarded in FY12 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY12, the Division awarded 14 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to discover new multiscale space-time computational methods for fluid-structure interaction problems, to determine control strategies and mathematical models for team coordination in networked systems, and to discover new methodologies for class comparison within high-dimensional genomic and phenotypic data. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Chung-Lung Chen, University of Missouri - Columbia; *Fluid-Structure Interaction Enabled Practical Rotorcraft Flow Simulator*
- Professor James Crutchfield, University of California - Davis; *Structural Complexity in Linguistic Systems*
- Professor Paul Dupuis, Brown University; Rare Events, *Control and Metastability of Weakly Interacting Particle Systems*
- Professor Eduardo Gildin, Texas A&M Engineering Experiment Station; *Local-Global Model Reduction for Large-Scale Models Integrating Systems-Theoretical Properties Research*
- Professor Curtis Huttenhower, Harvard University; *Scalable Biomarker Discovery for Diverse High-Dimensional Phenotypes*
- Professor Curtis Huttenhower, Harvard University; *The Human Microbiome as a Multipurpose Biomarker*
- Professor Gangaram Ladde, University of South Florida - St. Petersburg; *Network Dynamic Processes Under Stochastic Perturbations*
- Professor Hod Lipson, Cornell University; *Inverse Methods for Identifying Generative Models in Bio-Eco-Social Systems From Sparse Observations*
- Professor Dan Negrut, University of Wisconsin - Madison; *Homogenization-Driven Multiscale Approach for Characterizing the Dynamics of Granular Media*
- Professor Amir Shirkhodaie, Tennessee State University; *Recognition of In-Vehicle Group Activities*
- Professor Tayfun Tezduyar, Rice University; *Multiscale Space-Time Computational Methods for Fluid-Structure Interactions*
- Professor Yen-Hsi Tsai, University of Texas - Austin; *Visibility-Based Goal Oriented Metrics: Navigation and Path Planning Problems*

- Professor Gang George Yin, Wayne State University; *Consensus Control of Complex and Multi-scale Networks with Network Uncertainty and Adversary*
- Professor Jun Zhang, University of Michigan - Ann Arbor; *Semi-inner-products in Banach Spaces with Applications to Regularized Learning, Sampling, and Sparse Approximation*

2. Short Term Innovative Research (STIR) Program. In FY12, the Division awarded 12 new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to develop a novel Bayesian kernel classification model built around non-Gaussian prior distributions, determine new statistical process control approaches for anomaly detection in social interactions, and to establish mathematical models that characterize biological function. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Kash Barker, University of Oklahoma; *Bayesian Kernel Methods for Non-Gaussian Distributions: Binary and Multi-class Classification Problems*
- Professor Richard Charnigo, University of Kentucky; *Advances in Multivariate Nonparametric Regression*
- Professor Kathryn Coronges, U.S. Military Academy; *New Framework for Modeling Social Data*
- Professor James Damon, University of North Carolina - Chapel Hill; *Comparing Mathematical Models and Experimental Data for Intake Capacity Distributions for Plant Root Structures*
- Professor John Fricks, Pennsylvania State University; *Statistical Inference and Stochastic Simulation for Microrheology*
- Professor Chihoon Lee, Colorado State University - Ft. Collins; *Stationary Solutions of Constrained Stochastic Differential Equations Driven by Fractional Brownian Motions*
- Professor Jing Li, Arizona State University; *Novel Network Statistics for Modern Social Interaction Modeling and Inference*
- Professor Ulrich Neumann, University of Southern California; *Rapid Creation of Large-scale 3D Models*
- Professor Vilem Novak, University of Ostrava, Czech Republic; *Fuzzy Transforms*
- Professor Nicholas Ouellette, Yale University; *Characterization and Modeling of Insect Swarms Using Tools from Fluid Dynamics*
- Professor Gerald Penn, University of Toronto; *Mathematical Modeling for the Evaluation of Automated Speech Recognition Systems*
- Professor Allen Yang, University of California - Berkeley; *Geometric Sparse Representation For Complex Urban Terrain Modeling*

3. Young Investigator Program (YIP). In FY12, the Division awarded one new YIP project. The grant is driving fundamental research to discover new multiscale atomistic methods for modeling the structure of defects in modern multifunctional materials. The following PI and corresponding organization was the recipient of the new-start YIP award.

- Professor Kaushik Dayal, Carnegie Mellon University; *Multiscale Atomistic Method for Long-Range Electrical Interactions with Relevance to Multiphysics Calculations in Functional Materials*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY12 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Weak Social Ties: Quantification, Metrics and Modeling*; Durham, NC; 1-2 December 2011
- *Dynamics Days 2012*, Baltimore, MD; 4-7 January, 2012
- *International Conference on Mathematics and Numerical Analysis*; Los Angeles, CA; 4-6 April 2012
- *Numerical Methods, Biologically Inspired Algorithms, and Multi Objective Optimization*; Williamsburg, VA; 4-6 April 2012
- *Conference on Long-range Dependence, Self-Similarity and Heavy Tailed Statistics*; Chapel Hill, NC; 18-20 April, 2012

- *Dr. David Blackwell Memorial Conference on Mathematics, Probability and Statistics*; Washington, DC; 19-20 April 2012
- *XIX International Conference on Computational Methods in Water Resources*; Champaign, IL, 17-21 June 2012
- *2012 Conference on Stochastic Networks*; Cambridge, MA; 18-22 June 2012
- *Annual Meeting of the Society for Mathematical Biology*; Knoxville, TN; 25-28 July 2012

5. Special Programs. In FY12, ARO Core Research Program funds provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded two new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Mathematical Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Theories of Dynamic Modeling of 3D Urban Terrain. This MURI began in FY07 and was awarded to a team led by Professor Andrew Kurdila of the University of South Carolina. The goal of this research is to develop theory, algorithms, software, and experiments for the synthesis of urban terrain maps using dynamic point cloud sensor data. More specifically, the objective of this research is to develop theories (i) for capturing high-order topology through implicit representation of surfaces, (ii) for developing multiscale and adaptive algorithms that enable various resolutions of the rendered surface governed by the local density of the point clouds, (iii) for the fast computation of signed distances to the terrain surface thereby giving field of view from specified observation points, (iv) for the use of dynamic point cloud measurements for the navigation and control of autonomous vehicles in three dimensions, and (v) for change detection from point cloud observations taken at different times.

The MURI team has successfully developed (1) adaptive algorithms for representing point cloud data at compression ratios of the order of 100-to-1, (2) tree algorithms for classification and in non-rigid registration of 3D terrain data sets, (3) algorithms invariant under isometric mappings to compute intrinsic geometric quantities directly on point clouds and use them for registration, (4) consensus estimation and adaptive approximation from point cloud measurements by agents in a distributed network, (5) convergence rates for network consensus estimation, (6) efficient multigrid algorithms for approximation and (7) a non-myopic navigation approach for truly 3D applications that involve point cloud data. This research responds to the Army need for 3D urban terrain models for simulation, training, mission planning, operational situational awareness and vehicle navigation.

2. Designing and Prescribing an Efficient Natural-like Language for Bots. This MURI began in FY07 and was awarded to a team led by Professor Mitch Marcus at the University of Pennsylvania. The goal of this project is to develop theory that will eventually enable bots to both understand and to be understood by humans, ultimately enabling functional human-bot teams.

Fluent and effective communication between warfighters is imperative to convey orders and intent and to ensure adequate situational awareness. All unit members must continually exchange information as the environment changes. As autonomous bots move onto the battlefield, they will also need to participate in these complex linguistic interactions. This almost necessarily means equipping them with natural language capabilities. The Soldier whose native language is English can communicate a rich range of information and intentions in English with little appreciable increase in cognitive load, even when the Soldier is under high stress. Soldiers cannot compromise these abilities for the sake of the bots; therefore, this research strives to bring the bots to the level of the Soldier. This research effortis organized in nine synergistic areas: Machine Learning & Stochastic

Optimization, Human–Robot Interaction, Syntactic Analysis, Semantic Interpretation, Pragmatic Enrichment, Parameterized Action Representation, Formulating Specification for Robot Motion Planning, Corpus Collection, and Testbeds and Integrated Demonstrations.

In FY12, the team successfully integrated many of the important research directions, and many of its important components have been advanced. The team's work in joint inference is just now proving to be computationally feasible, whereas work based on previous algorithms proved to be unavoidably exponentially expensive and had to be abandoned. The team has ported natural language processing (NLP) components to the ARL-HRED robotic control system (see Section IV-D). The team has developed new concepts in models for computational pragmatics and its visualization through heat maps. This work has enabled asymmetric dynamics between human and bot speakers, and the team has shown where algorithms can best incorporate data from psychologists, especially for operations conducted under stress. Their movement into unsupervised learning and the shedding of old ontologies is promising.

3. Analysis and Design of Complex Multi-scale Networks. This MURI began in FY08 and was awarded to a team led by Professor Jean Walrand of University of California - Berkeley. The goal of this research is to invent new mathematical theories and techniques that will enable modeling, analysis and control of complex multi-scale networks. These theories will ultimately enable the development of a unified framework for understanding and exploiting complex behaviors of the network resulting from spatial and temporal heterogeneity and the interaction of network algorithms with traffic characteristics.

More specifically, the objective of this MURI is to: (i) understand the interaction of traffic statistics, including long-range dependence (LRD) properties, and control actions across timescales, from back-clocking and burstiness effects at the sub-round-trip-time (sub-RTT) timescale, congestion control at RTT timescales, inter-domain routing at the time scale of minutes or hours, to revenue maximization and peering structure on the scale of days and months, (ii) design strategies for controlling admissions of new connections, flows of admitted connections, and the pricing of connections taking into account the LRD property of the traffic, (iii) develop theories for maximizing network utilization in the presence of wired and wireless links (which typically pose significant challenges for the proper utilization of network resources by end-to-end rate control protocols), and (iv) design traffic-measurement techniques in a heterogeneous environment, which can have significant implications for monitoring, management, and security of the network. The new distributed algorithms for wireless networks that may result from this work have the potential of revolutionizing *ad hoc* networks by enabling the design of simple, robust, and efficient protocols. Improved WiFi protocols increase the throughput by a significant factor and the fundamental theoretical research by this MURI team on LRD will produce new mitigation methods such as optimal fragmentation and diversity routing.

4. Discovering New Theories for Modeling and Analysis of Multi-scale Networks. This MURI began in FY08 and was awarded to a team led by Professor Ness Shroff at the Ohio State University. The objective of this research is to invent new mathematical theory and techniques in order to enable modeling, analysis and control of complex multi-scale networks. In particular, the research will develop a mathematical theory and techniques for modeling, analysis, and control of complex multi-scale networks.

The research team is investigating multi-scale phenomenon and control of wireless systems including LRD in wireless systems, which is a consequence of the temporal and spatial complexity inherent in military networks. The research focuses on the impact of multi-scale phenomena on the control, performance, and security of these networks. This research will lead to a long-overdue union of stochastic control, statistics, queuing theory, complexity theory, and the distributed algorithms, which is necessary for the development of radically new strategies for controlling the increasingly complex military networks. In particular, the objective is to develop a unifying theory that is mathematically rigorous and leads to practically-implementable network control and distributed detection algorithms, thus providing an enormous tactical advantage for the U.S. military.

The research approach consists of three inter-related focus areas: (i) traffic modeling and analysis, (ii) network control, and (iii) information assurance. While the investigation covers both wired and wireless networks, it focuses heavily on the wireless portion of the overall networks, which is central to tactical communications and the Army's network centric operations, and is likely to have the most stringent resource constraints and greatest vulnerability to security breaches. The modeling approach takes into account the critical time scales in military networks, from user-level applications (*e.g.*, time-critical data), to the time-scale required for the operations of various protocols and resource allocation schemes; this is significantly different from the state-of-the-art in traffic modeling, where the network is viewed as a physical entity whose laws are being passively observed through traffic studies. The team is formulating optimization and distributed control problems for providing network services and studies the impact of LRD traffic on network control, performance, and security. The project is also developing an integrative approach that combines the LRD modeling and network control to obtain non-parametric or semi-parametric techniques for the distributed detection of information flow and flow changes needed for preventing security attacks. The research is characterizing the ability of flow to be detected as a function of flow rate, delay and memory constraints, and develops distributed detection schemes that guarantee vanishingly low detection error probabilities. The outcomes of this project will result in distributed, low-complexity, and robust control mechanisms for achieving high network performance, intrusion detection, and security. These outcomes will provide high performance, reliability, and information assurance in support of the Army's future Network-Centric Operations and Network Centric Warfare (NCW). Further, the rigorous and conceptually unifying mathematical techniques developed in the course of this work will enable a deeper understanding of the dynamics and control of large and complex networks.

5. Network-based Hard/soft Information Fusion. This MURI began in FY09 and was awarded to a team led by Professor James Llinas of the University at Buffalo. The goals of this research are to develop a generalized framework, mathematical techniques, and test and evaluation methods for fusion of hard and soft information in a distributed (networked) Level 1 and Level 2 data fusion environment.

During the first three years of this effort, the MURI team developed and refined the overall system concept for human-centered information fusion and information processing architecture and developed an evolutionary test and evaluation approach that proceeds from "truthed" synthetic hard and soft data to human-in-the-loop campus based experiments. The researchers created, refined and analyzed a counter-insurgency (COIN) inspired synthetic data set ("SYNCOIN") involving both hard and soft data. The MURI team completed human-in-the-loop data collection activities involving hard sensors. The team investigated frameworks for integration, test and evaluation of new algorithms and transition to Army operational environments. The researchers also developed a taxonomy for characterizing the human as observer (source characterization), and uncertainty characterization under environmental and observer characteristics. The team developed a software package "Tractor" for processing text messages in multiple stages and common referencing; evaluated syntactic and semantic processing techniques and selected GATE (General Architecture for Text Engineering) for syntactic processing and FrameNet for a semantic processing database. The MURI team refined a soft data association prototype that extends the traditional hypothesis generation-hypothesis evaluation-hypothesis selection paradigm for fusion of soft data and utilizes a data graph association process. It developed parallel data association algorithms (Hadoop/HBase/map reduction for handling large scale data and implemented state estimation algorithm using stochastic graph matching. Robust hard sensor fusion techniques for reliable characterization and semantic annotation of human behavior were developed. Calibrated experiments for testing and evaluation of new fusion techniques were carried out. New methods for representing uncertainty in soft data to support common referencing were developed. Concurrently conditional approach to possibility-probability fusion, imprecise uncertainty measure using belief structures, and aggregation operators to link types of monotonic set measures for uncertainty were investigated. Finally, the MURI team designed and implemented an infrastructure to support distributed information fusion using communication methods and protocols, extensions of Service Oriented Architecture (SOA) and Message Oriented Middleware (MOM) paradigms, optimized information flow and tasking, complex event processing, and utilization of community standard data representations.

6. Theories of Tomography of Social Networks. This MURI began in FY10 and was awarded to a team led by Professor Patrick Wolfe of Harvard University. The goal of this MURI is to develop quantitative procedures to identify, characterize and display, on the basis of externally observed data generated from passive and/or active procedures, covert social networks of asymmetric adversaries, that is, terrorist/insurgent networks.

The MURI team has developed a framework for quantifying the fundamental limits of detectability for embedded insurgent sub-networks. This first rigorous "signal detection theory" for networks enables the computation of these performance limits within a coherent mathematical framework and the development of algorithms that approach them. Trade-offs between algorithmic performance and computational requirements can now be explored using statistically principled methods. Further improvements involve modifying the probabilistic framework of communities using prior information on affinity. An in-depth investigation of network resilience and power relationships is underway to identify segments within networks that are most vulnerable to disruption.

7. Structured Modeling for Translation. This MURI began in FY10 and was awarded to a team led by Professor Jaime Carbonell at Carnegie Mellon University. The goal of this MURI is to investigate new concepts for language translation that use structured modeling approaches rather than statistical methods.

Whereas statistical approaches for machine translation (MT) and text analysis (TA) successfully harvest the low-hanging fruit for large data-rich languages, these approaches prove insufficient for quality MT among typologically-diverse languages and, worse-yet, are inapplicable for very low-resource languages. This research is venturing much further than just introducing syntactical structures into statistical machine translation (SMT) and will turn the process on its head (*i.e.*, start with a true linguistic core and add lexical coverage and corpus-based extensions as data availability permits). This linguistic core will comprise an enriched feature representation (morphology, syntax, functional semantics), a suite of core linguistic rules that operate on these features via powerful operators (tree-to-tree transduction, adjunction, unification, etc.), and prototype MT and TA engines to evaluate their accuracy and phenomenological coverage. Contrastive linguistic analysis will identify the major translation divergences among typologically diverse languages, feeding into the MT linguistic core. Once the core is built, coverage will be broadened through additional linguist-generated rules and via Bayesian constraint learning from additional corpora and annotations as available; learning with strong linguistic priors, respecting the linguistic core, is expected to require much less data than unconstrained corpus-based statistical learning. The initial efforts will focus primarily on African languages, such as Chichewa and Kinyarwanda (both from the Bantu family), Tumak (an Afro-Asiatic Chadic language), Dholuo (a Nilo-Saharan language), and for even greater typological diversity, a Mayan language, such as Uspanteko. In addition to designing, creating, documenting, and delivering the linguistic cores for the selected languages, this program focuses on delivering a suite of methods and algorithms (*e.g.*, tree-to-tree feature-rich transducers, proactive elicitors, rule interpreters) and their prototype software realizations.

The new powerful linguistic capabilities potentially generated by this research will enable the Army to perform rapid and principled construction of MT and TA systems for very diverse low-density/low-resource languages. This has the potential to provide the Army with new tactical capabilities for on-the-ground translation between deployed US forces and locals, especially in low density language regions. It also has the potential for new and improved capabilities for automated translation, automatic summarization, and textual analysis within the strategic intelligence communities.

In FY12, the MURI team has made a leap forward in developing the underpinning linguistic foundation and linguistic science. Their investigations on how to include human annotation in the system may very well change the way annotation is done and may achieve the same results with a fraction of the effort; this was very encouraging and is a possible transition after it has developed a bit more. The team has developed linguistically-targeted test suites that are an appealing alternative to the standard suites in evaluating the linguistics.

8. Optimal Control of Quantum Open Systems. This MURI began in FY11 and was awarded to a team led by Professor Daniel Lidar of the University of Southern California. The goal of this MURI is to show a high degree of fundamental commonality between quantum control procedures spanning all application domains.

This research is pursuing the development of a new mathematical theory unifying quantum probability and quantum physics, and this research is developing new ideas in quantum control that are presently in their infancy. Of particular importance is perhaps the most pressing quantum control frontier: real-time coherent feedback control of non-Markovian open systems. To address the project goal, the research team is studying unifying features of controlled quantum phenomena. The means for achieving quantum control is generally categorized as either open-loop control, adaptive open-loop control, real-time feedback control, or coherent real-time feedback control. Despite the operational distinctions between these control categories, the researchers aim to show that there is a strong relationship between all of these approaches to control, using algebraic and topological techniques. This linkage is expected to be significant for seamlessly melding these tools together in the laboratory to draw out the best features of each method for meeting new control challenges and overcoming inevitable laboratory constraints, in particular in the context of the proposed meso-scale laser and atomic Rb experiments.

9. Multivariate Heavy Tail Phenomena: Modeling and Diagnostics. This MURI began in FY12 and was awarded to a team led by Professor Sidney Resnick of Cornell University. The project aims to develop reliable diagnostic, inferential, and model validation tools for heavy tailed multivariate data; to generate new classes of multivariate heavy tailed models that highlight the implications of dependence and tail weight; and to apply these statistical and mathematical developments to the key application areas of network design and control, social network analysis, signal processing, network security, anomaly detection, and risk analysis.

More specifically, the researchers are investigating and developing statistical, mathematical, and software tools that will provide (i) flexible and practical representations of multidimensional heavy tail distributions that permit reliable statistical analysis and inference, allow model discovery, selection and confirmation, quantify dependence, and overcome the curse of dimensionality, (ii) heavy tailed mathematical models that can be calibrated which clearly exhibit the influence of dependence and tail weight and which are appropriate to the applied context, and (iii) exploitation of the new tools of multivariate heavy tail analysis to enable the study of social networks, packet switched networks, network design and control, and robust signal processing.

10. Associating Growth Conditions with Cellular Composition in Gram-negative Bacteria. This MURI began in FY12 and was awarded to a team led by Professor Claus Wilke of the University of Texas - Austin. The goal of this research is to develop methods to identify statistical association in multiple-input-multiple-output (MIMO) data using microbial growth and composition data.

To trace a microbe-causing disease to its source or to predict a microbe's phenotype in a given environment, it is necessary to be able to associate the conditions under which bacteria have grown with the resulting composition of the bacterial cell. However, the input and output data complexity – multiple, heterogeneous, and correlated measurements – poses an interpretational challenge, and novel methods for analyzing, integrating, and interpreting these complex MIMO data are sorely needed. The research team is thus comprised of experts in statistics, computational biology, computer science, microbiology, and biochemistry, with the goal of producing the following outcomes: (i) development of novel linear and nonlinear mathematical methods to associate bacterial cellular composition with growth conditions, (ii) identification of the types and ranges of growth conditions that lead to distinguishable cellular composition, (iii) identification of key compositional markers that are diagnostic of specific bacterial growth conditions, and (iv) assessment of model uncertainty, robustness, and computational cost. The MURI will develop capabilities in several novel areas of data analysis and statistics such as the analysis of MIMO data, the integration of side information into regression models, and inverse optimization approaches. In addition, the types of approaches developed in this project will advance DoD capabilities in bacterial forensics and allow natural pathogen outbreaks to be distinguished from intentional attacks.

C. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY12.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY12, the Division managed on new-start Phase I STTR contract, in addition to active projects continuing from prior years. The new-start contract aims to bridge fundamental discoveries with potential applications, including the development of modular parallel adaptive meshing capabilities for increasing the efficiency of numerical simulations.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY12, the Division managed one new REP award. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY12.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY12, the Mathematical Science Division managed seven new DURIP projects, totaling $1.0 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of information fusion, multiscale modeling of materials, front tracking methods, and unified mathematical models for solids, fluids, gases, and multiphysic interaction.

H. DARPA Economics of Collective Value Program

The objective of this program is to develop a theoretical framework that describes the dynamics of economic agents, transactions and price behavior, using a correspondence to physical non-equilibrium systems. ARO has collaborated with DARPA to develop this topic. ARO also manages this project as a step toward developing metrics which may also apply to more abstract areas such as social media: an area in which ARO has established a new research program. The framework provides a theoretical basis for the relationship of "value" and "price" as a scientific basis for economic systems. Price and value are in contrast to traditional theory, not synonymous. Traditional theories of value do not incorporate the complex dynamics of social systems. Value is determined by desire of an individual for a good, price is determined by collective agreements on transactions to transfer that good. In this work, the PI's new theoretical framework quantitatively reproduces the complex dynamics of economic agents and the resulting price behavior of commodity markets. The PI is mathematically modeling the mechanisms that underlie collective social behaviors, such as bandwagon effects, and has found evidence of their destabilizing force on the markets in the aftermath of the financial crisis (see FIGURE 1). The PI demonstrated how an unregulated economic activity, derived from the concept of a self-correcting stable economy, does not achieve market efficiency. This framework, introducing the perspective of complex systems into theories of price formation, provides a new scientific basis for economic systems.

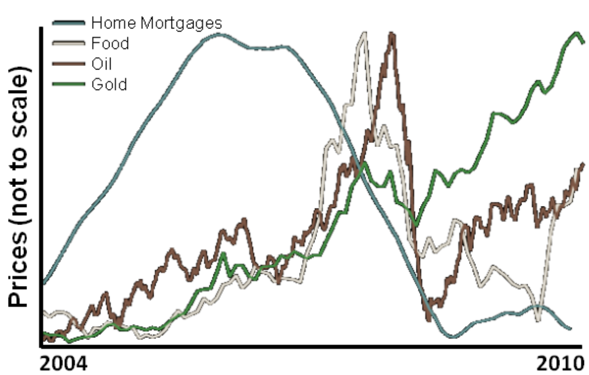

FIGURE 1

Historical commodity data. This commodity time series (2004-2010) plots relative changes in the prices of home mortgages (blue), food (yellow), oil (red), and gold (green), which are examples of the type of data used to text and validate theories developed by the research program.

I. DARPA Geometric Representation Integrated Dataspace (GRID) Program

The vision of the GRID program was to establish the theoretical foundations and pragmatic implications of a compressive representation format for high-resolution 3D data of all sensor modalities. The envisioned GRID format would have accurately encoded the 3D geometry and surface properties of objects at various spatial scales and would have provided efficient storage, application, and exchange throughout multiple industries.

There have been numerous attempts, often independent and industry-specific, to efficiently capture 3D geometry and surface properties. This program would have sought to unify disparate approaches in all three stages, namely, data format, encoding and rendering in automatic procedures. While there is strong interest in 3D land topography, this program also considers other areas such as manufacturing and biomedicine. The full GRID program was not funded by DARPA but, as part of the process for proposing the GRID program, the Mathematical Science Division identified and initiated three pilot projects which were supported via DARPA funding. Many of this program's goals were complementary to the research directions pursued by the Division's Dynamic Modeling of 3D Urban Terrain MURI.

J. DARPA Biochronicity Program

The DARPA Biochronicity Program builds on studies from the DARPA Fundamental Laws of Biology (FunBio) Program. ARO co-developed the Biochronicity Program, and currently co-manages the program as a core component of the ARO Biomathematics Program's emphasis on identifying the fundamental mathematical principles of biological structure, function and development applying across different biological systems and scales. The Biochronicity program in particular seeks to achieve a fundamental understanding of the role of time in biological functions in order to be able to manage the effects of time on human physiology. For example, biological clocks are involved in regulating virtually every function of the human body, yet exactly how time contributes to cell-cycle progress, growth, metabolism, aging, and cell death is unclear. In order to understand the coordination of timing on multiple scales in the human body, the Biochronicity program uses an interdisciplinary approach, involving empirical data sets, mathematical modeling, bioinformatics techniques, statistics, and data-mining, to identify common spatio-temporal instructions, or "clock signatures," regulating various physiological systems. Understanding how time regulates human biological processes should allow one to manipulate these processes so that one can for example improve trauma care on the battlefield by increasing the time available for medical treatment and surgery, as well as decrease the deleterious effects of age-related diseases and other infirmities. Along with the clear DoD relevance of the program, efforts in the Biochronicity program are leveraged by the Division's Biomathematics Program Area, Fundamental Laws of Biology Thrust.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Mathematical Sciences Division.

A. Sensing and Efficient Inference for Identity Management

Professor Carlo Tomasi, Duke University, Single Investigator Award

The goal of this project is to create the theoretical foundation for identity management when tracking multiple people by video-based urban physical sensor networks. In FY12, the researchers reformulated the problem as correlation clustering and conditions for partial solutions were identified. A theoretical framework for an approximate solution of the general problem of associating observations with individuals was developed on the basis of the graph partition framework developed in the previous year. In addition, sufficient conditions that allow associating tracks recorded by the same camera, but broken by occlusions, were established. A procedure for delineating the precise shape of objects being tracked in video that is consistent with the association algorithms has been developed. All of these theoretical results were implemented in algorithms that work at frame rate or faster, except for image feature extraction. Computational experiments based on preliminary, non-optimized implementation of the new theoretical results produce state-of-the-art performance, namely, ~1000 nodes in ~10 seconds (see FIGURE 2). When implemented in an optimized manner, the new theoretical approach is expected to be superior to competing methods.

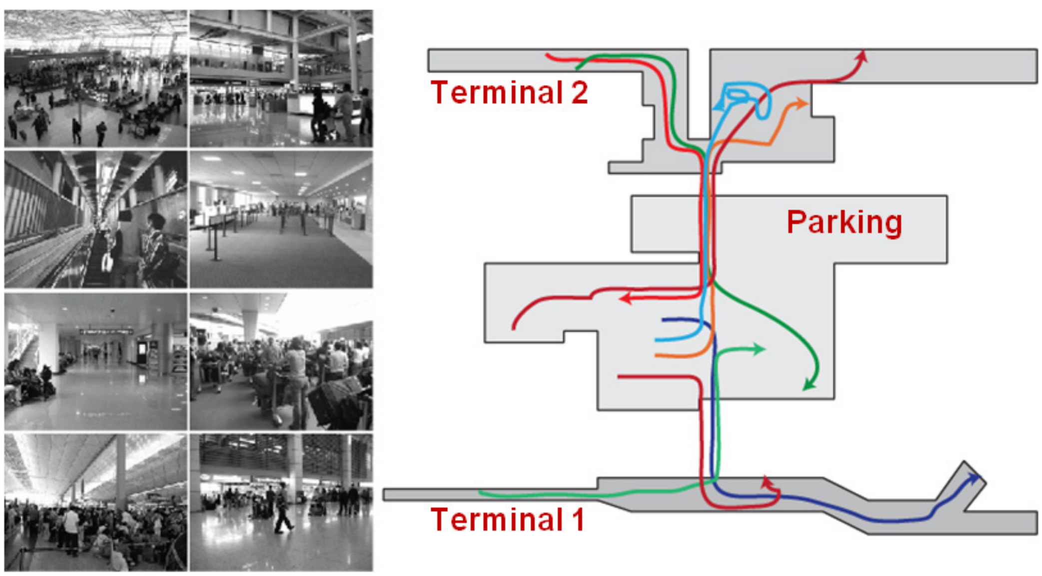

FIGURE 2

Identity management algorithms for tracking multiple people by video-based urban physical sensor networks. The input is video (left portion of figure), while the output (right) indicates "who went where" with correct identity being retained in spite of handoffs between video sensors and crossovers of targets in the video.

B. Mathematical Fundamentals of Semantics for High-Level Fusion

Professor Paulo Costa, George Mason University, Single Investigator Award

The goal of this project is to improve uncertainty management for High-Level Information Fusion (HLIF) systems. At present, HLIF researchers have to choose among various approaches for uncertainty representation and reasoning without a clear understanding of the mathematical appropriateness of each approach to HLIF problems. In FY12, the research team (i) performed an in-depth ontology-based analysis (see Figure 3) of the major requirements for representing and reasoning with uncertainty from the HLIF perspective, (ii) developed a set of use cases with enough complexity to cover the identified requirements, and (iii) defined a comprehensive set of criteria to evaluate how well a given methodology addresses the representational and reasoning needs of each use case. The PI is currently conducting an evaluation of two major uncertainty management approaches being used in HLIF research and development.

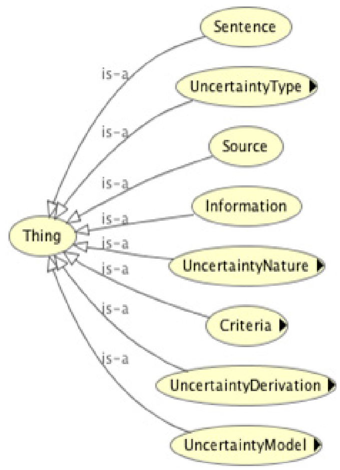

FIGURE 3

The ontology classes used for uncertainty representation. Recent progress in this project has led to improved understanding of the underlying ontology in the "uncertainty space", which enables future research to identify optimal frameworks for representation of uncertainty.

C. Principles of Three-Dimensional Modeling

Professor Avideh Zakhor, University of California - Berkeley, Single Investigator Award

The objective of this project is to develop the theoretical framework for efficient, high-resolution 3D geometric modeling based on input consisting of 2D images at irregular positions without GPS information. In the past, such modeling could be carried out only with more geospatial information. The approach proposed by Professor Zakhor results in the ability to extract the geospatial information from the 2D images. The two main foci of the PI's approach are localization and 3D model construction. The PI improved the localization by enhancing the feature basis on which pattern recognition among the 2D images takes place. Verification of the theoretically predicted improvement was provided by demonstrating a 22 cm position error over a closed-loop 60 m course (in contrast to position errors of many meters for competing methods). The 3D model was improved by (i) formulating it as a collection of planes (for example, representing ceilings, floors, walls and staircases), (ii) triangulating to develop a watertight representation of the planes for each of the scanned areas, (iii) smoothing to eliminate artifacts between local images, (iv) filling in holes by minimizing two energy functions for shape and texture (both based on similarities between the missing region and the rest of the object), (v) inclusion of thermography (heat maps) into the geometrical framework, and (vi) gridded approximate nearest neighbor searches for fast classification of geometric features. The theoretical framework developed by Professor Zakhor is of wide use, including and especially in the context of modeling the interiors of buildings. Previous efforts required stable, typically stationary platforms. The approach of the PI has been successfully tested using a backpack on a walking human being equipped with laser scanners and cameras to capture the geometry and texture of the building interiors (see FIGURE 4).

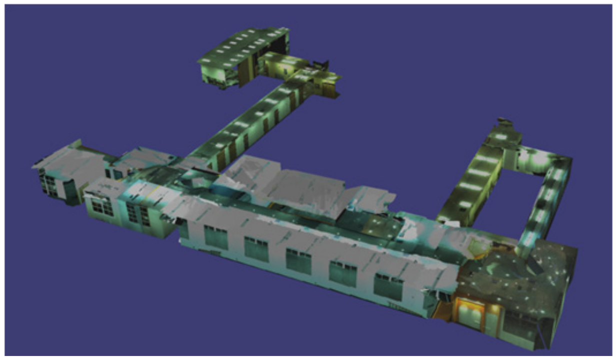

FIGURE 4

Model produced by GPS-denied indoor modeling system. Professor Zakhor's work has led to photorealistic models with minimal artifacts that are geometrically correct in spite of lack of GPS input and are suitable for training and mission rehearsal.

D. Algorithms for Modeling Insurgency

Professor Andrea Bertozzi, University of California, Los Angeles, Single Investigator Award

The goal of this project is to extend self-exciting point process models (see FIGURE 5) in order to explain spatio-temporal sociological processes underlying activity involving improvised explosive devices (IEDs), such as in Iraq. The empirical evidence on the basis of which this model was chosen was the dramatic temporal clustering of events in a database called the Iraq Body Count (IBC). The project involves both analysis of field data and constructive mathematical models with the plan to develop a mathematical framework in which to connect observational data with basic mechanistic models. The work builds on previous modeling of domestic crime done in connection with the Los Angeles Police Department. An important part of the research involves connections between geospatial patterns (such as urban and rural terrain, location of routine activities of potential offenders, and transportation routes) and clustering of events in space and time. Another part of the research involves the development of dynamic models to understand how to control and dissipate insurgent activity. Crime control is used as a proxy for insurgent behavior due to the immediate availability of data from local law enforcement agencies. Internet traffic data from a database of the U.S. Military Academy was used as source data. The connections between geospatial patterns (such as urban and rural terrain, location of routine activities of potential offenders, and transportation routes) and clustering of events in space and time that have been derived are at the front of the research in the field.

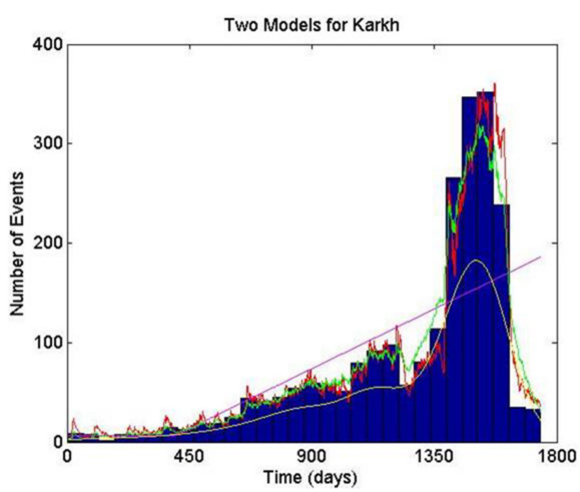

FIGURE 5

Events in Western Baghdad. Histogram (blue), estimate without/with self excitation (purple/red), smoothed background rate (green). The self-exciting point process model (red curve) provides accurate modeling of events in this data base while other models are less accurate.

E. Stochastic Analysis and Control of Transonic and Supersonic Aerodynamics
Professor S. Sritharan, Naval Postgraduate School, Single Investigator Award

The objective of this project is to develop a systematic mathematical theory for the robust real time feedback control and stochastic analysis of unsteady transonic aerodynamics of helicopter rotor blades, supersonic ballistic projectiles and propagation of blast waves in the presence of adverse external disturbances. Modern tools in stochastic analysis of discontinuous processes and control theory of nonlinear partial differential equations are combined to develop a penetrating theoretical foundation for the agile management of unsteady, highly vortical aerodynamics with shocks. In this research, the state space variables of the control system are physical quantities of fluid dynamics such as velocity field, vorticity field and pressure distribution. The state equations for control and stochastic analysis are the Euler equations for compressible rotational gas dynamics and the quasilinear unsteady potential equations of irrotational flows. These nonlinear hyperbolic and elliptic-hyperbolic type mixed equations are subjected to additive and multiplicative external disturbances modeled as Gaussian, Poisson and Levy type noise forces. Point vortex and turbulent shell models also give useful insight in the understanding of highly vertical structures associated with the helicopter blade tip aerodynamics. With H. Kunita's theory of stochastic characteristics for nonlinear hyperbolic systems, control and estimation problems were formulated. Main research directions are mathematical characterization of entropy solutions for stochastic hyperbolic systems of conservation laws, state estimation and feedback control analysis as well as assessment of the impact of noise in controlled and uncontrolled aerodynamic flows of the above type. Necessary conditions for optimal controls are worked out using a stochastic counterpart of the Pontryagin maximum principle while feedback analysis utilizes infinite dimensional Hamilton-Jacobi theory.

The scope of this basic research is critical for the Army's command and control and C4ISR at large as it seeks to develop a fundamental capability to enhance understanding as well as strategic and dynamic management of aerodynamic flows over helicopter rotor blades and ballistic projectiles subjected to adverse uncertainties. Breakthroughs in this research will impact the transonic aerodynamics of helicopter rotor dynamics as well as Army technologies such as combustion control, multiphase flows, and possibly to crumpling of surfaces in armored vehicles subjected to shell attack. A Directed Energy Weapon (DEW) such as a CO_2 Laser, Free Electron Laser or microwave directed energy weapons such as the Russian RANETS-E attacking a helicopter or a missile may be modeled as an abrupt noise forcing of Levy type and the estimation, control and mitigation techniques that were developed can give insight in to counter measures to such adversarial situations. Army's unmanned systems roadmap highlights the need for enhanced autonomy and this will in turn increase the importance of real time management of turbulence in aerodynamic configurations subject to uncertainties. This research program is at the heart of this paradigm.

In FY12, the investigator has demonstrated the following:

- Solvability of strong path-wise solutions to Navier-Stokes equations with Levy noise
- Solvability theorems for nonlinear filtering equations of infinite dimensional Fujisaki-Kallianpur-Kunita and Zakai equations that correspond to nonlinear estimation of stochastic Navier-Stokes equation with Levy noise
- Stochastic Lagrangian particle method for Euler flows with jump noise and their solvability theorems
- Stochastic particle method for nonlinear filtering equations for N-point vortex models with noise and convergence theorems

F. Achieving a Systems Level Understanding of Changing Cell Shape
Professor Tim Elston, University of North Carolina - Chapel Hill, Single Investigator Award

The goal of this project is to characterize and understand large-scale changes in cell morphology. An important property of all cells is their ability to sense and respond to their environment. For example, signaling molecules, such as hormones or growth factors, can lead to cell differentiation, proliferation, or migration. Understanding how the cytoskeleton and associated regulatory proteins function as an integrated system to generate changes in shape is a central challenge in cell biology. The morphological oscillations that occur in rounded cells constitute a mechanochemical prototype for studying regulation of the cytoskeleton by biochemical signaling networks as well as the biochemical properties of the cell that feed back to influence signaling. Computational modeling approaches are required to fully understand the self-emergent properties of the cytoskeletal system. Fortunately, the oscillating cell system has several features which lend themselves to computational approaches. First, modern technology such as probes and microscopes allow the spatiotemporal dynamics of the cortex and signaling molecules to be visualized and manipulated with unprecedented resolution. Second, the mechanical properties of the cortex can be interrogated and perturbed in the oscillating cell. Third, oscillating cells have a well-defined period and shape history that are easily measured and can be directly compared with mathematical models.

In FY12, the research team developed the computational tools required to simulate whole cell multiphase models and investigate potential mechanisms for generating sustained oscillations in cell shape (see FIGURE 6). Experiments involving novel reagents, live cell microscopy, and local mechanical measurements have allowed the team to revise their mathematical model for cell oscillations and show that the cortical actomyosin cytoskeleton plays an active role in the oscillations. Using high resolution confocal imaging, the research team demonstrated that during morphological oscillations, the actin cortex is reshaped and spontaneously polarizes toward alternate sides of the cell and the sites of high actin density correlate with active myosin, the protein that generates contractile forces. In addition, they showed, using biochemical methods, that the biochemical processes that regulate the oscillations are coupled to the biophysical mechanism generating the active forces required for the oscillations. The new model combines positive feedback to generate a focus of high RhoA activity, with a delayed feedback loop that causes the polarized site to move as a traveling wave. The feasibility of this mechanism was demonstrated using reaction-diffusion equations, and it is currently being incorporated into the multiphase model.

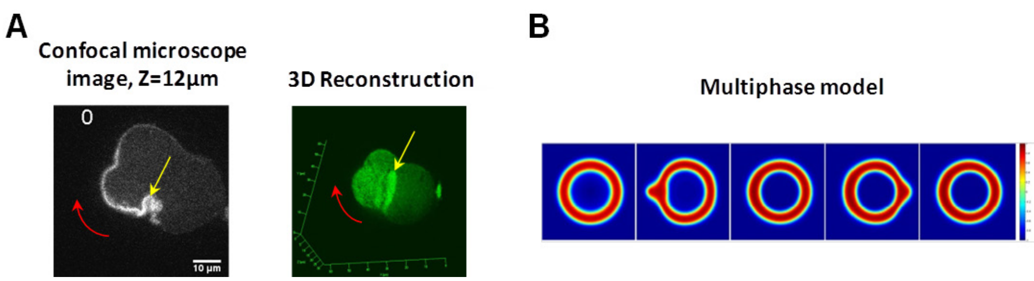

FIGURE 6

Cell changes during morphological oscillations. (A) Rounded cell undergoing large-scale oscillations in morphology. Left, slice from confocal microscope. Right, 3D reconstruction. (B) Simulation results of a multi-phase model demonstrating oscillatory behavior. In this model, RhoA activity generates contraction of the actin cortex.

By tightly integrating modeling and computational approaches with quantitative experimental measurements in live cells, this project is producing novel mechanochemical models for understanding global shape changes. A mechanistic understanding of this system will yield insights into the design principles that regulate the dynamic properties of the cell cytoskeleton that are key to cell division, motility and differentiation and the alterations that occur in pathological processes. The research results will have significant long-term impact on the understanding of wound healing, disease, and limb regeneration.

G. Multiscale and Multiphysics Numerical Methods for Mesoscopic Transport

Professor Wei Cai, University of North Carolina - Charlotte, Single Investigator Award

The goal of this project is to develop multi-physics and multi-scale fast numerical methods to simulate and understand current behaviors and optical properties of nano-scale devices, such as nano photo-voltaic solar cells and nano-scale bio-sensors that will enable advanced algorithms and tools in designs and simulations. This research has been focusing on an intrinsically multi-scale and multi-physics numerical approach for the study of transport and optical processes in these mesoscopic systems (*e.g.*, to study electron/hole transport, classical drift-diffusion and hydrodynamics models are not applicable inside quantum regions). However, in many other parts of the device, the behavior of the carriers can be sufficiently described by classical, less computationally expensive, models where the quantum interference effects are not dominant or important. This investigation is determining where and when quantum scales must be modeled.

In FY12, the PI investigated how to effectively employ either the full nonequilibrium quantum kinetics or the Wigner distribution to model far-from-equilibrium quantum processes. The PI also studied what other regions of the system are more-efficient continuum models, such as drift-diffusion and hydrodynamics models, acceptable from an accuracy and stability standpoint, and which to use and how to adapt them for passing information between scales. Investigations center around nano-devices involving quantum interference, many body scattering, nonlinear optical processes, and systems far from equilibrium, and develop methods that attempt to be both accurate and efficient, which are often dramatically different from classical approaches. Multiscale and multiphysics modeling of the transport and optical processes in nano-systems consists of a range of transport and optical response models involving increasing complexity to include more detailed physics. The strategy of this investigation in modeling and designing fast and accurate numerical methods for nano-scale systems is to gain clear understanding of the difficulties involved in applying each model at the appropriate spatial/time scales, and then creating hybrid approaches using various models to achieve the best computational efficiency and accuracy.

In FY12, the research team demonstrated a fast integral solver for Schrodinger equations for quantum dots in 3D layered media (see FIGURE 7). The new method is based on a novel fast computation of Green's functions in layered media and a decomposition of scattering wave in 3-D as superposition of many 2D Hankel waves. The latter is then computed by a wide band 2-D fast multipole method code also developed in this project. In addition, the research team developed a better understanding of the accuracy of device boundary treatment in Wigner quantum transport method in computing resonant tunneling diode (RTD). More specifically, the team quantitatively studied and described the effect of the contact size on the accuracy of the boundary conditions for the Wigner equation method for computing the I-V curve of the RTD. The researchers also developed an adaptive method for time dependent Wigner equations for simulating non-equilibrium behavior of nano-devices.

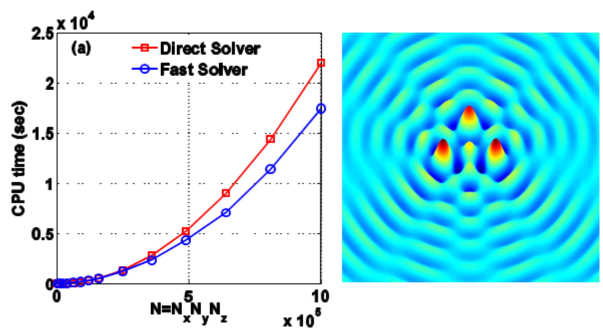

FIGURE 7

Numerical methods for quantum dots. The simulation of electron confinement by three quantum dots (right) requires expensive computations of the Helmholtz integral operator. Characteristics of the physical domain depend greatly on the scale; in this instance, the investigators characterize the device as very slowly varying in the horizontal direction as a ratio to the vertical and have developed a parallel fast algorithm for computing these operators. The graph (left) demonstrates a 23% speedup of this fast solver over the previously most competitive fast (direct) solver.

H. Modeling, Analysis, and Algorithms for Stochastic Control of Multi-scale Networks

Professor Ness Shroff, Ohio State University, MURI Award

The overall goal of this project is to develop a theory for modeling, analysis, and control of complex multi-scale networks to achieve high performance, reliability, and information assurance. The results of this research may ultimately support of the Army's future Network-Centric Operations and Network Centric Warfare. Multi-scale phenomenon is being investigated, including long-range dependence in wireless systems, which is a consequence of the temporal and spatial complexity inherent in military networks. Multi-scale phenomenon, if not managed appropriately, could result in excessive delays, packet loss, and instability. On the other hand, when well managed, one can potentially exploit the underlying correlations to make accurate predictions and better control the network. The impact of multi-scale phenomenon on the control, performance, and security of these networks is being studied. This research will lead to a long-overdue union of stochastic control, statistics, queueing theory, complexity theory, and the distributed algorithms, which are necessary for the development of radically new strategies for controlling the increasingly complex military networks. A specific objective is to develop a unifying theory that is mathematically rigorous and leads to practically-implementable network control and distributed detection algorithms.

Major accomplishments from FY12 include the completion of comprehensive statistical analysis for packetized voice traffic (VoIP) and Internet traffic, and the development of models that capture the traffic statistical properties and serve as a tractable basis for mathematical study for the traffic. Multifractal and Gaussian fractional sum-difference models for Internet traffic have been developed that can be used to generate synthetic traffic for network simulation in which only the traffic rate needs to be specified. New statistical models were also created for packetized voice traffic to understand queueing behavior such as delay and jitter. In the area of multi-scale network control, the team has developed delay-optimal policies for multi-hop wireless networks. In particular, sample-path optimality in trees and forest topologies were fully characterized. The accomplishments in the areas of inference and information assurance include development of fundamental limits on flow detection for preventing security attacks. It was demonstrated that timing traces at a few nodes in the networks can be used to detect information flows. The developed solution is applicable to detect wormholes in mobile ad hoc networks, and was validated through extensive experiments with sample VoIP traffic. The team also investigated traffic dependencies in practical systems, and developed low-complexity solutions to detect network anomaly with local information in intranet networks, discriminated client-keystroke from file transfers in monitoring systems, and characterized communication activities in online social networks. The researchers are continuing studies of the effects of long-range dependence phenomena on detection against MANET protocols.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers in FY12.

A. Algorithms for Modeling Insurgency

Investigator: Professor Andrea Bertozzi, University of California - Los Angeles, Single Investigator Award
Recipient: Concepts Analysis Agency

This project aims to develop a mathematical framework to connect observational data with basic mechanistic models, involving analysis of both field data and constructive mathematical models. An important part of the research involves connections between geospatial patterns and clustering of events in space and time, and sufficient development of dynamic models to understand how to control and dissipate insurgent activity. A better understanding of these processes may contribute to policy and security strategies to combat the critical national security challenges posed by terrorism and insurgencies.

The investigator has developed a code for "predictive policing" (predicting future insurgent-generated events), which has transitioned to the Concepts Analysis Agency for analyzing insurgency data from southwest Asia. This code, currently in a Matlab version, is based on a theoretical and empirical (mainly civilian crime) approach. It consists of agent-based modeling of 'hot spot' formation built from bottom-up behavior models (see FIGURE 8). Agent-based models enabled the development of custom statistics designed to answer specific behavioral questions that are less tractable in general statistical models. Methodologies of statistical physics and the mathematics of swarms were incorporated to develop formal models, which were then integrated with Geographic Information Systems data to explore spatial properties. At each stage of model development, empirical tests were conducted against civilian crime data, comparing simulated crime prevention interventions with known changes in urban planning and policing strategies. Simulations have also been carried out for analytical models where the model behavior can be rigorously tested against sound analytical expectations. Testing on real insurgency data is expected to start soon. Following further testing, the theoretical model will be adjusted based on the results obtained. The ultimate objective here is to adapt the underlying basis (and accompanying analysis) of the predictive policing code from a civilian criminal activity basis, such as in Los Angeles, to a high insurgency activity basis, such as in Afghanistan.

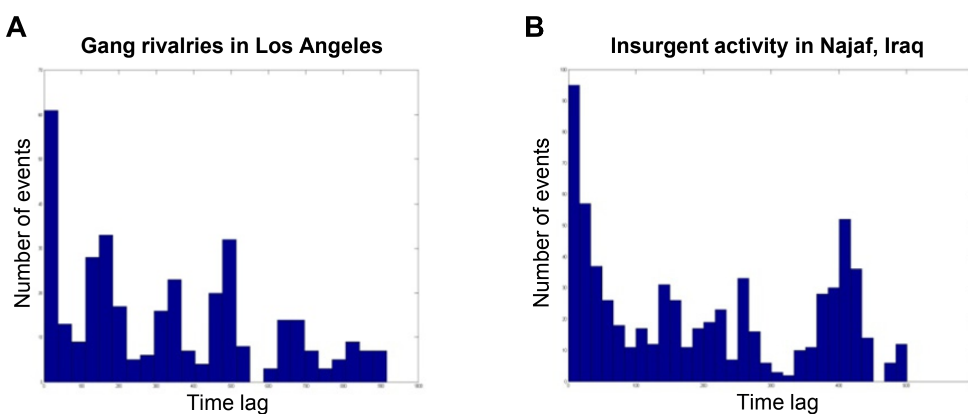

FIGURE 8

Comparing urban street crime with insurgent activity. Histograms of the number of events (y axis), such as IED activity or gang shootings are plotted vs. time between events (x axis) for (**A**) gang rivalries in Los Angeles and (**B**) insurgent activity in Najaf, Iraq.

B. Changepoint Detection for Network Intrusion Detection

Investigators: Professor Boris Rozovsky, Brown University, and Professor Alexander Tartakovsky, University of Southern California, MURI Award

Recipients: DoD and DoE

The goal of this research is to create innovative and easily implementable sequential hypothesis testing algorithms for computer network intrusion detection, where the sample size is not fixed in advance. Instead of a fixed sample size, data is evaluated as it is collected, and further sampling is stopped in accordance with a pre-defined stopping rule as soon as significant results are observed. Thus a conclusion may sometimes be reached at a much earlier stage than would be possible with more classical hypothesis testing or estimation, at consequently lower financial and/or human cost.

These sequential hypothesis testing algorithms have been developed based on the nearly minimax mixture sequential analysis technique created by Professor Tartakovsky of the University of Southern California. Discrete mixture sequential testing rules in statistical analysis arise naturally in certain important practical problems. One such problem is a multi-sample slippage problem where a statistician has to decide whether or not one of the populations has slipped outside the range of the rest of the populations, without specifying which one. To solve this multi-sample slippage problem, Professor Tartakovsky created nearly minimax mixture sequential hypothesis testing algorithms that will have certain important advantages over their continuous counterparts. The most important advantage is that they are easily implementable which is not usually the case using existing continuous mixture rules. Moreover, they are *second-order* asymptotically optimal with respect to the expected sample size for all discrete points (asymptotically suboptimal outside of these points).

These results have transitioned to CERDEC, where Professor Tartakovsky and researchers at the Intelligence and Information Warfare Directorate of CERDEC are now working together to develop a prototype intrusion detection system that can be implemented in the Army computer system for information assurance. Testing has shown that this statistical anomaly-based system provides reliable and rapid detection of cyber virus attacks (for the purpose of disrupting network services) with less than 12% false alarm rate. This is a significant improvement over the commonly used commercial anomaly detection software that has more than 30% false rate with the same detection delay time. These attacks are not easily amenable to detection by existing signature-based methods. Spatiotemporal clutter rejection and target tracking algorithms based on this research have been transferred to the DoD for testing and implementation (see FIGURE 9).

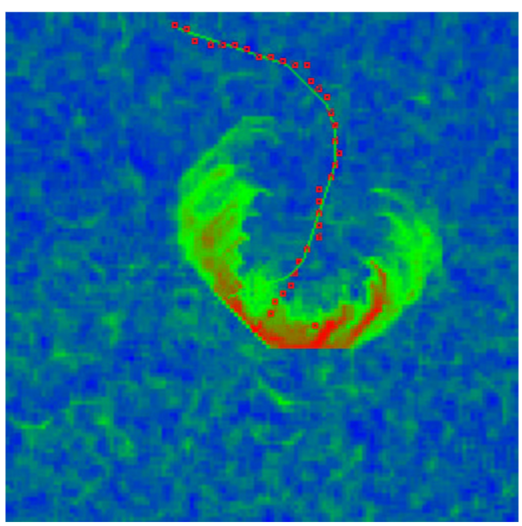

FIGURE 9

Simulation of spatiotemporal clutter rejection and target tracking algorithms. Dim Targets acquired under change point and nonlinear filtering methods.

C. Mathematical Imaging and Modeling of Cortical Spreading Depression and Wound Healing

Investigator: Professor Tim Elston, University of North Carolina - Chapel Hill, Single Investigator Award
Recipient: U.S. Army Medical Research and Materiel Command (MRMC)

The overall goal of this research is to develop a mechanistic understanding of cortical spreading depression (CSD) and epithelial wounds such as blisters and retinal detachments. Development of image analysis techniques, physiological models of spreading depression of brain activity, and mechanical models of blister formation and wound healing were carried out in parallel.

First, an image analysis algorithm was developed to better segment depression wave fronts in brain tissue confounded by extraneous anatomical features such as vasculature (see FIGURE 10). This work is currently being extended to allow identification of shapes in other images such as electron micrographs of bacterial cells. Accurate segmentation of bacterial boundaries allows for calculation of cell volumes and surface areas, which are important quantities for understanding cellular processes and function, as well as for better discrimination between different species. However, segmentation of bacterial cell boundaries can be challenging due to the graininess of the images, as well as confounding features such as sample holders and extraneous objects. To overcome these distractions, shape templates allow good identification of the objects with similar overall shape parameters before refining the segmentation using localized determination of the high contrast regions.

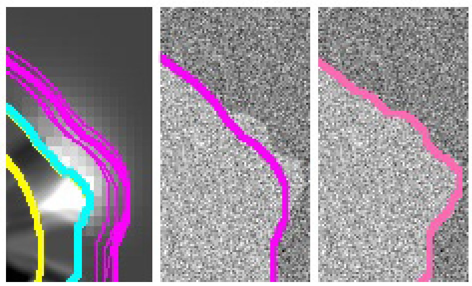

FIGURE 10

Improved capture of shape evolution. Tuning shape priors improved capture of shape changes as the front evolves (right panel).

A mathematical model of front propagation was also developed and incorporates metabolic processes that are fed by dynamically varying vasculature. The chief question investigated was whether vascular changes can qualitatively affect the dynamics of CSD. The main ingredients of the mathematical model uniquely included vascular dynamics and blood flow that control local oxygen level in the tissue and the subsequent ATP production. The investigators found that during CSD, vascular dynamics have very little effect on the overall dynamics, but that blood flow does affect the initiation of CSD as well as the refractory period following CSD.

Finally, a mechanical model of retinal detachment provided insight into how mechanical properties such as Young's moduli, and physiological processes, such as fluid pumping and resorption, conspire to destabilize or heal retinal detachments. The results predicted critical fluid pumping rates and cell adhesion strengths, below which retinal detachments are unstable to further growth. Extensions to the model have also been made to incorporate fluid drainage from lymphatic ducts and osmotic stresses arising from vascular leaking and inflammation, with relevance to understanding skin blister formation and healing.

This imaging and modeling work provides tools that will directly aid research into cortical spreading depression, migraine, nerve tissue trauma, retinal detachments, and identification of bacterial agents. These results transitioned to MRMC in FY12. MRMC scientists are currently specifically interested in using the results of this research to aid in the Army's treatment of burn victims, with other transitions to Army Medical Command scientists expected as the research matures.

D. Designing and Prescribing an Efficient Natural-like Language for Bots
Investigator: Professor Mitch Marcus, University of Pennsylvania, MURI Award
Recipient: Army Research Laboratory, Human Research Engineering Directorate (ARL-HRED)

The goal of this project is to develop theory that will eventually enable bots to both understand and to be understood by humans, ultimately enabling functional human-bot teams. Fluent and effective communication between warfighters is imperative to convey orders and intent and to ensure adequate situational awareness. All unit members must continually exchange information as the environment changes, and as autonomous bots move onto the battlefield, they will also need to participate in these complex linguistic interactions. This almost necessarily means equipping them with natural language capabilities. The Soldier whose native language is English can communicate a rich range of information and intentions in English with little appreciable increase in cognitive load, even when the Soldier is under high stress. Soldiers cannot compromise these abilities for the sake of the bots; therefore, this research strives to bring the bots to the level of the Soldier. This research effort, the Situation Understanding Bot Through Language and Environment (SUBTLE) project, is organized in nine synergistic areas: Machine Learning & Stochastic Optimization, Human–Robot Interaction, Syntactic Analysis, Semantic Interpretation, Pragmatic Enrichment, Parameterized Action Representation, Formulating Specification for Robot Motion Planning, Corpus Collection, and Testbeds and Integrated Demonstrations.

In FY12, the team developed and integrated many of its areas of research, including joint inferencing, natural language processing (NLP), computational pragmatics and its visualization, and incorporation of psychological data into models (see FIGURE 11).

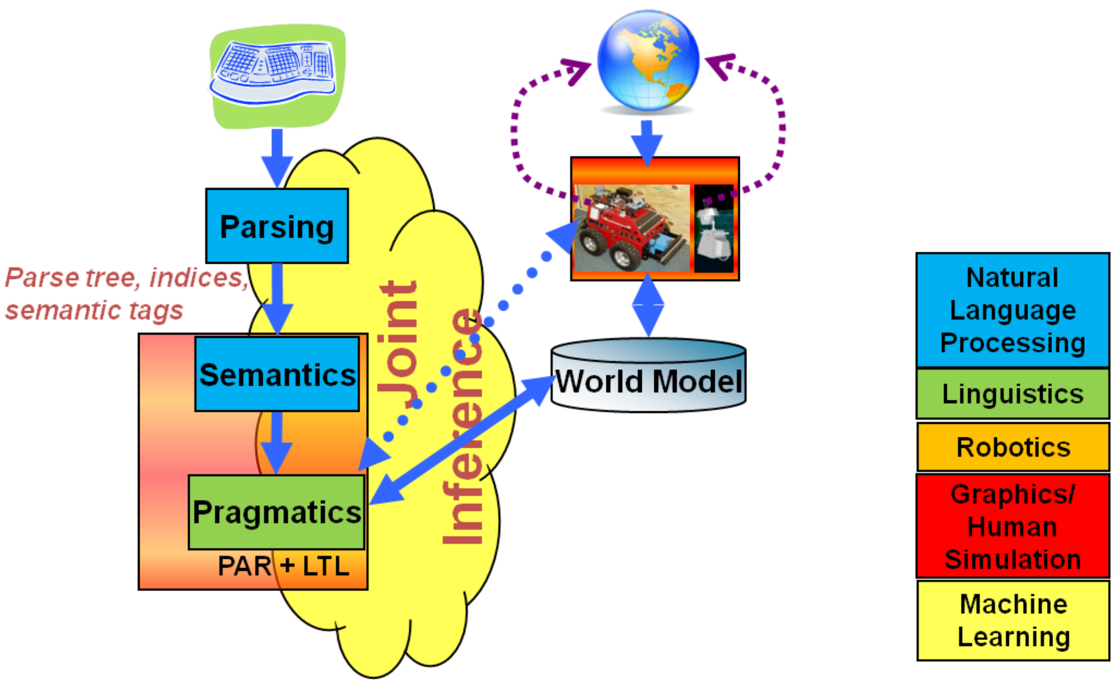

FIGURE 11

Situation understanding bot. System Incorporates formal models of language, develops techniques to analyze not only the utterance but also the speaker's implicit meaning, exploits the broad context of the environment, determines the adequacy of specifications through empirical, corpus-based methods, and works within the context of the real-time/high-stress situation of search and rescue

The NLP components that the team developed have been compiled, made more robust, and transferred to ARL-HRED. The research team modified the controller compiler to allow the MURI team's NLP components to interface with the ARL-HRED Symbolic and Sub-symbolic Robotic Intelligence Control System (SS-RICS). This was the first transition to ARL; ARL-CISD is also planning a similar transition, and the system will also transition to the AMC Systems Performance Office (AMC-SPO).

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Mathematical Fundamentals of Semantics for High-Level Fusion

Professor Paulo Costa, George Mason University, Single Investigator Award

The goal of this project is to improve uncertainty management for High-Level Information Fusion (HLIF) systems. At present HLIF researchers have to choose among various approaches for uncertainty representation and reasoning without a clear understanding on the mathematical appropriateness of each approach to HLIF problems. The project has (i) performed an in-depth ontology-based analysis (refer to Section III-B) of the major requirements for representing and reasoning with uncertainty from the HLIF perspective, (ii) developed a set of use cases with enough complexity to cover the identified requirements and (iii) defined a comprehensive set of criteria to evaluate how well a given methodology addresses the representational and reasoning needs of each use case. During the next year, the researchers will conduct an evaluation of two major uncertainty management approaches being used in HLIF, namely, Dempster-Shafer and Bayesian, and will report the results to the information fusion community at the FUSION 2013 conference. This research will also include a fundamental analysis of the main differences between the D-S and Bayesian approaches: (a) the formal mathematical properties of the formalisms being compared, (b) their applicability to the fusion problem under consideration and (c) their relative strengths and weaknesses. In this analysis, the ability to handle imprecisely defined concepts will be an important factor. (Probability theory and Dempster-Shafer theory have both been criticized for being restricted to propositions with “crisp” truth-values.) Also important will be the ability to handle incompleteness. At higher levels of information fusion, the approach chosen for representing uncertainty has a large impact on system performance that is hard to quantify or even to assess from a qualitative viewpoint. This project will provide information that will allow better choice of uncertainty representation in information fusion.

B. Control of Quantum Systems: Theory and Experiment

Professor Daniel Lidar, University of Southern California, MURI Award

The objective of this research is to develop new mathematical tools at the intersection of quantum probability physics for real-time coherent feedback control of non-Markovian quantum open systems. The ability to efficiently control the behavior of a large class of quantum systems is both fundamental and crucial to the future use of these systems for technological purposes. One of the most remarkable examples is the building of a computer which uses quantum mechanical effects to perform computations much more efficiently than any classical computer. This requires precise control of the dynamics of quantum systems. More generally, applications involving systems operating at a very small scale where the laws of quantum mechanics prevail, have become more and more common in many aspects of daily life (*e.g.*, nuclear magnetic resonance and laser spectroscopy). The development of general control principles for these quantum systems has the potential to greatly enhance their applications and is of fundamental importance. Many challenges and opportunities arise. Principally, de-coherence is the major obstacle to using the unitary evolution of quantum systems as a computational platform, so being able to mitigate de-coherence processes is of utmost importance. A complete theoretical grasp of de-coherence in its many manifestations is essential to this end and the team will focus on the development of new master equations and numerical techniques designed to model de-coherence. The standard model being developed, along with the master equation formalism applied to it will provide the community with the essential tools to study the quantum dynamics of systems coupled to reservoirs in the presence of feedback control. This will be an essential step in overcoming de-coherence effects, which currently pose severe limitations on the progress of quantum computing. The consequence of advancing understanding of coherent feedback control in open quantum systems is of both theoretical and practical significance. Theoretically the scientific community would have access to a validated methodology with which to study the dynamics of open quantum systems in the presence of coherent feedback control. Such techniques could then be applied to minimizing de-coherence that is a critical barrier to implementation of quantum computing. In addition to quantum computing there are other practical applications that would benefit from such advanced understanding. For example, reduction of quantum noise and generation of non-classical light in very small very efficient laser diodes could allow efficient *classical* photonic information processing at the chip scale. Quantum feedback control of a solid-state system would open a new avenue of scientific research and new field of applications. Classical feedback is used nearly everywhere and it is likely that feedback control of quantum systems will ultimately be used in many applications. As an illustration of an application of optimal quantum control to canonical phase measurement, a contour plot of the Wigner wave function, is shown in FIGURE 12.

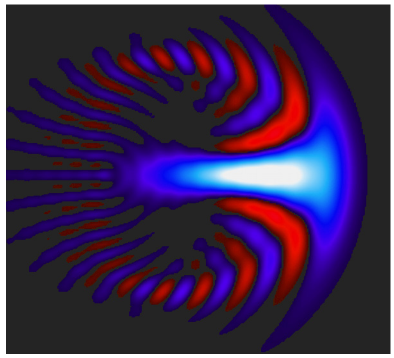

FIGURE 12

Contour plot of the Wigner function for a canonical phase state with 20 photons/phonons. This image illustrates an application of optimal quantum control to canonical phase measurement.

Initial studies are underway in all aspects of the research, theoretically and in the laboratory. Specifically, initial steps in developing an experimental and theoretical program that addresses the dynamics of open quantum systems in the presence of coherent feedback control have been implemented. This research will produce new fundamental understanding of quantum control of open systems and a set of tools for the precise control and analysis of a large class of quantum systems.

It is anticipated that in FY13, significant advances in efficient entanglement generation using stochastic control will be achieved. In particular, computational verification of proposed algorithmic improvements using super-operator algebra will be performed in order to study the effects of correlated randomness, and they will use powerful multi-parameter optimization tools to beat the effectiveness of the random unitary approach. In future years, the identification of realistic coherent control schemes that would be aggressive enough for de-coherence control are expected. In order to mesh this with research on the geometry of spin chains and rings, the team will investigate the effect of the environment on the quantum-mechanical geometry of spin chains and rings.

C. Disease Modeling via Large-Scale Network Analysis

Professor Inderjit Dhillon, University of Texas - Austin, Single Investigator Award

A central goal of genetics is to learn how the genotype of an organism determines its phenotype. The goal of this project is to address the implicit problem of predicting the association of genes with phenotypes or traits by developing a pragmatic data analytic method for linking specific genes to traits and diseases, especially polygenic traits, which are the most challenging to link with existing methods. In particular, predictive methods are sought that will be general enough to apply to potentially any genetic trait, varying from plant traits relevant to desirable agricultural properties to important human diseases. While the biological insight and capabilities to be gained from the research will be truly revolutionary, the mathematical models and techniques to be developed for the problem are also expected to advance the state-of-the-art in areas such as multiple sources in Positive-Unlabeled (PU) learning, side information in recommendation systems, social network analysis, sparse graphical models, and adaptive loss functions in matrix completion.

The problem of inferring associations between genes and phenotypes is posed as identifying missing links or the formation of new links in a social network. Unsupervised and supervised learning models are used, in both cases combining information from multiple species (see FIGURE 13). As an analogy with social networks, the interaction among genes is modeled as a social network and the associations between genes and phenotypes as an (bipartite) affiliation network. The task is then to predict links (or to discover missing links) in the bipartite networks. From the link identification perspective, the basic similarity-measured-based idea that the more similar two nodes are, the greater the probability of a link between them, is used. In the PU learning framework, a feature mapping is constructed that maps a gene-phenotype pair into a feature space of manageable dimensions and path-based features are constructed from the hybrid network. The research team is utilizing a biased Support Vector Machine (SVM) that is based on the idea that false negatives must be penalized heavily as they are known to be positive, while the false negatives much less as they are arbitrarily chosen from the large set of unlabeled examples.

Biologists have verified that some of the top gene-phenotype connections predicted by the investigator have been referenced in the literature, though their associations have not been established biologically. The team's experimental results indicate that combining multiple sources of information from different species significantly improves the quality of the prediction or classification. In addition, the team has shown how any quantitative measure of imbalance in a network can be used to derive a link prediction algorithm, and their new supervised machine learning-based link prediction method that uses features derived from longer cycles in the network outperforms all previous approaches, achieving good accuracy for sign prediction and effectively lowering the false positive rate.

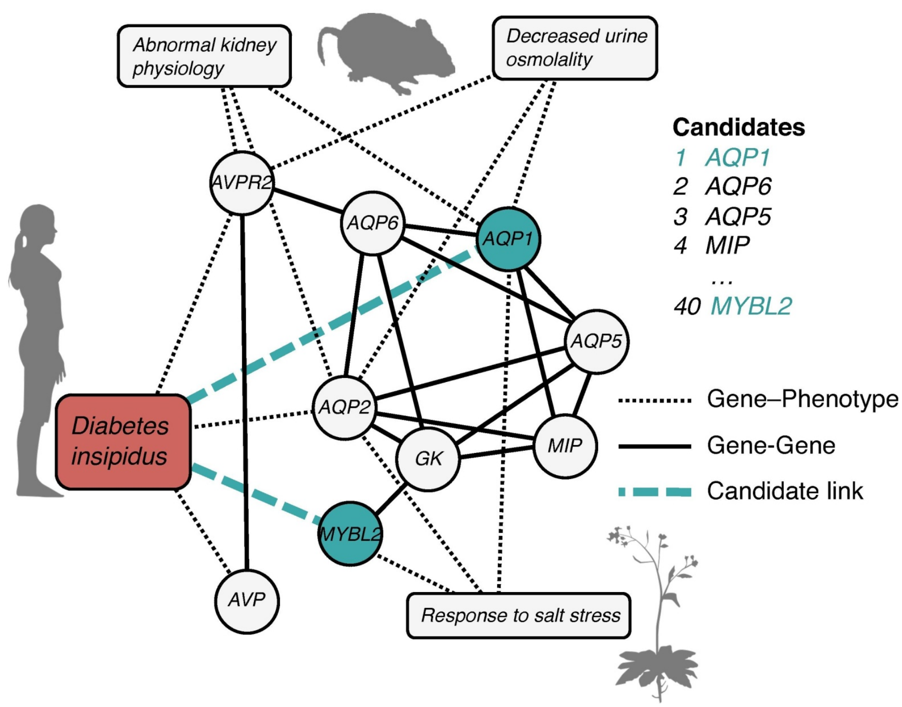

FIGURE 13

Combined gene-disease network in the neighborhood of the human disease *diabetes insipidus* and two highly ranked candidate genes, AQP1 (top ranked candidate) and MYBL2 (ranked as number 40). AQP1 is ranked higher than MYBL2 because it has more links to genes already associated with *diabetes insipidus,* and is also connected to more model organism phenotypes that are associated with genes for *diabetes insipidus*. Only genes and phenotypes that are close to both *diabetes insipidus* and the candidate genes AQP1 and MYBL2 are shown. Only human, plant and mouse are shown even though the actual data used is from 9 species.

It is anticipated that in FY13, the research team will produce better predictions, using a variety of methods. One approach is to combine multiple predictors, such as in a boosting framework. They also will further explore the PU learning framework and use other methods such as weighted logistic regression within this framework. Inferences on multi-partite networks composed of multiple species networks is a promising prospect that will be explored as well. In addition, wet-lab experiments will be initiated to confirm the predictions, and user-friendly prediction and visualization software will be developed and transitioned to Army scientists.

Any advance in the ability to link genes to traits will have immediate impact on understanding molecular mechanisms of the traits, identifying genetic targets relevant to manipulating the traits, and targeting and identifying genetic variants associated with the trait, thus enabling genetic diagnostics. Thus, progress on these fronts has the potential for major impacts on the understanding of the genetic basis of physical traits. The expected software and visualization tools will contribute greatly to the Army's and more generally the biology community's ability to analyze more diverse data sets, including polygenic traits. In addition, the mathematical techniques being developed will not only be applicable to linking genes with polygenic traits but to other areas of interest to the Army and to DoD, such as forensics and social network analysis.

D. Multiscale Modeling of Cementitious Materials
Professor Ram Mohan, North Carolina A&T University, PIRT Award

The objective of this project is to pursue new opportunities in data-based virtual modeling and multiscale modeling to achieve higher fidelity predictions and design capability in a variety of complex materials of interest to the Army. In FY13, new homogenization techniques and representative volume element concepts will be pursued and combined to model the coupling of scale-dependent phenomena in materials such as concrete and ceramics. These models will be informed by and tested against experimental data drawn from X-ray analysis and from existing databases such as those at NIST, with success being demonstrated by qualitative agreement of fracture distribution (location, width, length) of a dynamically loaded particular cementitious mix. Though the project will be only about half completed, it is anticipated that this will be the first year in which the team will be able to sketch the evolution of a multi-scale nano to continuum modeling methodology that includes scales from nanoscale material constituents to macroscopic deformation and failure behavior under dynamic loading conditions, to include molecular models, experimental morphology based microstructures, high resolution morphologies, and their variants of cementitious materials under dynamic loading ranging from its molecular material genome, micro, and higher length scales. It is anticipated that the team may also begin to obtain qualitative agreements of properties and failure behavior at micro and macro scales demonstrated for a particular dynamically loading cement mix.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Joseph Myers
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Program Manager, Probability and Statistics

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Science Advisor to the 18th Airborne Corps

Ms. Anna Mandulak
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C. Administrative Staff

Ms. Debra Brown
Directorate Secretary

Ms. Diana Pescod
Administrative Support Assistant

CHAPTER 10: MECHANICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2012* is to provide information on the programs and basic research efforts supported by ARO in FY12, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Mechanical Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY12.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mechanical Sciences Division supports research to advance the Army and Nation's knowledge and understanding of the fundamental properties, principles, and processes involved in fluid flow, solid mechanics, chemical reacting flows, explosives and propellants, and thedynamics of complex systems of relevance to the Army and the DoD. More specifically, the Division supports basic research to uncover the relationships to: (i) contribute to and exploit recent developments in kinetics and reaction modeling, spray development and burning, (ii) gain an understanding of extraction and conversion of stored chemical energy, (iii) develop a fundamental understanding that spans from a material's configuration to a systems response to create revolutionary improvements through significant expansion of the design landscape used to optimizing systems, (iv) advance knowledge and understanding governing the influence of inertial, thermal, electrical, magnetic, impact, damping, and aerodynamic forces on the dynamic response of complex systems as well as improving the inherent feature set of the components (*i.e.*, mechanisms and sensing) that comprise them, (v) provide the basis for novel systems that are able to adapt to their environment for optimal performance or new functionality, and (vi) develop a fundamental understanding of the fluid dynamics underlying Army systems to enable accurate prediction methodologies and significant performance improvement, especially with regard to unsteady separation and stall and vortex dominated flows. Fundamental investigations in the mechanical sciences research program are focused in the areas of solid mechanics; complex dynamics and systems; propulsion and energetics; and fluid dynamics. Special research areas have been continued in the Army-relevant areas of rotorcraft technology, projectile/missile aerodynamics, gun propulsion, diesel propulsion, energetic material hazards, mechanics of solids, impact and penetration, smart structures, and structural dynamics.

2. Potential Applications. In addition to advancing worldwide knowledge and understanding of properties and processes in mechanical sciences, research managed by the Mechanical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO research in the mechanical sciences could provide understanding that leads to insensitive munitions, tailored yield munitions, enhanced soldier and system protection, novel robotic, propulsion, and energy harvesting systems, and novel flow control systems and enhanced rotorcraft lift systems. In addition, mechanical sciences research may ultimately improve Soldier mobility and effectiveness by enabling the implementation of renewable fuel sources and a new understanding of energetic materials with improved methods for ignition, detonation, and control.

3. Coordination with Other Divisions and Agencies. The primary laboratory interactions of this Division are with the ARL Weapons and Materials Research Directorate (ARL-WMRD), ARL Vehicle Technology Directorate (ARL-VTD), ARL Sensors and Electron Devices Directorate (ARL-SEDD), the Joint IED Defeat Organization (JIEDDO), the U.S. Army Corps of Engineers (USACE), and various Army Research Development and Engineering Centers (RDECs), including the Aviation and Missile RDEC (AMRDEC), Natick Soldier

RDEC (NSRDEC), and the Tank-Automotive RDEC (TARDEC). The Division also facilitates the development of joint workshops and projects with Program Executive Office (PEO) Soldier and the Army Medical Research and Materiel Command (MRMC). In addition, the Division often jointly manages research efforts with ARO programs in the ARO Chemical Sciences, Materials Science, Mathematical Sciences, Computing Sciences, and Life Sciences Divisions, through co-funded efforts, projects, workshops, and committees. Strong coordination is also maintained with other Government agencies, such as the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the National Science Foundation (NSF), the National Aeronautics and Space Administration (NASA), the National Institute of Standards and Technology (NIST), and the Department of Energy (DoE). Several international efforts are also coordinated through the International Science and Technology office in London (ITC-London) and the Pacific (ITC-Pacific).

B. Program Areas

To meet the long-term program goals described in the previous section, the Mechanical Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of projects. In FY12, the Division managed research efforts within these four Program Areas: (i) Solid Mechanics, (ii) Complex Dynamics and Systems, (iii) Propulsion and Energetics, and (iv) Fluid Dynamics. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Solid Mechanics. The goal of the Solid Mechanics Program Area is to develop physically-based mechanics tools (theory, experiments, computation) for the quantitative prediction, control, and optimization of Army systems subjected to extreme battlefield environments. Army systems are frequently limited by material strength and failure. Solid mechanics research plays a crucial role in the prediction of strength, damage, and failure of Army materiel systems, structures and injuries of personnel under extreme loading conditions such as impact or blast as well as normal operating conditions. Research in computational and experimental solid mechanics forms the foundation of optimization tools to enhance performance while minimizing weight and volume, and its theories provide a strong link between the underlying physics of solids and the design of actual systems resulting in reduced development cost by minimizing the need for expensive system and field testing and it leads to novel ideas and concepts for revolutionary capabilities.

This Program Area is divided into two research Thrusts: (i) Multiscale Mechanics of Heterogeneous Solids, and (ii) Multiscale Mechanics of Biological Tissues. The goal of research in the Multiscale Mechanics of Heterogeneous Solids Thrust is to extend the design envelope of current and future Army structures for predictive continuum damage and cohesive models with a physical basis that is supported by computational modeling and experiments at the appropriate length and time scales. The objective of research in the Multiscale Mechanics of Biological Tissues Thrust is to understand how high rate loading of different durations and amplitudes may lead to cascading events starting at the cellular level that cause functional loss and impairment of human tissues and organs.

Research in this Program Area is focused on long-term, high risk goals that strive to develop the underpinnings for revolutionary advances in our military systems. It is developing the methods needed to take advantage of recent advances in new materials technology, including nanotubes, nanocrystaline solids, and bio-inspired and hierarchical polymeric- and nano- composites. As a result of the long-term vision of the program, some future applications are not yet imagined while others will lead to the creation of ultra-lightweight, high strength materials for applications such as lightweight armor, unmanned aerial vehicles (UAVs), unmanned ground vehicles (UGVs), and munitions.

2. Complex Dynamics and Systems. The goal of the Complex Dynamics and Systems Program Area is to exploit trans-disciplinary nonlinear science while vigorously pursuing new mathematical frameworks for the intelligent synthesis and exploitation of multi-dimensional flows in high-dimensional dynamical systems. This Program Area encompasses a significant shift away from traditional investment areas in legacy dynamics programs at ARO in order to capitalize on remarkable advances in the scientific understanding of *dynamical systems theory* (the study of the temporal evolution of abstract vector flows that are not necessarily mechanical in nature) and *non-equilibrium physics*. The programmatic strategy is to foster mathematically sophisticated, interdisciplinary, and hypothesis-driven research to elucidate classical physics and analytical methods pertinent to the foundations of a broad spectrum of ARL Major Laboratory Programs including: mobility, power and energy, sensors, lethality, and trans-disciplinary network science.

This Program Area is divided into two research Thrusts: (i) Mathematics and Control of Complex Dynamical Systems and (ii) Force Generation. The thrusts are comprised of Army-relevant problems in both low- and high-dimensional dynamical systems, and the exploitation of nonlinear and stochastic dynamic interactions at the nanoscale. New efforts in geometric biomechanics, neuromechanics, and granular dynamics have been initiated in respective thrust areas in low and high dimensional dynamical systems to inspire deep intuition for decentralized control, terramechanical interaction physics, and mathematical formalisms to enable solutions to agile robotic mobility problems. When considering the ubiquity of coupled oscillators and interdependent dynamic systems with underlying graph structure in a wide range of Army-relevant research programs from neuroscience to NEMS/MEMS frequency sources to networks, there is a resounding need for the establishment of a high-dimensional dynamical systems theory for which coherent structures, new understanding of attractors and bifurcations in high-dimensional phase space, state-estimation and control, heavy-tail distributions, and multiscale phenomena can be understood with an emphasis on implications for engineering design. Complicated multiphysics interactions as well as the inescapable manifestation of noise and nonlinearity at the nanoscale demands a complete understanding to push the boundaries of our ability to analyze and engineer infinitesimal systems. Accordingly, the Complex Dynamics and Systems program balances theoretical and experimental investigations and emphasizes interdisciplinary approaches in order to lay the foundations for the analysis of dynamic phenomena extensible to a wide range of more focused Army research programs.

3. Propulsion and Energetics. The goal of this Program Area is to explore and exploit recent developments in kinetics and reaction modeling, spray development and burning, and our understanding of extraction and conversion of stored chemical energy to ultimately enable higher performance propulsion systems, improved combustion models for engine design, and higher energy density materials, insensitive materials, and tailored energy release rate. Research in propulsion and energetics supports the Army's need for higher performance propulsion systems. These systems must also provide reduced logistics burden (lower fuel/propellant usage) and longer life than today's systems. Fundamental to this area is the extraction of stored chemical energy and the conversion of that energy into useful work for vehicle and projectile propulsion. In view of the high temperature and pressure environments encountered in these combustion systems, it is important to advance the current understanding of fundamental processes for the development of predictive models as well as to advance the ability to make accurate, detailed measurements for the understanding of the dominant physical processes and the validation of those models. Thus, research in this area is characterized by a focus on high pressure, high temperature combustion processes, in both gas and condensed phases, and on the peculiarities of combustion behavior in systems of Army interest. To accomplish these goals, the Propulsion and Energetics Program Area has two research Thrusts: (i) Hydrocarbon Combustion, and (ii) Energetics. The goal of the Hydrocarbon Combustion Thrust is to develop kinetic models for heavy hydrocarbon fuels, novel kinetics model reduction methods, surrogate fuel development, and research into sprays and flames, especially ignition in high pressure low temperature environments. In addition the Energetics Thrust focuses on novel material performance via materials design and development and materials characterization, and investigations (theoretical, modeling and experimental) into understanding material sensitivity (thermal and mechanical).

4. Fluid Dynamics. The vast majority of the Army weapon systems involve airborne vehicles and missile systems that are totally immersed in fluids. In turn, the performance of these weapon systems is greatly affected by the resultant forces imparted on them by the surrounding fluid. Consequently, developing highly accurate, stable, agile, and long-endurance weapon systems dictates the need for fluid dynamics research in the areas of interest to both rotorcraft vehicles and tactical missiles. In fact, the battlefield capability and tactical flight operations envisioned for the highly mobile Army of the twenty-first century can only be accomplished through scientific breakthroughs in the field of aerodynamics. Improving performances in every aspects of rotorcraft vehicle performance requires intensive fluid dynamic research in areas, such as, unsteady boundary-layer separation on the suction side of rotorcraft blades, unsteady rotor aerodynamic loads, wakes and interference aerodynamics, and computational fluid mechanics.

Ongoing research topics within this Program Area include the experimental and numerical determination of the flowfield over airfoils undergoing unsteady separation with subsequent dynamic stall, the development of micro-active flow control techniques for rotor download alleviation and dynamic stall control, and the development of advanced rotor free-wake methods to improve the predictive capability for helicopter performance, vibration, and noise. To ensure the accuracy and range of unguided gun-launched projectiles and the maneuverability and lethality of guided missiles and rockets, a thorough knowledge of the forces and moments acting during both launch and free flight is required. These objectives dictate research on shock boundary-layer interactions, compressible turbulence modeling, aft body-plume interactions, vortex shedding at high angle of attack, transonic body flows, and aerodynamic interference effects between various missile components. Examples of current studies in this subfield are the experimental study of aft body-plume-induced separation, and the use of direct numerical simulation, laser-Doppler velocimetry (LDV), and PIV techniques to investigate axisymmetric supersonic power-on/power-off base flows. Research initiatives on the aerodynamics of small unmanned aerial vehicles, both rotary wing and flapping wing, continue. Results indicate that the physics of vortex-dominated flight at low Reynolds number is quite different than that encountered for familiar high Reynolds numbers.

C. Research Investment

The total funds managed by the ARO Mechanical Sciences Division for FY12 were $19.2 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY12 ARO Core (BH57) program funding allotment for this Division was $6.2 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $3.6 million to projects managed by the Division. The Division also managed $6.5 million of Defense Advanced Research Projects Agency (DARPA) programs, and $1.0 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $0.1 million for contracts. Finally, $1.8 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY12 (*i.e.*,"new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research projects. Research projects are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts.

The following subsections summarize projects awarded in FY12 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY12, the Division awarded 30 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies of shock boundary-layer interactions, compressible turbulence modeling, high pressure, high temperature combustion processes, high rate loading of different durations and amplitudes and the exploitation of nonlinear and stochastic dynamic interactions at the nanoscale. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Erik Bollt, Clarkson University; *On Hierarchical Scales, Information Reduction Efficiency and Inference in Complex Systems*
- Professor Robert Candler, University of California - Los Angeles; *Energy Dissipation in Nanomechanical Resonators*
- Professor Ralph Chamberlin, Arizona State University; *Nonlinear Corrections to Temperature in Computer Simulations of Complex Systems*
- Professor Ioannis Chasiotis, University of Illinois - Urbana; *Mechanical and Ferroelectric Response of Highly Textured PZT Films for Low Power MEMS*
- Professor Aditi Chattopadhyay, Arizona State University; *A Stochastic Approach to Structural Health Monitoring of Advanced Composites*
- Professor James Crutchfield, University of California - Davis; *Intrinsic Information Processing and Energy Dissipation in Stochastic Input-Output Dynamical Systems*
- Professor Edward Dreizin, New Jersey Institute of Technology; *Electro-Static Discharge Sensitivity of Reactive Powders and Its Mitigation*
- Professor Mark Dykman, Michigan State University; *Studying Electron Transport in Nanowires Using Fluctuations of Nano-mechanical Vibrations*
- Professor John Eaton, Stanford University; *Turbulent Dispersion of Film Coolant and Hot Streaks in a Turbine Vane Cascade*
- Professor Somnath Ghosh, Johns Hopkins University; *Multi-Scale Analysis of Deformation and Failure in Polycrystalline Titanium Alloys Under High Strain Rates*
- Professor Mica Grujicic, Clemson University; *Concept Validation and Optimzation in Blast Mitigation*

- Professor Garth Hobson, Naval Postgraduate School; *Understanding and Mitigating Vortex-Dominated, Tip-Leakage and End-Wall Losses in a Transonic Splittered Rotor Stage.*
- Professor Anette Hosoi, Massachusetts Institute of Technology; *Developing Novel Frameworks for Many-Body Ensembles*
- Professor Yiguang Ju, Princeton University; *Multiscale Adaptive Large Eddy Simulation and Direct Numerical Simulation of Turbulent-Chemistry Interaction of Stratified Charge Ignition of JP-8 and Diesel Surrogate Fuels*
- Professor Aaron Katz, Utah State University; *Integration of Strand-based CFD Solution Procedures for Aerodynamics Simulations*
- Professor Kevin Lyons, North Carolina State University; *Studies of Hydrocarbon Flame Phenomena*
- Professor David Miller, Drexel University; *Autoignition Chemistry of Surrogate Fuel Components*
- Professor Michael McAlpine, Princeton University; *Buckled Piezoelectric Nanoribbons: Morphology, Nanomechanics, and Flexoelectricity*
- Professor Igor Mezic, University of California - Santa Barbara; *Dynamics of System and Applications to Net Zero Energy Facilities*
- Professor Hiroaki Nishikawa, National Institute of Aerospace Associates; *Fluid Dynamics: Intrinsically Efficient and Accurate Viscous Simulations via Hyperbolic Navier-Stokes Systems*
- Professor Antonio Palacios, San Diego State University; *Exploiting Symmetry to Study Coherent Self-Sustaining Dynamics in High Dimensional Nonlinear Systems*
- Professor Michelle Pantoya, Texas Technical University; *Understanding Multiphase Combustion of Metalized Nanocomposite Energetic Materials*
- Professor Terence Parker, Colorado School of Mines; *Optical Development and Phenomenological Studies of Spray Combustion*
- Professor Prashant Purohit, University of Pennsylvania; *Flexoelectricity in PZT Nanoribbons and Biomembranes*
- Professor David Rothamer, University of Wisconsin - Madison; *Fundamental Investigation of Jet Fuel Spray and Ignition Process in an Optically Accessible Piston Engine*
- Professor Mohammad Samimy, Ohio State University; *Understanding and Control of Basic Flow Elements Using NS-DBD Plasma Actuators*
- Professor Kalyanasundaram Seshadri, University of California - San Diego; *Study of Combustion of High Molecular Weight Hydrocarbon Fuels and JP-8 at Moderate Pressures*
- Professor Hareesh Tippur, Auburn University; *Development and Characterization of Novel Lightweight Transparent Materials*
- Professor Donald Thompson, University of Missouri - Columbia; *Theoretical Studies of Small-System Thermodynamics in Energetic Materials*
- Professor Mohammed Zikry, North Carolina State University; *Microstructurally Based Prediction of High Strain Failure Modes in Crystalline Solids*

2. Short Term Innovative Research (STIR) Program. In FY12, the Division awarded 17 new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to develop computational framework for the modeling and simulation of microscale fluid flows, discover multifunctional lightweight composites with tailorable interfaces that can provide enhanced dynamic strength, and develop new nonlinear models of molecular motor dynamics. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Subhashini Chitta, Flow Analysis Incorporated; *Analysis of Vorticity Confinement for Boundary Layer Dynamics*
- Professor Datta Gaitonde, The Ohio State University; *A Nanosecond Pulsed DBD Actuator model for LES of Stall Control*
- Professor Daniel Gauthier, Duke University; *Developing an Experimental Platform for Fundamental Research in Network Dynamics*

- Professor Henry Hess, Columbia University; *Determining Attachment Geometry and Interactions of Mechanically Coupled Molecular Motors in One-dimensional Arrays*
- Professor Timothy Kiemel, University of Maryland - College Park; *Closing the Loop: Integrating Body, Muscle and Environment with Locomotion Central Pattern Generators*
- Professor Ying-Cheng Lai, Arizona State University; *Multistability and Chaos in a Driven Nanowire System*
- Professor Alex Povitsky, University of Akron; *Vorticity Confinement Technique for Drag Prediction and Vortex Interaction*
- Professor Laxminarayan Raja, University of Texas at Austin; *Examining High-authority Aerodynamic Flow Control at Atmospheric Pressures*
- Professor Khalid Salaita, Emory University; *Molecular Force Meter to Image Force Propagation in Cells*
- Professor Henry Sodano, University of Florida; *Tailored Interfaces For High Strength Composites Across Strain Rates*
- Professor Anthony Stentz, Carnegie Mellon University; *Dynamic Mobility via Cellular Decompositions of Coordination Spaces*
- Professor Hongxing Tang, Yale University; *Control of the Dissipation Dynamics of Nanomechanical Resonator in Viscous Media*
- Professor Hongxing Tang, Yale University; *Synchronization of Two Remote Nanomechanical Oscillators*
- Professor Brian Thurow, Auburn University; *3-D Imaging of a Turbulent Boundary Layer with Adverse Pressure Gradient using a Plenoptic Camera*
- Professor Eric Tytell, Johns Hopkins University; *Cyclical Dynamics and Control of a Neuromechanical System*
- Professor Prakash Vedula, University of Oklahoma; *Novel Approaches for Computational Modeling of Microflows Based on Fundamental Kinetic Theory*
- Professor Youqi Wang, Kansas State University; *Ballistic Strength of Multi-layer Fabric System With Through-the-Thickness Reinforcement*

3. Young Investigator Program (YIP). In FY12, the Division awarded three new YIP projects. These grants are driving fundamental research, such as studies to investigate the effects of oscillating freestream Mach number on dynamic stall, quantification of empirical measurements from nonlinear oscillators, and development of advance state estimation techniques for complex systems. The following PIs and corresponding organizations were recipients of the new-start YIP awards.

- Professor James Gregory, Ohio State University; *Unsteady Aerodynamics: Time-Varying Compressible Dynamic Stall Mechanisms Due to Freestream Mach Oscillations*
- Professor Shai Revzen, University of Michigan; *Data Driven Floquet Analysis: Nonlinear Oscillators in Locomotion*
- Professor Jonathan Rogers, Texas A&M University; *State Estimation of Complex Dynamical Systems Using Belief Function Theory*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY12 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Parallel Computational Fluid Dynamics 2012 Conference*; Atlanta, GA; 21-25 May 2012
- *Locomotion Systems Science Workshop*; Arlington, VA; 29-31 May 2012
- *2012 Energetic Materials Gordon Research Conference;* West Dover, VT; 17-22 June 2012
- *2012 Princeton-CEFRC Summer Conference*; Princeton, NJ; 24-29 June 2012
- *Ninth International Symposium on Special Topics in Chemical Propulsion: Advancements in Energetic Materials and Chemical Propulsion*; Quebec City, Canada; 9-13 July 2012
- *Workshop on the Computation of Dynamic Stall at High Reynolds Number*; College Station, TX; 11 August 2012

- *2012 International Conference on Theory and Applications in Non Linear Dynamics*; Seattle, WA; 26-30 August 2012
- *22nd International Workshop on Computational Mechanics of Materials*; Baltimore, MD; 24-26 September 2012

5. Special Programs. In FY12, ARO Core Research Program funds provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded six new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

C. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Ultrafast Laser Interaction Processes for LIBS and Other Sensing Technologies. This MURI began in FY06 and was awarded to a team led by Professor Martin Richardson at the University of Central Florida. The objective of this research is to develop a theoretical understanding of femtosecond laser/materials interaction that is expressed in combined physical and chemical models, rigorously grounded by experimental characterization and detailed physical and chemical observations. These models will then be extended to the irradiation of complex sample matrices characteristic of chem/bio threat scenarios, and the use of advanced laser beam modalities, including femtosecond laser self-channeling (FLSC), with an ultimate goal to develop laser induced breakdown spectroscopy (LIBS) stand-off technologies at the kilometer range. This understanding is expressed in combined physical and chemical models, rigorously grounded by experimental characterization and detailed physical and chemical observations relevant to LIBS and other spectroscopic sensing techniques. The techniques include fluorescence and Raman scattering and resonance enhanced multi-photon ionization. The models will then be extended to irradiation of complex material samples characteristic of chemical and biological threat scenarios, and energetic materials such as those found in improvised explosive devices (IEDs).

2. Spray and Combustion of Gelled Hypergolic Rocket Propellants. Two MURIs in this topic area began in FY08. One team is led by Professor Stefan Thynell at the Pennsylvania State University, and the second team is led by Professor Stephen Heister at Purdue University. The objective of these MURIs is to understand the processes and mechanisms that control droplet formation, droplet collision and mixing, ignition, and energy release in gelled hypergolic propellants. The projects involve research in the areas of ballistic imaging, aerosol shock tubes, and ultra-fast laser diagnostics to capture reaction characteristics, and focus on fluid and gas dynamics, chemistry, chemical kinetics and reaction mechanisms, computational fluid dynamics with reactive chemistry, heat transfer, high-performance computing modeling and simulation, and advanced experimental diagnostic methods. The ultimate goal of the efforts is to gain understanding allowing for the science based design of gelled hypergolic propulsion injector and combustor systems. The pursuit of this research may also yield unexpected paths leading to the discovery of new concepts for hypergolic propulsion. The team led by Professor Thynell has developed an integrated research program comprising material science, chemistry, physics, and engineering to address various fundamental issues critical to the development of gelled hypergolic propellant (GHP) spray and combustion technologies for future rocket and missile propulsion systems. New techniques will be developed that will resolve the entire range of length and time scales (from atomistic to device levels). Emphasis will be placed on the microscale and macroscale processes that dictate the propellant interfacial dynamics and chemical initiation mechanisms, as well as the propellant atomization, mixing, and flame development. The team led by Professor Heister is investigating the rheological characterization of gelled propellants, non-Newtonian flow physics of gelled propellants, and the combustion physics of gelled hypergols.

D. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY12.

E. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY12, the Division managed one new-start STTR Phase I contract, in addition to active projects continuing from prior years. The new-start contract aims to bridge fundamental discoveries with potential applications, including the development of strain-modulated nanometer thin diamond structures with markedly enhanced electron mobility and biocompatibility.

F. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY12, the Division managed three new REP awards. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

G. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY12.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY12, the Mechanical Sciences Division managed six new DURIP projects, totaling $0.93 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of burning behavior of heavy fuels with suspended energetic nanoparticles for ignition and burning enhancement, effects of compressibility and freestream Mach oscillations on the three-dimensional development of rotorcraft dynamic stall, and electrical and thermal characterization of nanoscale piezoelectric structures.

I. DARPA Reactive Material Structures Program

The Mechanical Sciences Division is serving as the agent for the DARPA-sponsored Reactive Material Structures (RMS) program. This program was initiated in FY08 with an objective to develop and demonstrate materials/material systems that can serve as reactive high strength structural materials (*i.e.*, be able to withstand high stresses and can also be controllably stimulated to produce substantial blast energy). Research is investigating innovative approaches that enable revolutionary advances in science, technology, and materials system performance. These approaches touch on several Mechanical Sciences Division research areas, including: rapid fracture and pulverization of the material, dispersion of the particles, and material ignition and burning, all while achieving strength, density and energy content metrics. The vision of the RMS program is to be able to replace the inert structural materials currently used in munition cases with reactive material structures that provide both structural integrity and energy within the same material system along with the ability to rapidly release the energy upon demand.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Mechanical Sciences Division.

A. Nonlinear Multiscale Modeling of 3D Woven Fiber Composites Under Ballistic Loading

Professor Suvranu De, Rensselaer Polytechnic Institute, Single Investigator Award

The objective of this project is to develop a multiscale computational method for the nonlinear damage and failure analysis of 3D orthogonal woven fiber composites (3D OWC) under ballistic loading. The nonlinear damage and failure analysis that employ experimentally obtained physically based parameters can provide reliable estimate of the performance of the armors leading to the design of improved armor.

An advanced *meso-scale* partitioned damage model has been developed for 3D OWC that exploit their unique geometrical architecture and damage modes to study the characteristics of high speed projectile impact events. This method divides the sources of constitutive nonlinearities into meso-scale regions of fiber and the remaining bulk matrix. This division allows implementing a state-of-the-art high strain rate and large deformation polymer model to capture rate effects from the matrix. In addition, although the pre-failure behavior of the fiber is treated as linear elastic, nonlinearities appeared through strain rate dependent failure initiation as well as progressive damage modes. This physically motivated meso-scale division greatly reduced the number of arbitrary parameters and yielded predictions which were in very good agreement with existing ballistic penetration experiments.

In FY12, the investigators found that both the through thickness or Z-fibers and bulk matrix rate effects can improve ballistic resistance depending on the momentum of the projectile and dimension of the plate (see FIGURE 1). However, in the penetration range, competing nonlinearities tended to nullify each other producing both localized effects and potential crack nucleation sites through wave propagation. The effect of Z–fiber on damage distribution was not straightforward and analysis of both fiber and matrix damage modes has explained many of the unique damage features of 3D OWC.

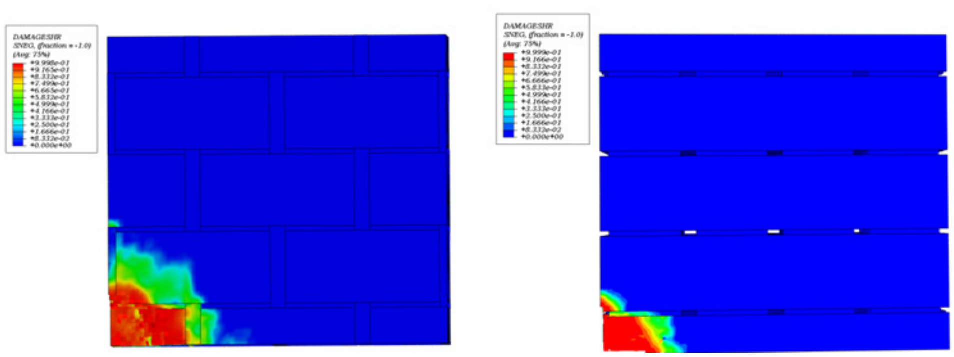

FIGURE 1

Through-thickness or Z-fibers and bulk matrix effects. Strike face matrix shear damage for 3D OWC (right) and layered composite (left) at t=4ms, which shows that the Z-fibers are unable to arrest matrix shear damage. Thus, in spite of the fact that actual terminal damage is highly localized the matrix damage at Z-fiber sites has potential for void growth and interlaminar cracks thereby reducing the ability of Z-fibers to act effectively during future impact events, which is interesting because the purported benefits of Z-fibers over stitched composites are that it does not physically damage the composite structure. However, the simulation revealed that Z-fibers can still cause damage to the underlying structure indirectly during dynamic loading because of the matrix damage. This conclusion was experimentally observed by Pankow *et al.* 2011 during shock loading of these panels. This also indicates that Z-fibers can easily de-bond from other fibers through shear failure at the interface. This is also a commonly observed mode of failure when 3D OWC are loaded in tension. *[Callus et al. 1999]*

B. Phase-field Modeling and Computation of Crack Propagation and Fracture

Professors C. Landis and T. Hughes, The University of Texas - Austin, Single Investigator Award

The goal of this research is to develop computational modeling methods that are able to describe the propagation and interaction of multiple cracks. To this end the investigators have applied a phase-field description for fracture. The phase-field methodology has emerged as a powerful tool for modeling the evolution of microstructures and the interactions of defects in a wide range of materials and physical processes. Phase-field methods can be implemented to simulate large-scale evolution of material microstructure and defect motion without the need to explicitly track interfaces or defects.

One of the strengths of this modeling approach lies in the fact that there are no extra rules required within the theory that dictate when a crack should nucleate, grow, change direction, or split into multiple cracks. Cracks and their growth emerge as solutions to the governing partial differential equations of the model. This allows for the development of numerical methods where the research is focused on uncovering the best procedures for solving the differential equations, which have small length-scale boundary layers about the cracks, as opposed to developing ad hoc rules to track crack nucleation and evolution. In particular, a unique and striking feature of the approach is that all calculations are performed entirely on the initial, undeformed configuration. There is no need to disconnect or eliminate elements, or introduce additional discontinuous basis functions, as is commonly done in existing computational fracture mechanics techniques.

This approach results in enormous simplification of the numerical implementation, and a simple and direct pathway from two-dimensional to three-dimensional applications, which for existing methodology usually proves to be at least cumbersome, if not prohibitively complex. Furthermore, the approach is general in that higher-order finite elements and recently developed isogeometric analysis procedures can be utilized just as easily as low-order elements, for which most all existing methods are restricted to. This creates the potential, for the first time, of higher-order accuracy in fracture mechanics numerical simulations (see FIGURE 2). The phenomena of crack nucleation, crack branching, and fragment formation are all captured naturally in both two and three-dimensional simulations. The red-blue colors in essence represent the opposite sides of an iso-surface in the phase-field. The smaller "balls" of red and blue are locations where initial damage was placed randomly within the sample and the red-blue colors indicate crack surfaces.

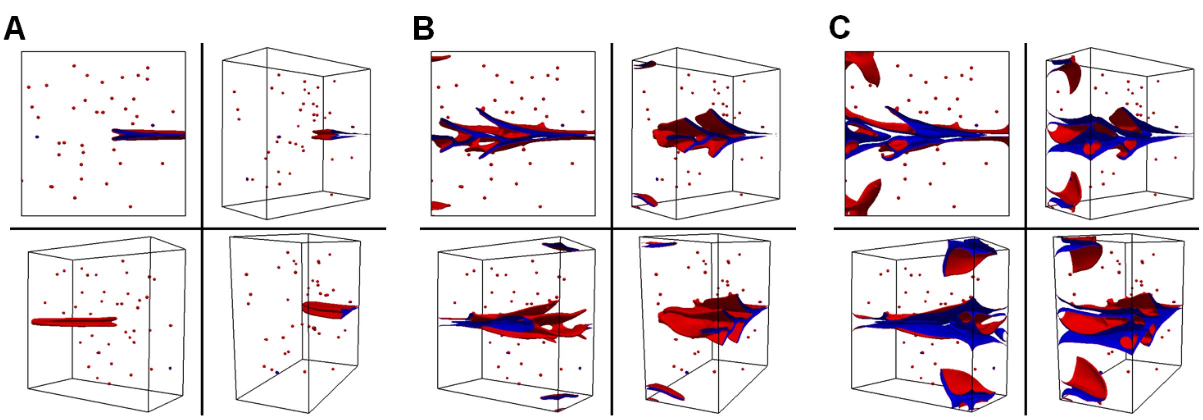

FIGURE 2

Three-dimensional example of application of phase-field fracture modeling to dynamic crack initiation and growth in a defected material. The panels illustrate four viewpoints of the same box (**A**) nucleation, growth and the onset of branching of an initial crack, (**B**) multiple branching of the initial crack and the nucleation of secondary cracks, and (**C**) evolution of the crack fronts and in particular the turning and twisting of 3D crack fronts. It is worth noting the very complex topology of the initial crack with one side of the crack being branched and the other side relatively smooth with a complex transition in the topology towards the middle.

C. Microstructure-Sensitive Fatigue Design of Notched Components

Professor Gbadebo Owolabi, Howard University, HBCU-MI and REP Awards

The overall objective of this research is to develop and implement robust simulation-based strategies for microstructure-sensitive notch root analysis and fatigue design that account for complex interactions between the material's microstructure and the notch-root stress and strain gradients for safety-critical components such as turbine disks and blades. The approaches to be developed in this work will more closely couple the selection or design of the material microstructure with the notch root fatigue resistance, thereby enabling true 'microstructure-sensitive' fatigue design. Recently, a new probabilistic framework to analyze the fatigue potency of notched components as a function of a material's microstructure, notch size, and applied strain, ε(t) amplitudes has been developed. This probabilistic framework employs computational micromechanics to conduct multiscale modeling of actual microstructures with appropriate microstructure length scale dependence as a function of geometry, notch size, and notch root acuity (*i.e.*, stress gradient and peak stress).

For each loading condition, 40 different realizations of grains within the notch root region were implemented with randomly assigned orientation distribution to obtain an initially isotropic effective medium while gathering information regarding variability among instantiations. To reduce computational time, the notched specimen geometries were decomposed into three regions: an outermost region far from the notch root, where isotropic linear elasticity is used, a transition region employing macroscopic J2 cyclic plasticity theory along with isotropic linear elasticity to minimize effects of discontinuity between the exterior field and the notch root domain which employs 3D crystal plasticity simulations, each grain having anisotropic (cubic) elastic behavior. The domain decomposition for a double edge-notched plate with notch root radius of 1000 μm is shown in FIGURE 3. The actual dimensions of the crystal plasticity region were chosen in a way that ensures that the distribution of micro slip at the notch region is fully captured. Notch root plasticity is small scale in such cases. The simulation results were used to identify and classify important microstructural features. Mathematically consistent and physically meaningful methods were developed to incorporate the effects of these features on localized plastic deformation and fatigue performance at both microstructure and geometric notch root scales.

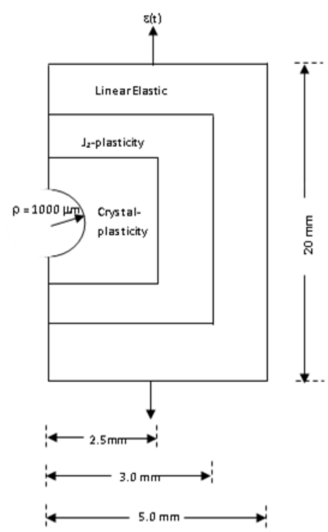

FIGURE 3

Domain decomposition of half of a double edge-notched plate with semicircular edge notches. The schematic shows the domain decomposition for a double edge-notched plate with notch root radius of 1000 μm.

Statistical information regarding the distributions of stress/strain gradients and fatigue indicator parameters obtained from simulation results were also used in the development of a new microstructure-dependent fatigue notch factor and the associated sensitivity index. Numerical results show that the local driving force for fatigue crack formation can vary significantly between different microstructures (see FIGURE 4). The developed probabilistic framework will assist in the design of notched structural components for low probability of failure and can potentially be used to support design projections for microstructures that have not yet been processed. As part of the ongoing work for this project, the probabilistic framework which has been implemented for a single-phase oxygen-free high conductivity (OFHC) copper material has been further extended to multiphase materials such as nickel-base super alloys with non-metallic inclusions in order to improve the prediction of high cycle fatigue of safety-critical components such as turbine engine disks and blades employing these materials. This approach can be used in conjunction with limited experiments to help validate a new material or manufacturing technique to create a variant form of an existing material.

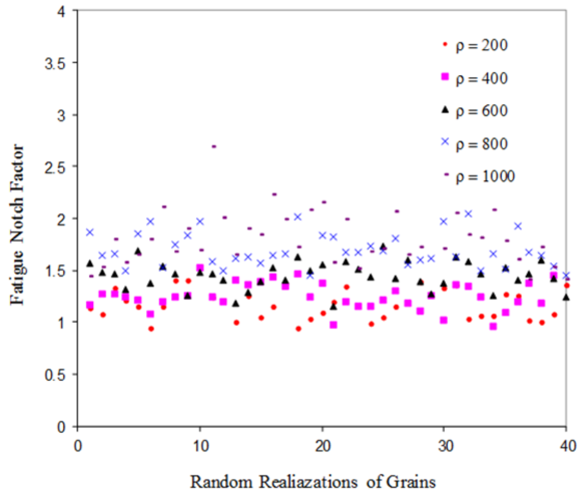

FIGURE 4

Distribution of microstructure-dependent fatigue notch factor. The data plot displays the distribution of microstructure-dependent fatigue notch factor for 40 random realizations of grains at the notch root with notch root radii ρ ranging from 200 μm to 1000 μm.

D. Dynamics of Systems of Systems: An Operator Theoretic Approach
Professor Igor Mezic, University of California - Santa Barbara (UCSB), Single Investigator Award

The objective of this project is to develop mathematical tools to analyze the dynamics of large-scale interconnected system of systems. These tools are a combination of operator-theoretic, geometric dynamical systems methods and graph-theoretic methods. More specifically, the project will extend analysis methods based on Koopman operator properties to include stable and unstable motions as well as developing methods in Generalized Laplace Analysis for a large class of nonlinear interconnected dynamical systems. The investigator will couple these operator-theoretic methods to graph theoretic analysis that will rely on spectral analysis of the interconnection graph associated with a dynamical system. The coupling is enabled by the fact that both approaches are spectral. The new theory will be able to treat discrete and continuous, stochastic and deterministic, and hybrid systems within a single framework. Experimental validation and real-world effectiveness is also being pursued. This aspect involves developing effective algorithms for energy efficiency in complex dynamical systems and testing them on an existing testbed site.

Several research contributions were made in FY12. First, a novel algorithm for computing global isochrons of high-dimensional dynamics was developed. The concept of isochrons is crucial for the analysis of asymptotically periodic systems. Generally, isochrons are sets of points that partition the basin of attraction of a limit cycle according to the asymptotic behavior of the trajectories. However, computing global isochrons in the whole basin of attraction is difficult and existing methods are inefficient in high-dimensional spaces. In this context, researchers presented a novel algorithm is based on the notion of Fourier time averages evaluated along trajectories. Such Fourier averages were shown to produce eigenfunctions of the Koopman semigroup associated with the system. As a result, isochrons are obtained as level sets of those eigenfunctions. The change of paradigm from a geometric one to operator-theoretic one enabled a breakthrough extension of the theory to high-dimensional spaces. The method was validated by several examples of increasing complexity, including the 4-dimensional Hodgkin-Huxley model (see FIGURE 5). In addition, the framework naturally extends to the study of quasiperiodic systems and motivates the definition of generalized isochrons of the torus. In a similar fashion, investigators extended the concept of linearization around stable (unstable) equilibria or periodic orbits to the whole basin of attraction for both discrete diffeomorphisms and flows. Progress in this regard was also enabled by the same paradigm change to an operator-theoretic point of view.

Theoretical progress has also been subject to experimental testing. Professor Mezic and his students applied operator-theoretic techniques to the problem of simplifying the description of complex systems. In particular, as an example of a complex system, researchers examined the energy dynamics of a large building on the UCSB campus. Despite the growing sophistication of building modeling tools, errors can arise from approximations made in building model creation. Researchers addressed the issue of model zoning. That is, how the volume of a building is divided into regions where properties are assumed to be uniform. A systematic approach to creating zoning approximations was introduced to investigate the effect of zoning on simulation accuracy. Using the Koopman operator, temperature history of rooms produced by a building simulation can be decomposed into Koopman modes. These modes identify dynamically significant behavior which will form a basis for the creation of zoning approximations.

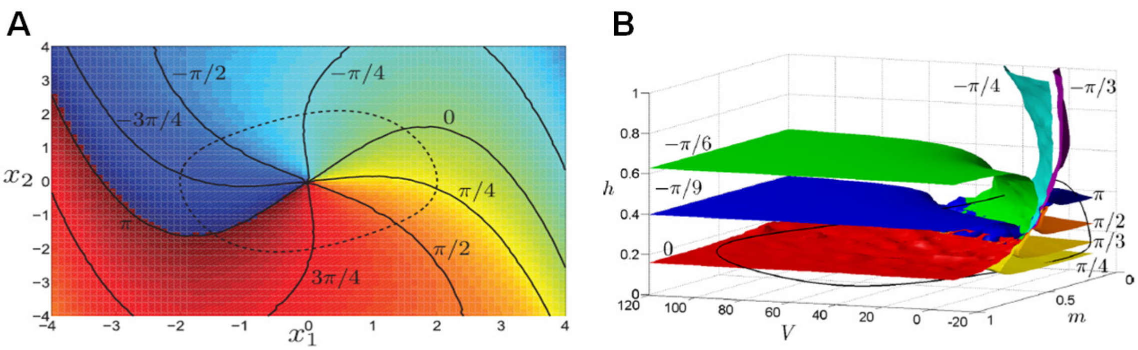

FIGURE 5

Spectral approach to isochron determination. (**A**) Isochrons (solid black lines) are shown to be the level sets of Fourier averages of a typical nonlinear oscillator. Previous methods for calculating isochrones could not extend to high dimensions while the operator theoretic methods have been shown to extend readily (**B**) for a Hodgkin-Huxley model which is central to dynamics in neuroscience.

In addition, uncertainty in the dynamics of complex systems was explored. Specifically, whole-building energy models take information about the building structure, multidimensional loading, and disturbances and predict long-time energy performance. In FY12, the researchers investigated how parametric uncertainty influenced uncertainty via a control-oriented frequency-based robustness assessment as well as a study of how uncertainty influences the network structure of a building by investigating the spectral gap of its graph Laplacian.

E. Understanding Locomotion and Interaction Physics in Granular Media

Professor Daniel Goldman, Georgia Institute of Technology, Single Investigator Award

The goal of this research project is to develop new understanding of the physics of intrusion in dry and wet granular states through biological experiments and multi-body models. Robotic devices that can move effectively on and within complex ground like sand and soil have promising applications in military tasks such as reconnaissance and rescue. Many organisms developed diverse locomotion methods and extraordinary locomotion capabilities on and within complex grounds to escape predators, regulate temperature, and hunt for prey. Discovery of principles of biological locomotion had aided the design of robots with excellent mobility on the surface of hard, level ground. Central to this research project is the hypothesis that creation of devices with capabilities to move on and within complex ground also requires discovery of interaction principles used by organisms that are masters of these environments. An integrative approach, which includes animal experiments, physical experiments, and theoretical/numerical modeling, has led to the discovery of some fundamental principles of locomotion in and on dry granular media in previous studies. Professor Goldman and his students have utilized these principles to create a sand-swimming robot with performance comparable to the animal and have developed limb control strategies to allow effective legged movement on dry sand.

In FY12, major progress has been made in a number of areas. First, researchers demonstrated that power consumption in biological sand-swimming is proportional to the frequency of undulation at low speeds (a quasi-static regime). Experimental validation followed from a numerical simulation prediction that head drag is important in determining the motion of a sand-swimmer and consumes significant energy. The domain of validity for empirical force laws was examined with a multibody robot, where actuator torque and segment power were found to be maximal near the center of the body and decrease to zero toward the head and the tail. Approximately 30% of the net swimming power was dissipated in head drag. This confirmed earlier results that friction forces dominate locomotion within dry sand. These results were then utilized to examine the surface intrusion physics of a shovel-nosed snake to understand how the animal can swiftly bury itself.

Following these studies, the research team hypothesized that legs moving in granular media in the vertical plane can also be obtained by linear superposition of forces on each infinitesimal segment of the legs. The researchers developed a model element of a leg (simplified as a plate) in granular media and measured stresses as a function of the plate's depth, orientation, and movement direction in the vertical plane to develop resistive force laws for legs. The model showed that resistive force laws accurately predicted forces on model legs of a variety of shapes that move in granular media with prescribed kinematics. Experimental validation was accomplished with a small legged robot and indicated that resistive force laws accurately predicted the robot speed using a variety of leg shapes and stride frequencies (see FIGURE 6).

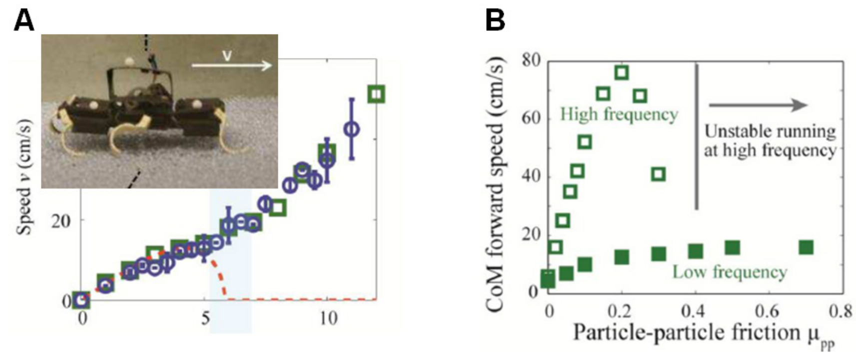

FIGURE 6

Granular Physics Meets Robotics. These multi-body intrusion studies in granular matter were found to be highly accurate for (**A**) predicting the speed of legged locomotion (blue circles: experiment, green squares: simulation). By varying inter-particle friction, (**B**) researchers examined stability boundaries for locomotion. At low frequencies, hydrostatic-like forces generated during the yielding of the granular material led to solidification of the material, and the robot moved as if walking on a solid surface. At high frequencies inertia of the grains being accelerated became important and forces became hydrodynamic-like.

This model was the first to capture the complex dependence of forces on depth, morphology, and kinematics in granular media and predicts legged locomotor performance. These force laws have also appeared to be convincingly universal in a variety of granular media of different particle size, density, friction, and compaction. Insight gained from fundamental studies of the intrusion physics was then utilized to study the locomotion mechanics of a legged robot to reveal limits of stability. These results will be used to advance the design and control of small robots in deformable terrains. Furthermore, the work was awarded "Best Student Paper" distinction at the 2012 Robotics: Science and Systems conference.

F. Multiscale Adaptive Large Eddy Simulation and Direct Numerical Simulation of Turbulent-Chemistry Interaction of Hydrocarbon Ignition

Professor Yiguang Ju, Princeton University, Single Investigator Award

The objective of this project is to develop a new, high fidelity, multi-scale, space, physics and chemistry Adaptive Large Eddy Simulation and Direct Numerical Simulation (MA-LES/DNS) method to gain a fundamental understanding of turbulent-chemistry interaction of highly stratified charge ignition of JP-8 and diesel surrogate fuels, with detailed chemistry. To achieve this, the research will provide a new turbulent combustion method which enables multi-physics, time-dependent, and accurate turbulent combustion modeling with detailed chemistry. The research project includes four research thrusts: (i) development of an error controlled dynamic model reduction method using multi-generation path flux analysis method, (ii) development of a chemistry and physics adaptive large eddy simulation and direct numerical simulation method to model turbulent chemistry coupling, (iii) development of a chemistry adaptive, multi-timescale method for efficient integration of conservation equations with detailed chemistry, and (iv) modeling of high pressure, turbulent ignition and combustion of diesel surrogate mixtures in a highly fuel stratified turbulent flow.

A comprehensively reduced mechanism of diesel surrogate using a multi-generation path flux analysis method (PFA) has been achieved. The detailed kinetic mechanism of the Aachen diesel surrogate (a mixture of 80% n-decane, and 20% 1,2,4-trimethylbenzene) *[Honnet et al.]* with 118 species is comprehensively reduced by using the multi-generation PFA method. The new, comprehensively reduced mechanism has 93 species and is compared with the detailed mechanism (113 species) for a wide range of equivalence ratio (0.6-1.6), initial temperature (300-1500 K), and pressure (1-50 atm). The results revealed that the comprehensively reduced mechanism captures both PSR extinction and the temperature dependence for normal and low temperature flame branches. FIGURE 7 shows the comparison between the reduced and detailed kinetic mechanisms for ignition delay time at pressure of 50 atm and various equivalence ratios. The reduced mechanism shows excellent agreement with the detailed mechanism in both high temperature and negative temperature coefficient regions. The deviation in ignition delay time was <10%, which is smaller than the corresponding experimental error.

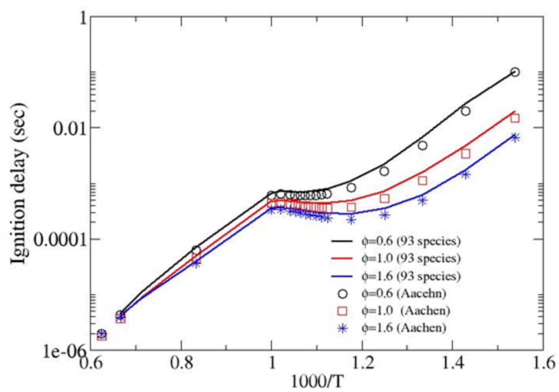

FIGURE 7

Comparison between the reduced and detailed kinetic mechanisms for ignition delay time. The data plot displays a comparison of ignition delay time between reduced and the detailed Aachen mechanism at P=50 atm and φ = 0.6, 1.0, and 1.6.

Even with a comprehensively reduced mechanism, two challenges remain to be solved. First, although the comprehensively reduced mechanism of diesel surrogate mixture has a high predictability, the size of the reduced mechanism is still large (93 species), which is not efficient to be directly used in turbulent combustion modelin. A series of computations for n-heptane shows that the active species number changes dramatically during the ignition process. Therefore, an introduction of dynamic adaptive chemistry (DAC) reduction in ignition modeling at different time steps can provide additional increase of computation efficiency. Second, although a reduced mechanism is generated by DAC, the reduced kinetic mechanism is still stiff. A robust and efficient method is needed to integrate the conservation equations with the locally reduced chemistry.

The research team has developed a dynamic adaptive chemistry with multi-time scale method (DAC-MTS) to overcome the above two technical challenges. It has been demonstrated that the computation efficiency and the validity of this method are demonstrated by using two different kinetic mechanisms, one large detailed n-heptane mechanism *[Curran et al.]* with 1034 species and 2539 reactions and the present, comprehensively reduced diesel surrogate model (93 species). These results are shown in FIGURE 8.

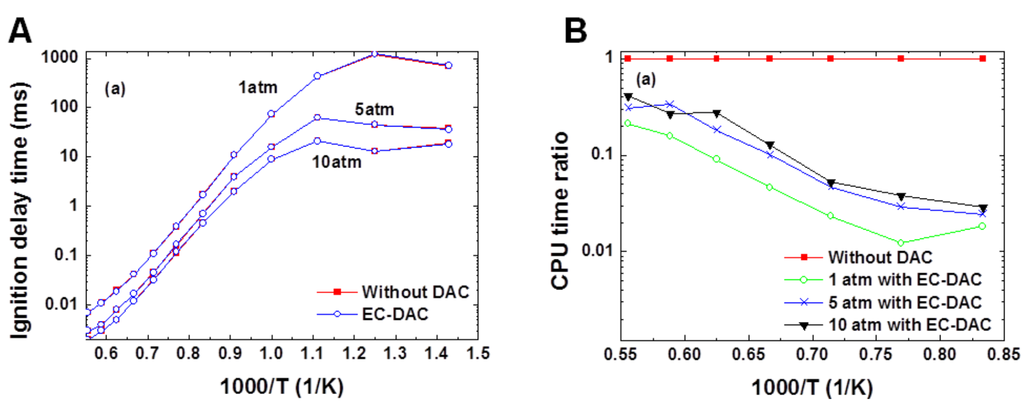

FIGURE 8

Diesel surrogate model of n-heptane ignition. The data plots display (**A**) comparison of ignition delay time and (**B**) computation efficiency with and without DAC for n-heptane/air mixture ignition at equivalence ratio of 0.5.

G. Characterization of Ignition and Combustion of Nanowire-based Energetics

Professor Xiaolin Zheng, Stanford University, Single Investigator Award

The objective of this research is two-fold. First is to develop new characterization methods to investigate the ignition and combustion properties of nanoenergetics which require only milligram level of samples and to develop models to predict their scale up behaviors. The other objective is to tune the ignition and propagation speeds of nanoenergetics by designing their nanostructures and/or using nanomaterial additives (e.g., carbon nanotubes, and graphene oxides). To achieve these objectives, the researchers are working to develop a camera flash ignition method to ignite Al nanoparticles (NPs) and use Al NPs as ignition promoters to ignite other solid, liquid and gaseous fuels. They will extend the camera flash ignition method to Al micron particles (MPs) by addition of WO_3 NPs for enhanced light absorption and oxygen supply. Al MPs are much more difficult to ignite optically than Al NPs since Al MPs have lower light absorption and higher ignition temperatures. A solution phase synthesis method is to be developed to coat/ deposit nanostructured metal oxides on Al particles for thermites with improved chemical uniformity, and the formed thermites have 25 times higher propagation speeds than mechanically mixed Al and metal oxide particle thermite mixtures. Finally, carbon-based additives will be used to modify the ignition and burning properties of energetic materials without introducing solid impurities.

The researchers have successfully realized a low power camera flash ignition (<1J/cm^2) for nano-thermites and further applied this ignition method to Al MPs (see FIGURE 9). The flash ignition is based on photothermal effect, for which the particles absorb the photons of the flash and convert the photon energy to heat. When the temperature rise exceeds the particle ignition temperature, flash ignition occurs. Al MPs are much more difficult to ignite by flash than Al NPs because Al MPs have lower light absorption and higher ignition temperatures. Nevertheless, Al MPs are safer to handle, cheaper, and have higher energy density (or less dead volume of the oxide layer) than Al NPs. Tungsten trioxide (WO_3) NPs were introduced to lower the minimum ignition energy of Al MPs and successfully realized flash ignition of Al MPs. WO_3 NPs play two roles when mixed with Al MPs: (i) increasing the light absorption and (ii) improving the oxygen supply inside the Al MPs where gaseous oxygen is difficult reach and replenish.

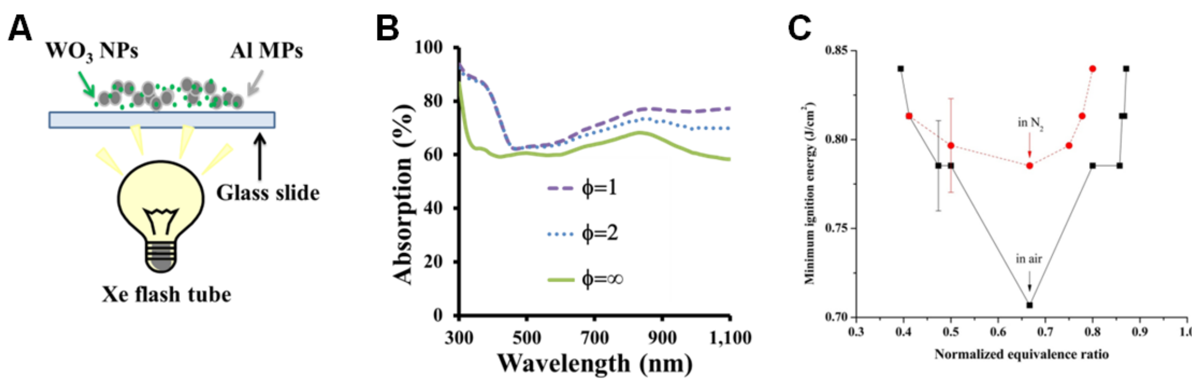

FIGURE 9

Low power camera flash ignition for nano-thermites applied to Al MPs. (A) Schematic of the experimental setup for flash ignition of the mixture of Al MPs (d = 2m) and WO_3 NPs (d = 100nm). (B) Light absorption spectrum of Al MPs/WO_3 NPs films with different fuel to oxidizer equivalence ratios. (C) Minimum flash ignition energy vs. equivalence ratios in air and nitrogen gas for the mixture of Al MPs and WO_3 NPs.

The researchers have designed and built a new and simple microchannel device with integrated optical fiber sensors to measure the propagation speeds of nanoenergetics. It should be noted that a microchannel has larger surface to volume ratio and larger heat loss rate compared to large scale channels, but it requires significantly less amount of materials for each test (typically 7 to 15mg) and can provide quick and simple qualitative comparison between different samples. In parallel, researchers have pioneered a precipitation method for the synthesis of Al/CuO core/shell particles with the goal of reducing the diffusion length between the fuel and oxidizer. The Al/CuO core/shell MPs, in comparison to mixtures of Al MPs and CuO NPs of same equivalence ratio, were found to have better chemical homogeneity and physical contact between Al and CuO, so that the core/shell MPs also exhibited much larger burning rates measured by the microchannel device (see FIGURE 10) and much lower minimum ignition energy measured by TSC. When the same core/shell structure was applied to

Al NPs, similar enhancement in ignition and burning rate were observed. Researchers believe that the core/shell structure is a general and effective means by which to tune the ignition and combustion properties of Al particles.

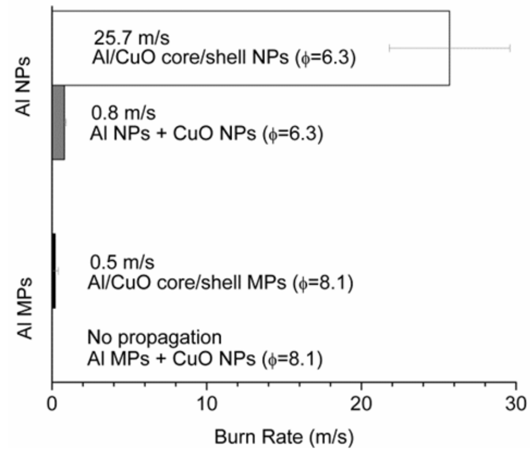

FIGURE 10

Comparison of burning rates of Al/CuO core/shell particles vs. a mixture of Al particles (both NPs and MPs) and CuO NPs. The burning rates are measured by a microchannel integrated with the photodiodes (microchannel width is 500m).

Finally, the research team has blended carbon-based nanomaterials, such as carbon nanotubes, graphene oxides, into energetic materials to control their ignition and combustion properties. There is interest in carbon-based additives because their combustion product is mainly CO_2, which brings in no impurity. Graphene oxide was synthesized by the improved Hummers method. Results demonstrated that both carbon nanotube and graphene oxides can function as a flame retardant and reduced the flame propagation speeds (see FIGURE 11).

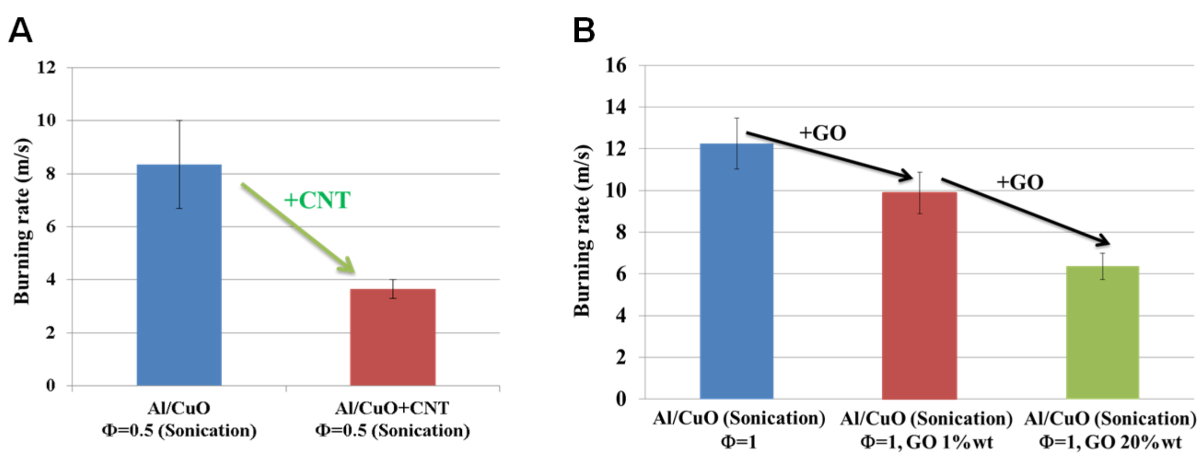

FIGURE 11

Effect of carbon nanotube and grapheme oxide additives on the burning rates of Al NPs and CuO NPs mixtures. The burning rates were measured by a microchannel integrated with the photodiodes and the microchannel width was 1 mm. (**A**) The burning rate comparison between Al/CuO NPs (Φ=0.5) vs. Al/CuO NPs (Φ=0.5) with 1% wt carbon nanotube addition. (**B**) The burning rate comparison between Al/CuO NPs (Φ=1) vs. Al/CuO NPs (Φ=1) with 1% wt and 20%wt grapheme oxide addition. For both carbon nanotube and graphene oxide functioned as a flame retardant and reduced the burning rates significantly.

H. A Nano-Second Pulsed Dielectric Barrier Discharge Model for Large-Eddy Simulations of Stall

Professor Datta Gaitonde, Ohio State University, STIR Award

The phenomenon of stall, in which flow separates from the surface of an airfoil section and results in reduced lift and increased drag, is a major factor limiting helicopter performance. A potentially revolutionary approach to alleviating this problem is to use low inertia, high-bandwidth pulsed plasma devices. Recently developed nanosecond pulsed dielectric barrier discharges (NSDBDs) have demonstrated flow control authority at speeds ranging from low subsonic to high supersonic with relatively small power inputs. In particular, the researchers can substantially delay the appearance of stall even at take off velocities, making them potentially scalable for practical use. The mechanism by which this occurs remains unknown, and limits evolution of an effective control strategy. The objective of this project is to use the proposed NSDBD model to explore plasma-based flow control strategies that are applicable to static and dynamic stall. Further insight into the physics, especially of the manner in which the energy is transformed from thermal to acoustic with concomitant effects on coherent structures and turbulence, will greatly facilitate exploitation of this revolutionary technology. Large Eddy Simulations (LES) can provide this breakthrough. However, a combined first principles fluid and plasma dynamic analysis is unfeasible and will remain so for the foreseeable future because of the massive computational resource requirement. To address this shortcoming, researchers have developed a simpler actuator model anchored in quiescent experiment to successfully reproduce the key effects. The model is then deployed with LES using a very high-order spectral-like scheme to analyze helicopter blade flow.

The model was developed by reproducing three key observations (i) wave structure, (ii) wave speed and (iii) power input. The wave structure is comprised of a semi-circular segment with a "tail". A two-parameter Gaussian heating distribution was demonstrated to successfully generate this structure. The heating volume determines the initial location of the disturbance. The subsequent relaxation of the wave speed to acoustic then precisely matches the observed location of the actuator-generated wave at any instant. Post facto estimates of the power injected into the flow agree very well with the experimental observation, providing confidence that the model faithfully reproduces the effect of the actuator at the primary fluid scales of interest. The applicability of this model to perform LES is demonstrated on a NACA0015 airfoil at 15 degree angle of attack (see FIGURE 12). The uncontrolled flow is fully separated at the leading edge, with the shear layer exhibiting rapid breakdown into turbulence after the development of non-linear and spanwise undulations. The process of flow attachment is successfully simulated with an actuator pulsed at the same frequency as in the experiment. This rich dataset is being mined to understand the fluid response in terms of transients and the impact on coherent structures.

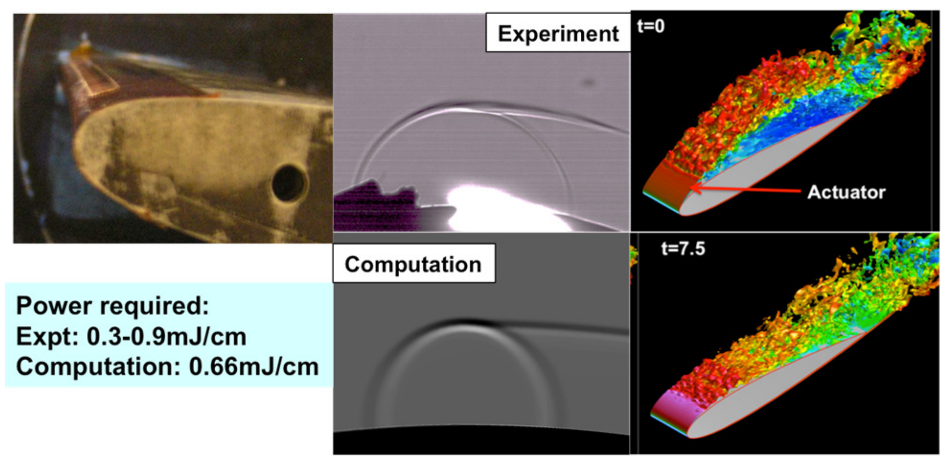

FIGURE 12

NSDBD Control of Stall. The panels illustrate the physical configuration, wave structure and vorticity with and without control on NACA 0015 flow. *[AIAA 2012-0184]*

These pioneering results have brought to bear advanced simulation methods together with massively parallel systems to address some of the most vexing problems in helicopter aerodynamics of interest to the Army. The results guide control strategies as well as scalability analyses. Additionally, the results have dual-use implication, since the main basic research conclusions can be easily transferred to the dynamics of wind-turbines and commercial fixed wing aircraft. This work was performed in collaboration with Dr. B. Glaz (ARL) and was supported by computer resources from DoD HPCMP and Ohio Supercomputer Center.

I. Intrinsically Efficient and Accurate Viscous Simulations via Hyperbolic Navier-Stokes System
Dr. Hiroaki Nishikawa, National Institute of Aerospace, Single Investigator Award

This project aims at generating an intrinsically efficient and accurate Computational Fluid Dynamics (CFD) solver based on First-Order Hyperbolic System Method (FOHSM). Ever-growing computing power is allowing the use of high-fidelity CFD models in engineering analysis and design for complex flow fields. However, practical aerodynamic simulations are so computationally demanding that current CFD methodologies are not able to produce accurate solutions at affordable cost, especially for vortex-dominated flows critical to Army applications such as rotor-craft wake computations. The FOHSM is a generalized numerical approach that is applicable to the solution of a wide class of partial-differential equations. In this project, the FOHSM has been implemented to the hyperbolic form of the Navier-Stokes system of equation with the goal of achieving efficient and accurate vorticity prediction for unsteady aerodynamic systems that are critical interest to many Army applications.

The CFD algorithm in this research is geared towards the development of high-order methods for the viscous terms (second derivatives). FOHSM is a unique and radical approach of casting the viscous terms into a hyperbolic system by including derivative quantities such as viscous stresses and heat fluxes. That is, methods developed for hyperbolic systems can be applied directly to the viscous terms. Potentially, it offers three major benefits: (i) straightforward construction of high-order viscous schemes, (ii) one order higher accuracy in the derivative quantities, (iii) improved efficiency by eliminating the numerical stiffness associated with second derivatives. The researchers obtained noteworthy preliminary results in FY12 using second-order unstructured finite-volume schemes based on a conventional method and FOHSM (see FIGURE 13). Orders of magnitude faster convergence to the steady solution as well as superior accuracy in the viscous stress and the heat flux by FOHSM were observed.

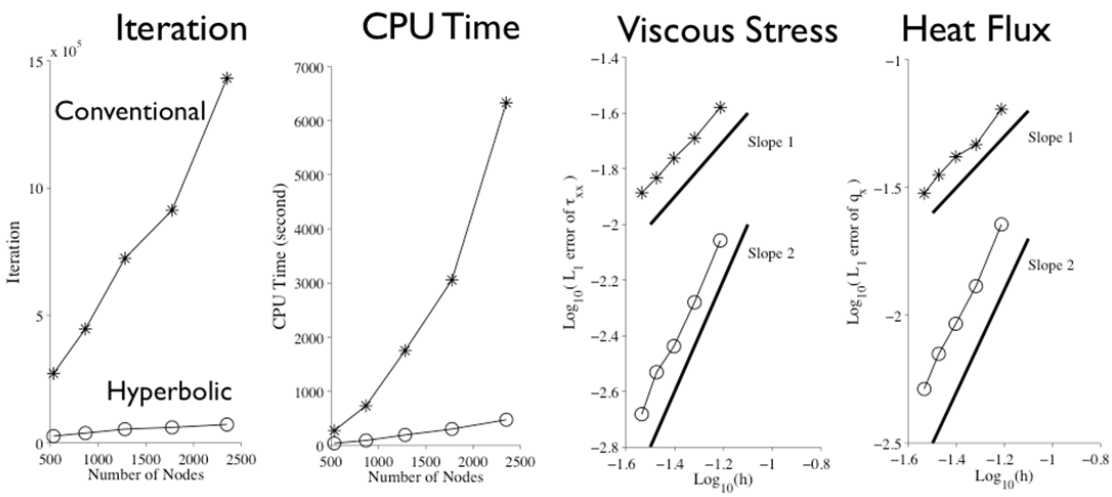

FIGURE 13

Results of second-order unstructured finite-volume schemes. The plots display a comparison between a conventional method (stars) and the hyperbolic method (circles) for a viscous shock problem on irregular triangular meshes. *[Nishikawa et al., 2011]*

J. Time-Varying Compressible Dynamic Stall Mechanisms Due to Freestream Mach Oscillations
Professor James Gregory, Ohio State University, YIP Award

The objective of this study is to investigate the effects of time-varying, compressible flow on rotorcraft dynamic stall through experiments in an unsteady flow wind tunnel. To pursue this goal, the researchers are utilizing a 6” x 22” transonic wind tunnel modified to enable Mach oscillations, while independently varying the angle of attack and the freestream velocity. For these studies, the Mach number, Reynolds number, and reduced frequency are all matched to critical flight conditions for this investigation. Advanced diagnostic techniques such as fast-responding pressure-sensitive paint (PSP) and particle image velocimetry (PIV) are also being used to study the fundamental details of the dynamic stall process under time-varying compressible conditions. This work is specifically focusing on unsteady shock/boundary layer interactions that drive the dynamic stall process, in order to determine the significance of the causal mechanisms.

The researchers have studied dynamic stall on a NACA 0012 airfoil has been studied with pressure-sensitive paint (see FIGURE 14). Here the phase averaged pressure coefficient distributions show the abrupt lift stall, a transient that is readily captured by the fast-responding PSP. Furthermore, the full PSP data sets reveal spanwise gradients in the pressure distribution that are critical for the three-dimensional compressible dynamic stall phenomena. These features were studied in detail for this investigation. PIV results from a thin airfoil in steady transonic flow illustrate the inherent unsteadiness of the shock-boundary layer interaction and its impact on the stall characteristics. Further investigations with a dynamically oscillating freestream are expected to produce much more substantial unsteady shock/boundary layer interaction. The PIV technique is currently being used in conjunction with PSP to understand the effects of compressibility on the three-dimensional dynamic stall phenomena.

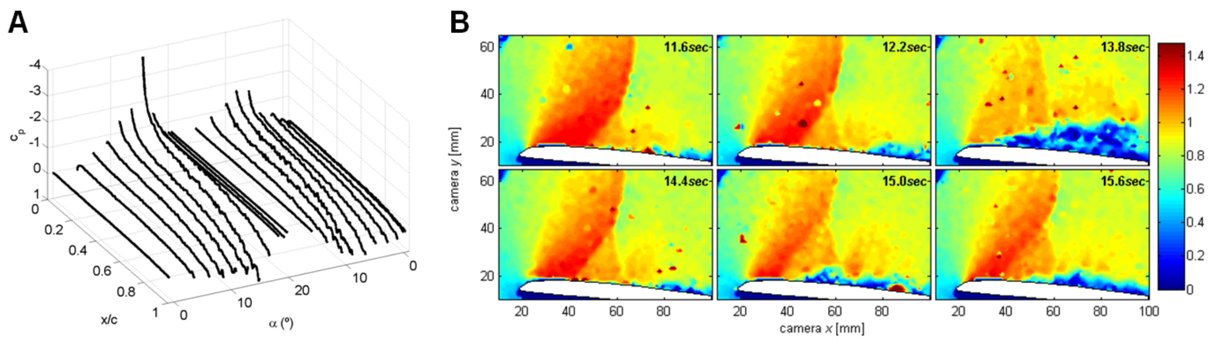

FIGURE 14

PSP measurement of pressure coefficient profiles and Mach number Contours. (A) PSP measurement of pressure coefficient profiles along the airfoil chord at various angular positions: NACA 0012, k = 0.012, M∞ = 0.3. (B) Representative set of raw PIV samples. Contours of Mach number are plotted for the thin airfoil at M∞ = 0.75, Rec = 5 × 106, and α = 8°.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Robust Stability and Control of Multi-body Vehicles with Uncertain Dynamics and Failures

Investigator: Professor Rama Yedavalli, Ohio State University, Single Investigator Award
Recipient: Tank and Automotive Research, Development and Engineering Center (TARDEC)

The objective of this research is to investigate mechanical principles that could ultimately improve stability and handling qualities (*e.g.*, roll-over stability, lane-change maneuver stability, etc.) of military, off-road, unmanned multi-body ground vehicles within as wide operating envelope as possible under the presence of uncertainty in vehicle model parameters as well as under failure modes. A major innovative approach, developed through this period was to design nominal controllers based on the Extended Coupled Linear Quadratic Regulator technique. In this technique, the control coupled output is regulated in an LQR (Linear Quadratic Regulator) framework, clearly delineating the coupling effect between the control and output which in turn is exploited to design controllers of reduced control effort for a given performance objective.

Professor Yedavalli examined both traditional interval parameter theory and newer ecological sign stability theory to study uncertainty. Researchers developed a robust control algorithm based on ecological sign stability for an entire class of vehicles without any need for redesign, resulting in substantial savings in development costs. These results were transitioned to TARDEC to develop a robust control design algorithm for vehicle testing.

B. Spray and Combustion of Gelled Hypergolic Propellants for Future Rocket and Missile Engines: Ignition and Reaction of Gelled Hypergolic Propellants in Microreactors

Researcher: Professor Rich Yetter, Pennsylvania State University, MURI Award (co-PI)
Recipient: Orbital Technologies Corporation (ORBITEC)

The objective of the originating research is to develop a fundamental understanding of the processes and mechanisms that control droplet formation, droplet collision and mixing, ignition, and energy release in gelled hypergolic propellants. Micro-reactors were developed under this work to study the reaction processes at the interface of the two hypergolic fluids in a carefully controlled fluid environment (the micro-reactor). Several of these reactors have been supplied to ORBITEC for use with their own studies on Gelled Hypergolic Propellants (GHPs), as well as other reactive systems under study by the company for potential future use in their developing rocket systems. Each of the reactors has a main-channel with a width of 240 µm, a total length of 1 cm and a depth of 55~60 µm. Stainless steel manifolds are used to flow the reactants through the micro-reactors. These manifolds help avoid using hypodermic tubing which would cause a large pressure drop in the system The manifolds also provide a safe and secure way of collecting the exhaust fumes and residual salt from the reactions. The inlets and outlets of the manifold to the reactor are sealed using Kalrez o-rings to prevent any leakage of the chemicals. A high speed camera can be used to visualize all the flows while fine-wire thermocouples are used to simultaneously record the exit temperatures of the products from the micro-reactors (see FIGURE 15).

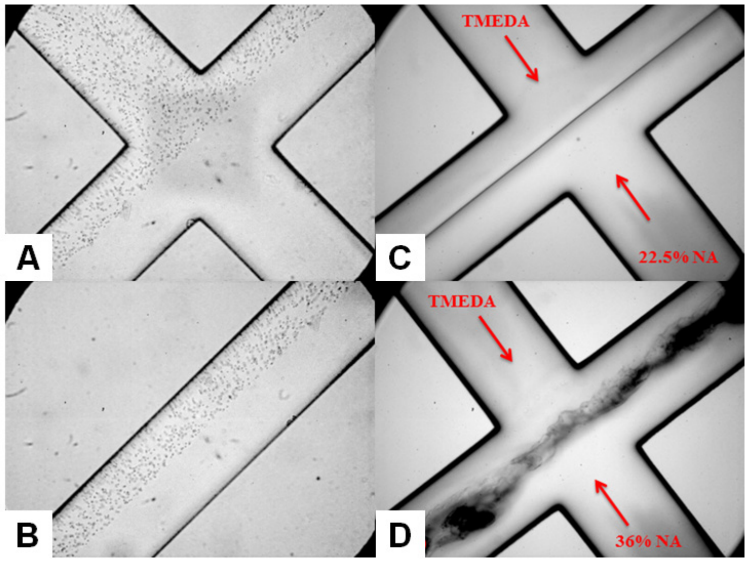

FIGURE 15

Examining the reaction between TMEDA and nitric acid. (A) Cold flow testing of micro-reactor using micro-spheres to visualize flow at stagnation zone. (B) Cold flow visualization downstream of the stagnation zone showing very little broadening of diffusion interface. (C) Visualization of flow in stagnation flow micro-reactor during reactions between TMEDA and nitric acid at lower nitric acid concentration. (D) Precipitation of salt in micro-reactor once concentration of nitric acid is raised beyond a certain limit and a large amount of reaction starts occurring in the reactor

C. Effect of Protective Devices on Brain Trauma Mechanics Under Idealized Shock Wave Loading

Investigator: Professor Namas Chandra, University of Nebraska - Lincoln, Other Army Programs Award
Recipient: ARL-WMRD, Natick Soldier Research, Development and Engineering Center (NSRDEC)

The goal of this project is to understand the fundamental material and mechanical behavior of protective systems in mitigating brain trauma under blast loading conditions. Professor Chandra and colleagues have built a very unique blast facility that can precisely regenerate field IED conditions of blast overpressure, duration and impulse which may lead to identifying injury mechanisms of TBI. Three shock tubes were developed and used for small animal studies and full head/neck surrogate studies with and without helmets for the Army surrogate head form. These studies revealed that flexural deformation induced by pressure loading is the primary loading mechanisms for soldiers in the theater for primary blast loadings leading to mild traumatic brain injury (mTBI). These results have transitioned to ARL-WMRD and NSRDEC, where the researchers are participating in collaborative research to conduct field explosion studies to validate shock tube blast profiles. Once validation and calibration is complete, the shock tubes can then be used to identify injury mechanisms of TBI.

D. Understanding and Mitigating Vortex-Dominated, Tip-Leakage and End-Wall Losses in a Transonic Splittered Rotor Stage

Investigator: Professor Garth Hobson, Naval Postgraduate School, Single Investigator Award
Recipients: ARL-VTD, NASA, Naval Air Warfare Center - Aircraft Division

The objective of this research effort is to develop an understanding of vortex-dominated, tip-leakage and end-wall losses in a transonic “splittered-rotor compressors.” The requirement for higher thrust-to-weight ratios in modern jet engines leads to a reduced number of stages at increased loading per stage or blade row. The usual limit of low diffusion in a compressor passage between two blades can be exceeded by using a tandem splittered cascade instead of a single blade row.

In the 1970s Wennerstrom and Hearsey designed a 2.76:1 pressure ratio and 68% efficient transonic compressor rotor. Since computational analysis has matured to the level where design optimization can be performed with such variables as airfoil shape and spacing of the main and splitter blades. As clearance-to-span ratios increase in high-pressure ratio compressors, so too will the chord-to-clearance ratio. Hence the logical conclusion to attempt to overcome the associated tip clearance loss with strategically placed partial blades within the main passage. Aggressive forward sweep of the main airfoil blades has been used in the current design to achieve moderate pressure rise, with good efficiency (80%) and a flow range of approximately 20%.

Recently the PI and his colleagues computed the flow through the Wennerstrom splittered rotor (see FIGURE 16). These computations have accurately predicted the performance of the team's splittered transonic rotor. The in-house design will be built and tested to verify the performance predicted. Detailed flowfield measurements in the tip leakage region will be performed to determine the interaction of the main tip leakage vortex with the splitter blade in the passage.

Collaborations with the Aerospace Industry and DoD Labs are underway as the logical application of this technology is in small turboshaft engines that power Army Helicopters. Benefits to the warfighter are longer persistence, larger payloads, longer range, increased speed and lower cost of ownership.

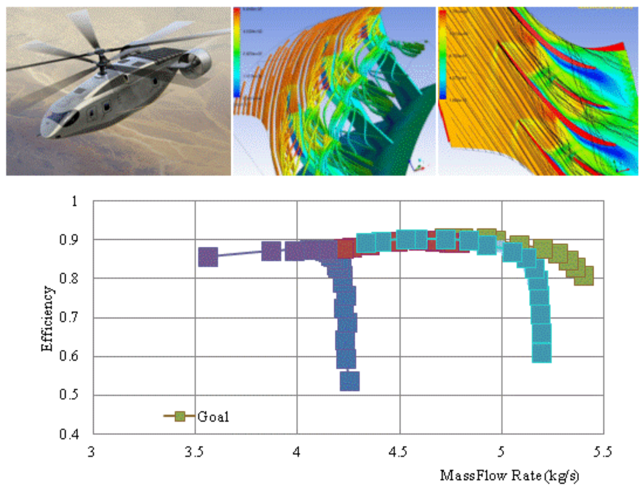

FIGURE 16

Experimental comparison of massflow rates versus efficiency with model predictions. The panels illustrate the efficiency of the Wennerstrom splittered rotor design compared with the target goals.

E. Microstructurally Engineered Armor System for Enhanced Survivability via Optimal Energy and Momentum Dissipation

Investigator: Professor Mohammed Zikry, North Carolina State University, Joint Improvised Explosive Device Defeat Organization JIEDDO) Award

Recipient: ARL-WMRD

The objective of this research project is to focus on the development of modeling and experimental techniques that span the nano to the macro scales. The ultimate goal is to develop a new class of high strength, blast resistant lightweight aluminum alloys. Researchers at North Carolina State University in cooperation with the California Institute of Technology have been working to optimize and develop a new class of high strength and lightweight aluminum alloys for armored systems subjected to high rate and severe loading conditions associated with IED events. The project has resulted in new state-of-the-art aluminum armor alloy technology that is providing a critical link between macroscopic dynamic response, microstructural characteristics and inelastic mechanisms at relevant length and time scales. It should be noted that the ballistic evaluation of the 2139-T8 aluminum alloy has been qualified as a Long-Term Armor Strategy (LTAS), presently being developed for two Military Specifications, and it has been incorporated into the Stryker Underbody Kit. The research team has transitioned these findings to ARL-WMRD, which is using these findings to enhance parallel applied research efforts and help develop new and significantly improved armor designs. There have been significant transitions to private industry where the computational techniques and optimization methods have been used to improve processing and synthesis techniques for high strength aluminum alloys.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Tailoring Interface Properties with High Strength Across Strain Rates

Professor Henry Sodano, University of Florida, STIR Award

The goal of this research project is to develop a new approach to the design of composite materials with an ultimate payoff being the creation interfaces that behave optimally across strain rates. The science required to define these new systems requires a multidisciplinary approach that incorporates chemistry, materials science and engineering and thus may make impacts across disciplines. The results of the work will impact the performance and design approach used for armor systems and primary structural components that require a higher level of toughness to potential ballistic impact. The goal is to produce a novel multifunctional material with tailorable interfaces such that under static loading the nanowires act to strengthen the interface, but under impact or a ballistic event, readily separate from the fiber due to the brittle nature of the ceramic nanowires, thereby allowing the tough fiber to carry the load. The nanowires may also provide increased friction with the fiber, as demonstrated by the use of shear thickening fluids pioneered by Dr. Eric Wetzel at ARL and Professor Norman Wagner at the University of Delaware.

ZnO is a ceramic material that can be grown in a variety of geometries at the nanoscale and when grown as a nanowire provides control over the wire diameter, length, location and spatial density. The PI will attempt to create advanced composites by growing single crystal ZnO nanowires on the surface of the structural fiber to functionally grade the interface, improve the interfacial bond and enhance load transfer between the fiber and matrix material. Micrographs of ZnO nanowires grown on carbon fiber clearly demonstrated the ability to control the morphology of the interface, which will allow for variation of the interfacial properties to create multifunctional materials with optimized structural and ballistic properties (see FIGURE 17).

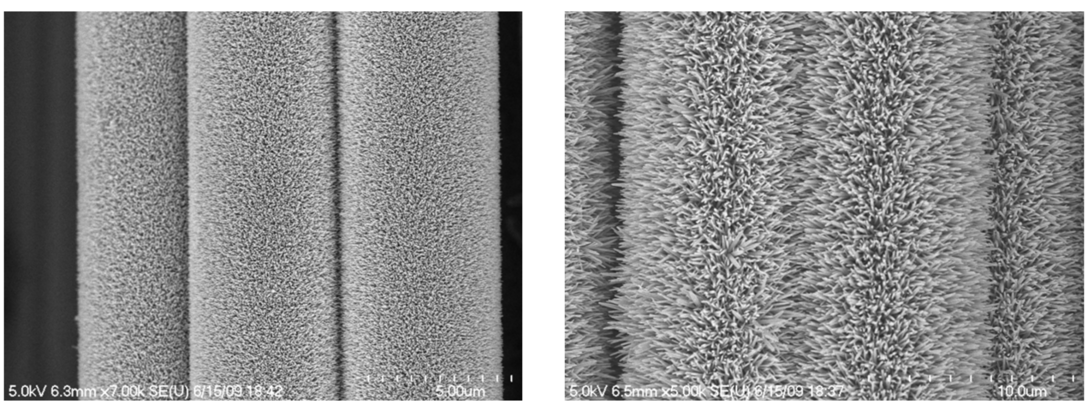

FIGURE 17

Micrographs of ZnO nanowires grown on carbon fiber. ZnO nanowires grown on carbon fiber at two different lengths demonstrating the controllable nature of the ZnO interphase.

This approach is completely novel and no prior research has been performed to study the high strain rate behavior of functionally graded fiber interfaces. Furthermore, the growth of ZnO on reinforcing fibers was developed by the PI and is the first whiskerization technique compatible with polymer fibers thus providing an opportunity for significant fundamental and applied impacts. Lastly, the concept of a multifunctional system designed for optimal behavior across strain rates is new and holds great promises for reducing the weight and complexity of armor systems as well as the ballistic resistance of structural components.

It is anticipated that in FY13 the investigator will (i) develop the functionalization and nanowire growth process such that the interface strength can be controlled, (ii) develop a testing methodology using a piezoelectric stack actuator to measure the single fiber pullout strength as a function of strain rate, (iii) perform high strain rate testing to measure the interfacial strength of the single fibers, and (iv) use results to develop a theory defining the role of the nanowires in increasing the interfacial and interlaminar strength as well as the failure mechanism and stress/strain distribution.

B. Molecular Interpenetrated Polymer Composites
Professors Hareesh Tippur (PI) and Maria Auad (co-PI), Auburn University, Single Investigator Award

Professors Tippur and Auad recently demonstrated the feasibility of processing transparent 'interpenetrating polymer networks' (IPNs) by combining stiff (PMMA) and tough (polyurethane) constituents in different proportions, both polymerized simultaneously in the presence of each other. By controlling the process kinetics, phase separation has been overcome to preserve optical transparency of the resulting IPN. However, in view of processing and scaling up difficulties associated with MMA, an epoxy system with polyurethane has been proposed in the current work to achieve the same goal. These novel polymer networks, termed Molecular Interpenetrated Polymer Composites (MIPC), show superior processability as adhesives or sheets with different fractions of stiff and tough constituents while being optically transparent. Furthermore, unlike IPNs, MIPC offer cross-links between the constituent phases.

In the first part of this research, investigation of process kinetics, weight fraction and molecular weight of the constituents, inclusion of nanoscale reinforcements, are among the issues to be investigated as an alternative transparent armor material. High strain rate characterization of MIPC and other transparent materials is the second part of this research. Failure behavior of these materials in monolithic and layered configurations will be studied by subjecting them to impact loading using a variety of full-field optical methods and high speed imaging. A new optical technique based on Digital Image Correlation (DIC) method and the elasto-optic effect exhibited by transparent solids will be developed for studying MIPC. This new methodology will complement existing experimental mechanics methods for material characterization at elevated rates of loading.

It is anticipated that in FY13, the researchers will demonstrate the feasibility of MIPC concept, perform preliminary mechanical characterization (DMA, tension tests, and fracture tests) and optimize the MIPC composition. The goal of the project will be to conceive and demonstrate the concept of creating a MIPC using epoxy based bis-GMA-acrylate copolymers to form the rigid phase and different precursors (disocyanate, diol and polyol) needed to generate the flexible polyurethane system, and to study the tensile and fracture performance of MIPC samples will be studied under quasi-static and dynamic loading conditions.

C. Understanding Locomotion and Interaction Physics in Wet Granular Media
Professor Daniel Goldman, Georgia Institute of Technology, Single Investigator Award

A major gap in scientific understanding concerning the dynamics of solid and structural interactions with soft/granular media translates into stifled progress and innovation regarding the efficiency and operational range of future ground-based autonomous and non-autonomous lightweight Army robotic systems. These interactions are complicated by the physics of granular media, wherein mobility may be hampered or, as recently discovered, augmented by the fact that granular media can exhibit a hybrid of both solid and fluid-like phases of matter. Since granular media is a prototypical far-from-equilibrium dynamic system dominated by friction, there exists incomplete fundamental understanding of how the spatiotemporal dynamics of these regimes and phases develop and propagate in the presence of external forces. However, by drawing inspiration from and quantitatively analyzing many soil and desert dwelling organisms specialized for locomotion within complex media, scientists will build upon recent progress in the physics of intrusion in dry granular media toward a new and hitherto unexplored understanding of multi-body interactions upon and within wet granular matter (granular media with interstitial fluid).

It is anticipated that in FY13, Professor Goldman will develop a substrate preparation system that allows creation of repeatable initial states of wet granular matter for which experiments in drag and intrusion with flat plates will elucidate empirical force laws. These force laws will build the foundation for a predictive force theory applicable to more complex shapes and multi-body structures such as legged and undulatory mechanisms. In parallel, the research team will develop and experimentally test a discrete-element-model approach to cohesive granular matter based on first principles concerning the capillary fluid pressure at the particle contact points. In future years, the investigators plan to demonstrate quantitative prediction and experimental validation of intrusion forces on small objects in wet granular matter states.

D. Combustion of High Molecular Weight Hydrocarbon Fuels and JP-8 at Moderate Pressures
Professor Kal Seshadri, University of California - San Diego, Single Investigator Award

The objective of this research is to understand and characterize combustion of high molecular weight hydrocarbon fuels in laminar non-uniform flows at elevated pressures up to 2.5MPa. Both experimental and kinetic modeling studies will be carried out. They include critical conditions of extinction and auto-ignition, and flame structure. The scientific questions that will be answered by this work are (i) How does pressure influence the critical conditions of extinction and auto-ignition? (ii) What surrogate best reproduces selected combustion characteristics of JP-8 at atmospheric and moderate pressure? (iii) What are possible chemical kinetic mechanisms for these surrogates? (iv) What is the influence of pressure on kinetic models?

Towards accomplishing these goals, in FY13 the researchers will design and build a counterflow burner for carrying out experiments on high molecular weight hydrocarbon fuels and jet fuels in particular JP-8 at elevated pressures up to 2.5 MPa. Many of these fuels are liquids at room temperature and pressure. A number of scientific questions can be addressed from experimental data obtained using this system. Experimental studies will be carried out using the condensed fuel burner employing the counterflow configuration. In this configuration, a gaseous oxidizer flows over the vaporizing surface of a liquid-fuel. The oxidizer is a mixture of air and nitrogen. A High Pressure Combustion Experimental Facility (HPCEF) has been constructed at the University of California at San Diego. The main part of this facility is a pressure chamber made from stainless steel. The counterflow burner will be placed inside this chamber. Nitrogen will be introduced into the chamber to establish and maintain the pressure at the desired level. The fuels to be tested will include jet fuels, in particular JP-8. Critical conditions of extinction and auto-ignition will be measured for various values of pressure in the range 0.1 MPa to 2.5 MPa. Temperature profiles will be measured using thermocouples. Kinetic modeling will be carried out employing a detailed mechanism. Results will be compared to models and used in further developing and validating the kinetic models.

E. Hover Test Facility for Mach-scaled, Coaxial, Counter-Rotating Helicopter Rotors
Professor Jayant Sirohi, The University of Texas - Austin, DURIP Award

Army requirements for next-generation helicopters call for significantly higher forward flight speed and enhanced payload capability. However, in a conventional helicopter, the forward flight speed is fundamentally limited by the aerodynamics of the main rotor. As the flight speed increases, compressibility effects on the advancing side and stall on the retreating side of the rotor disk decrease the propulsive efficiency. The rigid, coaxial, counter-rotating (CCR) rotor concept was introduced to address these issues. The XH-59A demonstrator aircraft featured a CCR rotor system with turbojet engines for auxiliary propulsion during high-speed flight. The XH-59A was developed in the 1960's and flight testing continued into the early 1980's, proving the potential of the concept, while demonstrating the need to improve rotor efficiency and reduce airframe vibrations.

In spite of the successful demonstrations of helicopters with CCR rotor systems, detailed experimental data on such rotors is lacking. Detailed measurements of velocity distribution in the rotor wake, and the effect of rotor separation, lift offset, rotor phasing and rotor speed reduction in forward flight are essential for fundamental understanding of CCR rotor systems. To address this need, the hover test facility at the University of Texas at Austin was developed with support from a DURIP award (see FIGURE 18). When completed, this facility will test reduced-scale single as well as CCR rotor systems at full-scale tip Mach numbers, in hover. The facility consists of a rotor test stand located inside a building with a high ceiling, and a control/observation room. The rotor test stand has a synchronous belt transmission driven by a 100 HP hydraulic motor. The entire transmission assembly can be removed and installed in the test section of a wind tunnel for forward flight testing. The unique coaxial rotor transmission features hub-mounted load cells that can measure individual rotor loads in the rotating frame. Electrical power, data and control signals are transferred between the fixed frame and rotating frame through slip rings.

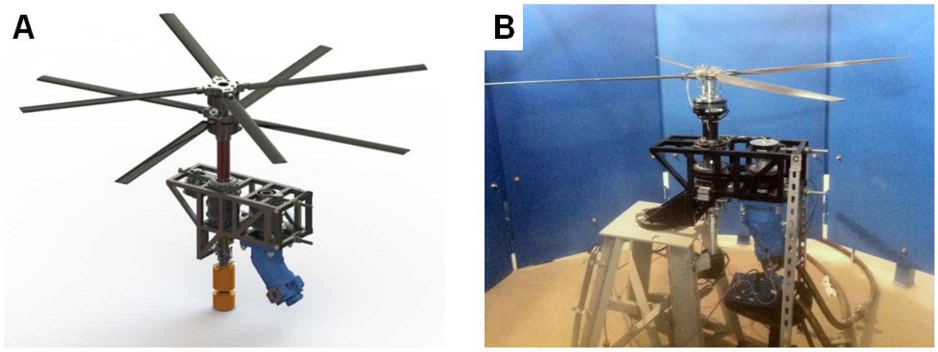

FIGURE 18

University of Texas at Austin hover test facility supported by a DURIP award. Components of the facility include (A) the coaxial, counter-rotating rotor test stand, and (B) the test stand showing 0.15 scale Bell 412 rotor with hub-mounted load cell.

At present, the test facility is being validated by performing detailed tests on a 0.15 scale Bell 412 rotor system. The anticipated outcome of this project will be a set of benchmark data (loads, rotor wake) on a 6ft diameter, Mach-scale CCR rotor system, including measurement of the effect of different parameters such as rotor separation, lift offset, rotor phasing and variable rotor speed. These data will be used for validation of analytical tools being developed by the Army as well as industry, and will be a key enabler in the development and risk reduction of next-generation, high-speed helicopters with CCR rotor systems.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Ralph Anthenien
Division Chief (Acting)
Program Manager, Propulsion and Energetics

Dr. Frederick Ferguson
Program Manager, Fluid Dynamics

Dr. Larry Russell
Program Manager (Acting), Solid Mechanics

Dr. Samuel Stanton
Program Manager, Complex Dynamics and Systems

B. Directorate Scientists

Dr. Thomas Doligalski
Director, Engineering Sciences Directorate

Mr. George Stavrakakis
Contract Support

C. Administrative Staff

Ms. Pamela Robinson
Administrative Support Assistant

CHAPTER 11: NETWORK SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2012* is to provide information on the programs and basic research efforts supported by ARO in FY12, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Network Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY12.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Network Sciences Division supports research to discover mathematical principles to describe, control, and to reason across the emergent properties of all types of networks (*e.g.*, organic, social, electronic) that abound all around us. The unprecedented growth of the internet, the tremendous increase in the knowledge of Systems Biology, and the availability of video from US military operations have all led to a deluge of data. The goal of the Network Sciences Division is to identify and support research that will help create new mathematical principles and laws that hold true across networks of various kinds, and use them to create algorithms and autonomous systems that can be used to reason across data generated from disparate sources, be they from sensor networks, wireless networks, or adversarial human networks, with the resulting information used for prediction and control. Given that network science is a nascent field of study, the Network Sciences Division also supports basic research on metrics that are required to validate theories, principals and algorithms that are proposed.

2. Potential Applications. In addition to advancing worldwide knowledge and understanding of networks, the research efforts managed in the Network Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO through network science research may provide new and revolutionary tools for situational awareness for the Solider and new regimes for command, control and communication for the Army. Furthermore, work supported by ARO through the Network Sciences Division could lead to autonomous systems that work hand-in-glove with the Soldier.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Network Sciences Division frequently coordinates and leverages efforts within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). In addition, the Division frequently coordinates with other ARO Divisions to co-fund research efforts, identify multi-disciplinary research topics, and to evaluate the effectiveness of research approaches. For example, interactions with the ARO Computing Sciences Division include promoting research to investigate game-theoretic techniques that could lead to better cyber situational awareness and to address concerns about performance and resilience to cyber attacks in ad-hoc dynamic wireless networks in a uniform fashion. The Network Sciences Division also coordinates efforts with the Mathematics Division to pursue studies of game theory that address bounded rationality and human social characteristics in a fundamental way. The Network Sciences Division coordinates with Life Sciences on studies at the neuronal level to understand human factors in how decisions are made under stress. Lastly, the Division's Program Areas interface with the Mechanical Sciences Division to understand the interplay between learning and manipulation and locomotion in robotic systems. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

To meet the long-term program goals described in the previous section, the Network Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY11, the Division managed research efforts within these four Program Areas: (i) Multi-agent Network Control, (ii) Decision and Neuro Sciences, (iii) Communications and Human Networks, and (iv) Intelligent Networks. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Multi-agent Network Control. The objective of this Program Area is to develop the theory and tools, through appropriate application and creation of relevant mathematics, to ultimately model, analyze, design, and control complex real-time physical and information-based systems, including distributed and embedded, networked autonomous and semi-autonomous, non-linear, smart structures, and decentralized systems. This Program Area invests in fundamental systems and control theory and relevant mathematical foundations for areas of control science such as multi-variable control, non-linear control, stochastic and probabilistic control distributed and embedded control, and multi-agent control theory. Further, the Program also involves innovative research on emerging areas such as control of complex systems and theories for the design of large heterogeneous multi-agent teams with desired emergent behaviors. This Program Area is divided into two research Thrusts: (i) Intelligent Control and (ii) Multi-agent Systems. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. The Intelligent Control Thrust involves research topics focusing on non-traditional approaches to control with focus on the Army's interest in basic research on intelligence, embedded in a single agent operating in highly uncertain, clustering, and complex environments. The Multi-agent Systems Thrust involves research focused on extending the mathematical foundations of distributed system theory, with a focus on basic research in the massive-scale, low cost, highly distributed agents cooperating over networks in highly uncertain, clustering, and complex environments. In addition, research focuses on the design of emergent behavior for heterogeneous multi-agent systems, accommodative-cooperative-collaborative theory of multi-agent behavior and interaction, and multi-player/multi-objective game theory.

2. Decision and Neuro Sciences. The goal of this Program Area is to advance frontiers of mathematics and neuroscience to support timely, robust, near-optimal decision making in highly complex, dynamic systems operating in uncertain, resource-constrained environments. This Program Area involves two major research Thrusts: (i) Mathematical Modeling of Neural Processes and (ii) Stochastic Optimization and Modeling. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. The Mathematical Modeling of Neural Processes Thrust addresses innovations to quantitatively model decision behaviors in neural-anatomical or other observable measures to explain how factors such as complexity, uncertainty, stressors, social and other dynamics affect decisions. The Stochastic Optimization and Modeling Thrust addresses advances in mathematical algorithms to better address stochastic data properties common in highly dynamic, heterogeneous and complex operational environments and in environments with ill-conditioned and varying information such as in dynamic complex social contexts. Based on operations-research methodologies such as modeling, simulation and numerical optimization, this Program Area includes a significant multi-disciplinary emphasis, specifically with neuroscience, to address the complex, multi-dimensional decision frameworks in today's asymmetric warfare.

3. Communications and Human Networks. The goal of this Program Area is to better understand the fundamental scientific and mathematical underpinnings of wireless communications and human networking, their similarities, and the interactions between these two networks. This Program Area is divided into two research Thrusts: (i) Wireless Communications Networks and (ii) Human Networks. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. The Wireless Communications Networks Thrust supports research efforts to discover the fundamental network science principles as they apply to the wireless multi-hop communications systems, while the Human Networks Thrust identifies and supports research to better understand social network structures from heterogeneous data, the structures effect on decision making, and the interaction of communications and human networks. The research efforts promoted by this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications could include wireless tactical communications, improved command decision making, and determining the structure of adversarial human networks.

4. Intelligent Networks. The goal of this Program Area is to develop and investigate realizable (i.e., computable) mathematical theories, with attendant analysis of computational complexity, to capture common human activity exhibiting aspects of human intelligence. These studies may provide the foundation for helping augment human decision makers (both commanders and Soldiers) with enhanced-embedded battlefield intelligence that will provide them with the necessary situational awareness, reconnaissance, and decision making tools to decisively defeat any future adversarial threats. This Program Area is divided into two research Thrusts: (i) Integrated Intelligence and (ii) Adversarial Reasoning. These thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long term goal. The Integrated Intelligence Thrust supports research efforts to discover the mathematical structuring principles that allows integration of the sub-components of intelligent behavior (such as vision, knowledge representation, reasoning, and planning) in a synergistic fashion, while the Adversarial Reasoning Thrust area brings together elements of Game Theory, knowledge representation and social sciences to reason about groups/societies in a robust manner. The research efforts promoted by this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications could include robotic unmanned ground and air vehicles, reasoning tools for wild life management, and decision making tools in the context of command, control, communications, computers, intelligence, surveillance and reconnaissance (C4ISR).

C. Research Investment

The total funds managed by the ARO Network Science Division for FY12 were $25.2 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY12 ARO Core (BH57) program funding allotment for this Division was $5.2 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $4.7 million to projects managed by the Division. The Division also managed $15.2 million of Defense Advanced Research Projects Agency (DARPA) programs. Finally, $0.1 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY12 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research projects. Research projects are developed by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts.

The following subsections summarize projects awarded in FY12 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY12, the Division awarded 22 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to characterize optimal decision making mechanisms using neurophysiological measures, investigate new metacognitive architectures for autonomous systems, and determine the influence of network structure on the dynamics of large discrete-state networks. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor William Anderson, Johns Hopkins University; *Biophysical Model of Cortical Network Activity and the Influence of Electrical Stimulation*
- Professor Roger Brockett, Harvard University; *Continuum Models for Multi-Agent Cooperative Control*
- Professor Pamela Cosman, University of California - San Diego; *Robust Mobile Communications*
- Professor Michael Cox, University of Maryland - College Park; *The Metacognitive Loop and Learning Goal States*
- Professor Daniel J. Gauthier, Duke University; *Fundamental Experimental Research on the Dynamics of Physical Networks*
- Professor Paul Glimcher, New York University; *Neurobiologically Validated Models of Errors in Decision-Making: Strategies for Remediation and Detection*
- Professor Laurent Itti, University of Southern California; *Detection and Interpretation of Low-Level and High-Level Surprising and Important Events in Large-Scale Data Streams*
- Professor Michael Jensen, Brigham Young University; *Propagation Analysis and Performance Assessment for Multi-Antenna Communications*
- Professor Minjun Kim, Drexel University; *Microbiorobots for Manipulation and Sensing*
- Professor Whee Ky (Wei Ji) Ma, Baylor College of Medicine; *Measuring and Modeling Attentional Limitations in Split-Second Visual Decisions*
- Professor Chjan Lim, Rensselaer Polytechnic Institute; *Theoretical and Computational Studies of Tipping Points and Community Detection in Social Networks*
- Professor Edward Ott, University of Maryland - College Park; *The Role of Network Structure in the Dynamics of Discrete-State Systems*

- Professor Matthew Peterson, George Mason University; *Electroencephalogy Feedback In Decision-Making*
- Professor Ioannis Poulakakis, University of Delaware; *Constructive Control Algorithms*
- Professor Ramesh Rao, University of California - San Diego; *Cognitive Protocol Stack Design*
- Professor Johannes Royset, Naval Postgraduate School; *Estimation and Uncertainty Quantification of Stochastic Systems*
- Professor Ashutosh Saxena, Cornell University; *Integrative Perception and Action*
- Professor Paulo Shakarian, U.S. Military Academy; *Combinatorial and Scalable Initiation in Complex Networks*
- Professor Roger Wets, University of California - Davis; *Estimation and Uncertainty Quantification of Stochastic Systems*
- Professor Ji Hyun Yang, Naval Postgraduate School; *Understanding Optimal Decision Making Using Neurophysiological Measures*
- Professor Luke Zettlemoyer, University of Washington; *Instruction via Interactive Grounded Learning*
- Professor Qing Zhao, University of California - Davis; *Stochastic Online Learning in Dynamic Networks under Unknown Models*

2. Short Term Innovative Research (STIR) Program. In FY12, the Division awarded seven new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to discover new techniques for understanding the context, meaning and trends emanating from social media, determine trust of data over networks, and to investigate advanced signal processing methods. The following PIs and corresponding organizations were recipients of new-start STIR awards

- Professor Ing-Ray Chen, Virginia Polytechnic Institute and State University; *Dynamic Trust Management in Delay Tolerant Networks*
- Professor Judith Gelernter, Carnegie Mellon University; *Mapping Social Media Messages*
- Professor Yingbo Hua, University of California - Riverside; *Feasibility of Full-Duplex Radio*
- Professor Xiaoli Ma, Georgia Tech Research Corporation; *Realizing Lattice-Reduction-Based Detectors*
- Professor Nikolaos Sidiropoulos, University of Minnesota - Minneapolis; *Sparse Latent Factor Models for Social Network Analysis and Tensor Completion*
- Professor Lori Sheetz, United States Military Academy; *Modeling Contemporary Decision-Making Environments: Education as a Decision Support Tool*
- Professor Wesley Snyder, North Carolina State University; *Detection of Low-order Curves in Images using Biologically-plausible Hardware*

3. Young Investigator Program (YIP). In FY12, the Division awarded one new YIP project. This grant is driving fundamental research to understand the role of domain adaptation in the context of statistical machine learning. The following PI and corresponding organization was the recipient of the new-start YIP award.

- Professor Fei Sha, University of Southern California; *Domain Adaptation for Intelligent Systems in Changing Environments*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY12 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Fourth International Workshop on Network Science for Communication Networks (NetSciCom)*; Orlando, FL; 25-30 March 2012
- *Fifth Annual North American School of Information Theory*; Ithaca, NY; 19-22 June 2012
- *Summer School on Algorithmic Economics*; Pittsburgh, PA; 6-10 August 2012
- *Workshop on Populations & Crowds: Dynamics, Disruptions and their Computational Models*; Los Angeles, CA; 6-7 September 2012

5. Special Programs. In FY12, ARO Core Research Program funds provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded four new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Network Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. A Unified Approach to Abductive Inference. This MURI began in FY08 and was awarded to a team led by Professor Pedro Domingos at the University of Washington. The goal of this research is to investigate Markov Logic Networks as a model to study human cognition, specifically the process of human analysis of seemingly disparate, voluminous data to explain the most possible cause for a set of observations.

Abduction is the process of generating the best possible explanation for a set of observations. While this calls for generation of a logical argument, observed data invariably contain inconsistencies. The research team has been investigating the use of Markov Logic Networks, a formalism that combines first order predicate logical and statistical reasoning to combine logical rigor with soft constraints, to capture domain knowledge. The task of generating explanation can then be looked upon as the inverse of forward chaining with the greatest probability/weight. To make such an automatic system scalable/practical this research effort involves (i) cognitive science based heuristics for guiding generation of most likely proof trees, (ii) integration of low level sensor data with potential imprecision into the reasoning process, and (iii) parallel and distributed schemes for speeding belief propagation and proof construction, etc. Finally, the MURI team is working on several case studies to validate their approach; this includes generation of explanation for how a Capture the Flag game is played, based on GPS traces. The ability to fuse information of different kind, and to reason about it at higher cognitive level, is relevant to improving situational awareness for Soldiers and commanders in a battlefield.

2. Neuro-Inspired Adaptive Perception and Control. This MURI began in FY10 and was awarded to a team led by Professor Panagiotis Tsiotras of the Georgia Institute of Technology, with participation from researchers at the Massachusetts Institute of Technology and the University of Southern California. The objective of this MURI is to investigate a new paradigm based on "perception/sensing-for-control" to achieve a quantum leap in the agility and speed maneuverability of vehicles. The team will leverage attention-focused, adaptive perception algorithms that operate on actionable data in a timely manner; use attention as a mediator to develop attention-driven action strategies (including learning where to look from expert drivers); analyze the saliency characteristics of a scene to locate the important "hot-spots" that will serve as anchors for events; make use of fused exteroceptive and proprioceptive sensing to deduce the terrain properties and friction characteristics to be used in conjunction with predictive/proactive control strategies; and will study and mimic the visual search patterns and specialized driving techniques of expert human drivers in order to develop perception and control algorithms that will remedy the computational bottleneck that plagues the current state of the art.

This MURI will have significant benefits for the Army in the field and off the field, such as increasing vehicle speed and agility in direct battlefield engagements, as it will increase the chances of evading detection by the enemy or of escaping an ambush. As confirmed by several Army studies, the difficulty of successfully engaging and hitting a target increases disproportionately with the target speed. Support logistics will also become safer and more effective as even moderate increases in speed can largely increase the capacity of convoys and the throughput of the supply lines of materiel. Finally, the results of this research will contribute to the development of realistic off-road high-speed simulators for training special forces and other military and government personnel.

3. Scalable, Stochastic and Spatiotemporal Game Theory for Adversarial Behavior. This MURI began in FY11and was awarded to a team lead by Professor Milind Tambe of the University of Southern California, with participation from researchers at UCLA, Duke University, Stanford University, UC Irvine and California State University at Northridge. The objective of this MURI is the development of game theory formalisms that account for bounded rationality, scalability of solutions, real-world adversaries, and socio-temporal issues. The technical approach to be followed by the team will involve a mix of behavioral experiments and development of theoretical formalisms to characterize individual human behavior and that of adversarial groups; it is expected that psychological theories such as prospect theory and stochastic theories for coalitional games will play equal part in the technical development. The results of this MURI may have significant impact on diverse applications of the Army such as scheduling of resources for ISR and for monitoring of contracts while building nations or societies.

C. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY12.

D. Small Business Technology Transfer (STTR) – New Starts

No new starts were initiated in FY12.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY12, the Division managed three new REP awards. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE)—New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The PECASE winners for each calendar year are announced by the White House in the last quarter of the fiscal year. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Computing Game-Theoretic Solutions for Security in the Medium Term. The objective of this PECASE, led by Professor Vince Conitzer at Duke University, is to build on earlier work in Game-Theoretic solutions for security games (being deployed at LAX airport and by US Coast Guards) to extend it to longer-term settings. This includes optimizing the parameters of the game (such as the number and types of resources deployed). It also involves developing techniques for extensive-form, repeated, and stochastic security games, as well as learning in security games, to move beyond single-period models. The work has the potential to lead to both improvements in existing applications and entirely new applications. The project will combine techniques from artificial intelligence, algorithms, combinatorial optimization, (machine) learning, and game theory (including behavioral game theory).

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY12, the Network Science Division managed three new DURIP projects, totaling $0.6 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of neural networks, wireless networks and perception-driven robotic systems.

H. DARPA Anomaly Detection in Multiple Scales (ADAMS)

The ADAMS program is an effort to understand how insider threats to an organization (such as Maj. Nadal Hassan or Robert Hansen) can be predicted based on changes in behavior of individuals, or a small group of people within an organization. At a technical level this program involves mining incredibly large graphs (based on normal human activity) in a manner that is cognizant of human behavior, which reduces to computational challenges in managing and reasoning of large datasets, statistical reasoning techniques to find black swans, and efforts to manage uncertainty in both data and reasoning techniques. This program is managed on behalf of DARPA through the Network Sciences Division, Intelligent Networks Program.

I. DARPA Structured Social Interactions Module (SSIM)

The SSIM program is an effort to discover what makes certain soldiers, policemen and ethnographers effective in new environments (*e.g.*, a different culture to their own) making them "Good Strangers." Typically, Good Strangers can operate in a new environment without upsetting the local population and are good at understanding social mores without being taught what they are. This program engages social scientists to identify physiological coping mechanisms and psychological characteristics of Good Strangers, and artificial intelligence experts to devise new Social Science cognizant computer-based simulation and training algorithms. This program is managed on behalf of DARPA through the Network Sciences Division, Intelligent Networks Program.

J. DARPA Social Media in Strategic Communication (SMISC)

The SMISC program is an effort to understand and control strategic communication that takes place over social media. Recent events in Madagascar, North Africa (especially the Arab Spring) and in Bangalore suggest that social media could and does play a major role in bringing together mobs and crowds in unpredictable ways. The SMISC program aims to develop solutions that could be used to understand development of memes over social media and potential techniques to influence the formation or dissipation of memes. This program is managed on behalf of DARPA through the Network Sciences Division, Intelligent Networks Program.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Network Sciences Division.

A . Understanding Collective Motion and Swarms of Micro-scale Objects at Low Reynolds Number

Professor Paulo Arratia, University of Pennsylvania, Single Investigator Award

The objective of this research is to investigate and develop strategies to generate and control the collective motion and swarms of micro- and/or nano-scale objects/particles immersed in fluids. Due to their small length scales, the motion of such small objects is often described by low Reynolds number (*Re*) equations in which linear viscous forces dominate nonlinear inertial forces. In this low *Re* regime, an object immersed in fluid cannot propel itself unless specially designed and powered so that its motion is not reciprocal. Two alternative strategies for propulsion of artificial swimmers at low *Re* are being pursued. The first strategy relies on manipulation of the fluid rheological properties in order to break the system time-symmetry constraints. The second strategy relies on a "collective motion" approach, which uses simple, generic particles that cannot propel themselves individually, but that can work together by hydrodynamic interactions to move as a group.

During FY12, investigators developed experimental methods to fabricate small (~1 μm) paramagnetic ellipsoidal particles of aspect ratio up to 1:6. This method relies on stretching paramagnetic spherical colloidal particles in a uniform magnetic field. Also, the investigators developed well-controlled, force-free driving mechanisms in order to actuate "swimming particles" in viscous Newtonian and complex fluid environments. These results culminated in the first experimental evidence of 'artificial swimming' using simple reciprocal forcing at low *Re* by carefully manipulating the fluid rheological properties (see FIGURE 1).

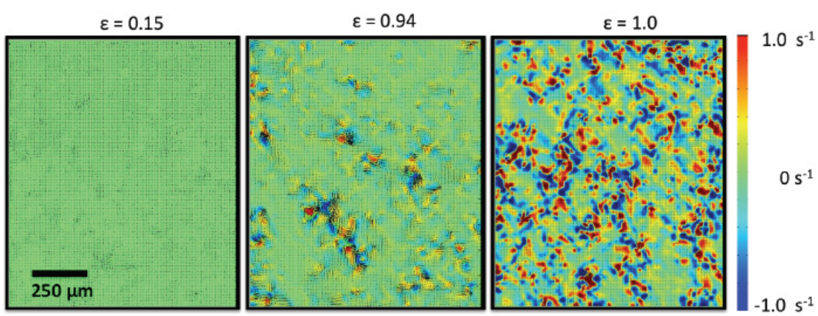

FIGURE 1

Coherent structures due to multi-agent motion. New imaging methods show vorticity fields generated by a swarm of synthetic swimmers. The particles are reoriented harmonically by an external magnetic field and suggest close particle-particle interactions cause net particle motion across one actuation cycle of individual particles. The preliminary results suggest that an increase in strain amplitude from the magnetic actuation results in collective behavior.

B. Theoretical Foundations of Wireless Networks

Professor Alejandro Ribeiro, University of Pennsylvania, Single Investigator Award

The goal of this research is to develop a formal theory that will provide a scientific basis for the design of multi-hop wireless tactical networks by using optimization techniques. Fading (*i.e.*, random variations in channel gains) is a unique property of wireless communications which leads to a much more difficult optimization problem. Also unlike wired networks, the sum transmission rate optimization problem in wireless random access networks is not convex, due to power and bandwidth allocation problems as well as interference. The problem is also infinite dimensional and has a positive duality gap between the primal and dual problems.

Professor Ribeiro has been able to reformulate the optimization problem in order to eliminate the duality gap, which makes the optimal solution to the dual problem the same as the primal problem. Also, the resulting dual problem is finite dimensional and convex, which significantly simplified the optimization. In addition, a distributed optimization algorithm has been derived for this problem, based on Newton's method, which speeds up convergence by an order of magnitude. Since the algorithm is decentralized, it can run on individual network nodes, with only local network information, thus reducing overhead.

C. Cultured Neural Network

Professors Thomas Shea (PI) and Holly Yanco (co-PI), University of Massachusetts - Lowell, Single Investigator Award

The goal of this joint project between the ARO Network Science and Life Science Divisions is to develop an innovative approach to study learning behavior in cultured neural networks, using multi-electrode arrays (MEAs) for analysis of neuronal activity. This new methodology allows for tracking neural responses, including learning behaviors, in a highly controlled experimental setting. Two variations on commonly accepted techniques to increase the precision of extracellular electrical stimulation include: (i) the use of a low-amplitude recorded spontaneous synaptic signal as a stimulus waveform and (ii) the use of a specific electrode within the array adjacent to the stimulus electrode as a hard-grounded stimulus signal return path. The investigators found that both variations remained compatible with manipulation of neuronal networks. In addition, localized stimulation with the low-amplitude synaptic signal was found to allow selective stimulation or inhibition of otherwise spontaneous signals. These findings revealed that minimizing the area of the culture impacted by external stimulation allows modulation of signaling patterns within subpopulations of neurons in culture.

In FY12, the investigators developed a self-contained system in which cultured neurons receive sensory input from the environment, process the input, and generate motor functions (see FIGURE 2). The goal of feeding a digitized camera signal (sensory input) to cortico-hippocampal neurons cultured on multi-electrode arrays (the "neuronal network" that will process the information) and transmission of resultant neuronal signals to a digitally-controlled robotic arm capable of complex manipulations (motor output) was achieved. The neuronal cultures function as rudimentary central nervous systems. The resulting cultures are capable of long-term potentiation, which is the basis for learning. Established training regimens were utilized to refine the response capabilities of the neuronal network, including differential responses following observation of friendly or potentially hostile targets prior to retaliation. The extent of training and responsiveness has been correlated with that of standard artificial neural networks in order to improve performance of artificial neural networks.

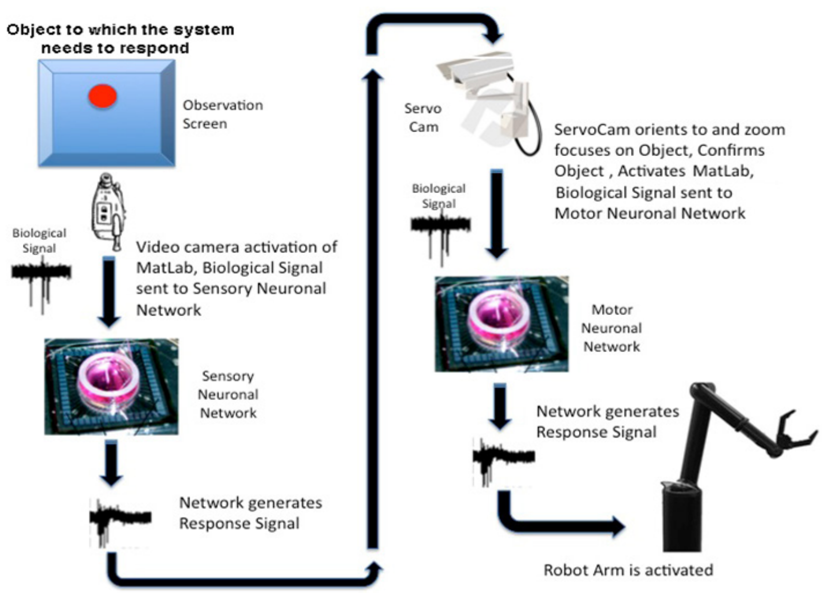

FIGURE 2

Flow of information: from visual signal to movement of a robotic arm. The diagram shows observation screen recorded by video camera, which is then translated by a MATLAB program into a "biological" signal that the sensory neural network can interpret. The sensory neural network then produces response signal which is interpreted by another MATLAB program, sending another biological signal to the motor neural network which then produces a signal to activate the robot arm.

D. Optimally Managing Dynamic Server-to-Customer Systems
Professor Laura McLay, Virginia Commonwealth University, YIP Award

The objective of this research is to develop new mathematically-based algorithms to identify optimal dispatching policies for server-to-customer systems. One important approach has used a mixed-integer programming model for enforcing priority list policies in a Markov decision process model. Since the optimal solution is dependent on Markov state variables, it may not always correspond to a simple set of rules when implementing it in practice. Restricted policies that conform to a priority list for each type of customer may be desirable for use in practice. A priority list policy is an ordered list of servers that indicates the preferred order to dispatch the servers to a customer type subject to server availability. However, traditional methods that constrain the Markov decision process to only consider structured policies like priority lists expand the state space.

Professor McLay is investigating a new constrained Markov decision process model for identifying optimal priority list policies. The new constrained model is novel in that it is formulated as a mixed integer programming model that does not extend the Markov state space and can be solved using standard mixed integer programming algorithms. An important finding is that the optimal mixed integer programming solutions have objective function values that are close to those of the unrestricted model and are superior to those of heuristics. Another area of work within this project includes development approaches that address models of human behavior. As a complement to existing tools for meeting this need, this work is based Herrnstein's Matching Law, a model of choice behavior developed in operant psychology. These behaviors can be introduced into preexisting optimization problems as a set of constraints. This procedure generates non-convexities in the resulting optimization problem's feasible region, but this work shows that, for problems with separable, Lipschitz continuous Matching Law constraints, these non-convex optimization problems may be approximately solved using separable programming. The approach is demonstrated by applying it computationally to a family of assignment problems. These formulations expressed as assignment problems demonstrate how numerical optimization can be used to assess the real-world relevance of matching which addresses human behavioral dynamics.

E. Learning in the Presence of Unawareness
Professor Joseph Halpern, Cornell University, Single Investigator Award

The objective of this research is to establish a new Decision Theory where lack of knowledge is well accounted for, and not merely based on traditional notions of sets of probabilities. For this research, the investigator is considering a setting where an agent's uncertainty is represented by a set of probability measures, rather than a single measure. Measure-by-measure updating of such a set of measures upon acquiring new information is well-known to suffer from problems; agents are not always able to learn appropriately. To deal with these problems, the researchers use weighted sets of probabilities, a representation where each measure is associated with a weight, which denotes its significance. In FY12, the PI designed a natural approach to updating and a natural approach to determining the weights. He showed how this representation can be used in decision-making by modifying a standard approach to decision making, minimizing expected regret, to obtain minimax weighted expected regret (MWER). Finally, the PI has invented an axiomatization that characterizes preferences induced by MWER both in the static and dynamic case.

F. Unified Theory for Perception and Planning
Professor Mark Campbell, Cornell University, Single Investigator Award

The objective of this research is to develop a unified theory for perception and planning to enable reasoned and intelligent planning as opposed to traditional reactive planning. Both object- and map-centric heterogeneous sensor fusion methods are being developed for detection, tracking and identification. Innovations may include the development and use of a probabilistic ground model as well as parts-based computer vision methods in order to improve tracking in cluttered environments. Ultimately, human-like driving behaviors are sought using a nonlinear, constrained optimization based path planner. Innovations include the incorporation of probabilistic models of the environment into the optimizer, including vehicle and obstacle locations, and obstacle motion. Formal guarantees will be explored for both vehicle stability, as well as numerical solutions. The unified theory will be analyzed and verified through a three step process, ranging from theoretical analysis to empirically driven simulations to full sized, robotic testbed validation.

This research resulted in several noteworthy accomplishments in FY12. First, the researcher developed a scalable method for reducing obstacle predictions, which is critical for planning in highly dynamic and complex environments. Second, a new terrain model based on Markov Random Fields was developed which probabilistically fuses general sensory information into a representation that is much easier to reason about in tracking, planning and control. Third, the investigator developed a new method for fusing information across a network of robots, which is robust to network configuration and changes. Fourth, a method for fusing stochastic maps across a network of robots was developed.

In FY13, the research team anticipates the publication if (i) a new method for fusing negative information, such as from occlusions, which dramatically improves tracking robustness, (ii) a new method for dynamic obstacle anticipation based on Gaussian Processes, and (iii) experimental validation of tracking, anticipation and trajectory planning algorithms on an autonomous vehicle.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Game Theoretic Approach to Spectral Sensing, Tracking, and Exploitation

Investigator: Professor Qing Zhao, University of California - Davis, Single Investigator Award
Recipient: Communications and Electronics Research and Development Center (CERDEC)

This project focuses on extending the learning techniques based on multi-armed bandit theory developed under the ARO project to support distributed battlefield environments and multi-dimensional performance metrics. A major objective of this 6.2 project is to transition the distributed learning algorithms developed under the ARO project to the CERDEC-STCD CNEDAT (Cognitive Network Design and Analysis Toolset) currently under development.

CERDEC is interested in establishing virtual network backbone via connected dominating sets (CDS) in unknown communication environments. Professor Zhao has been extending learning techniques developed under the ARO project to this more complex problem. Finding the minimum CDS even under known deterministic models is NP-hard and there is no study on learning algorithms for CDS under unknown and random network models. Leveraging extensive research experience on real-time learning, primarily developed under the ARO project, Professor Zhao has developed a learning algorithm with strong performance that scales with both the time horizon and the network size. Distributed implementations of the learning algorithms and the simulation platform are currently being developed for incorporation into the CNEDAT simulation platform. This will allow the characterization of the performance, convergence, and overhead of the learning algorithms for a number of typical military mobile ad hoc networking scenarios.

B. Cortical Networks Underlying Rapid Decision Making

Investigator: Professor Paul Sajda, Columbia University, Single Investigator Award
Recipient: ARL Human Research and Engineering Directorate (ARL-HRED)

The objective of this project is to investigate, using multimodal neuroimaging, the cortical networks involved in rapid decision making. The search for targets and anomalies in imagery/video occurs in the face of highly changing contextual information, such as current geo-politics, SIGINT, and HUMINT. How analysts do this, what differentiates an expert analyst from a novice, and what can be done to better train and prepare analysts and soldiers for making rapid decisions in the face of increasing complexity and uncertainty are all questions of substantial national security interest. In this project, the research team is attempting to couple high temporal resolution, single-trial analysis of electroencephalography (EEG) with simultaneously acquired fMRI to infer the constituent cortical networks of rapid decision-making in the human brain. Simultaneously acquired EEG/fMRI will enable more precise identification of cortical networks underlying rapid decision-making, including those processes involved in integration of contextual information and accumulation of multiple sources of evidence.

Professor Sajda has been very active in pursuing technology transition within the Army research community, particularly with the Translational Neuroscience Branch at ARL-HRED. Professor Sajda's collaborations with ARL-HRED have led to transition funding (6.2) of the basic science results which are the focus of this ARO project. Researchers at ARL-HRED have been working on methods to decode neural signatures of targets and task relevant events when presented using rapid serial visual presentation (RSVP). Through a transition to ARL-HRED, Columbia University's capability of simultaneously measuring EEG and fMRI has enabled ARL-HRED to gain a more comprehensive picture of the nature of the cortical networks involved during this task. This helps to guide the design of EEG electrode montages for fieldable systems, as well as potentially yield new insights for applications (*e.g.*, training). ARL-HRED have also been testing and developing a variety of single-trial EEG decoding algorithms. Columbia University has worked with ARL-HRED to analyze classifiers and EEG data collected in the MRI scanner.

C. Toward Algorithmic Advances for Solving Stackelberg Games
Investigator: Professor Milind Tambe, University of Southern California, Single Investigator Award
Recipient: U.S. Coast Guard

The goal of this research is to account for bounded rationality and, in particular, human behavioral models of risk assessment in devising strategies for solving security games. In particular, Professor Tambe has (i) developed tractable mathematical models including human behavior based on work in Psychology and Decision Science literature, especially that of Prospect Theory and Quantal Response Equilibirum Theory, (i) carried out an empirical evaluation of games with models of human behavior, and (iii) devised techniques for solving massive security games by making use of solution structure. The resulting algorithms have transitioned to the U.S. Coast Guard for use in solving problems related to resource allocation, such as scheduling patrol boats in the Boston Harbor and in NY/ NJ ports. The U.S. Coast Guard is now planning to extend deployment of the PROTECT system (algorithms based on Quantal Response Equilibrium) to other ports across the nation.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Continuum Models for Multi-Agent Cooperative Control

Professor Roger Brockett, Harvard University, Single Investigator Award

The objective of this research is to uncover a set of unifying principles that will advance the understanding of mobile agents moving under cooperative control. Despite two decades of progress concerning flock dynamics and empirical studies of animal behavior, rather few general principles capable of providing guidance about treating flocks as engineering systems have emerged. This project emphasizes a flexible control theoretic approach to multi-agent problems as opposed to focusing on systems for achieving a particular objective.

During FY13, research will study control theoretic versions of some common models based on a discrete collection of agents and as well as continuum models. The effort stands apart from earlier work based on continuum descriptions by virtue of its focus on control problems as opposed to providing a description of naturally occurring phenomena. In particular, the investigator will use applied analysis methods involving the partial differential equation description of ensembles and control theoretic methods for stabilization and trajectory optimization. Successful work in this direction will serve to broaden the conceptual underpinnings of the field of control by showing that cooperative flock dynamics can be seen as an extension of what has been previously understood and used by control engineers. It will also serve to clarify the potential for practical application of an important class of cooperative multi-agent systems.

B. Estimation and Uncertainty Quantification of Stochastic Systems

Professor Johanne Royset (PI), Naval Postgraduate School, and Professor R. Wets (Co-PI), University of California - Davis, Single Investigator Award

The objective of this research is to develop a flexible framework for estimation of density functions, regression curves, performance functions, and other quantities that systematically incorporates hard information derived from physics-based sensors, field test data and computer simulations, as well as soft information from human sources and experiences. The framework will be based on *epi-splines* for consistent approximation of infinite-dimensional optimization problems arising in the estimation process. Epi-splines could be viewed as constrained splines. However, their construction does not follow the standard spline-fitting techniques and they are focused on approximation instead of interpolation. Preliminary results indicate that the framework is highly promising computationally as well as theoretically (see FIGURE 3).

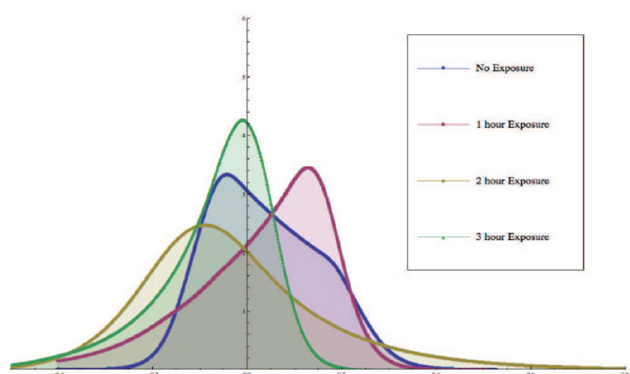

FIGURE 3

Preliminary results of estimation of epi-splines approximation of infinite-dimensional optimization problems arising in the estimation process. The data plots display an approximation of data related to U.S. Marine cognitive ability after waterborne motion using unimodal constraint and expectation constraint.

The project is a joint effort between the Naval Postgraduate School and the University of California, Davis, and focuses on two main thrust areas: (i) complex systems subject to random input parameters and development of epi-spline-based procedures for constructing functional models of the system as well as for estimating probability density functions, moments, quantiles, and rare events of the resulting random system performance, and (ii) in the context of target detection, tracking, and situational awareness, development of constructed epi-spline-based procedures for information fusion of 'hard' data from physics-based sensors with 'soft' contextual information and predictions from human sources pertaining to past, current, and future time periods. It is anticipated that in FY13 the investigators will develop epi-spline based procedures for information fusion. The anticipated results will provide fundamental advances in these areas in terms of theoretical understanding of statistical estimation, function approximation, and uncertain quantification as well as new model formulations and computational methods.

C. Propagation Analysis and Performance Assessment
Professor Michael Jensen, Brigham Young University, Single Investigator Award

The objective of this research is to model and experimentally verify the radio propagation channel that would be typical for dismounted soldiers, including multi-antenna scenarios. The use of multi-antenna systems on vehicles to increase throughput and reliability of tactical communications has been the topic of recent investigations. Multi-antenna systems can also improve the performance of dismounted soldiers. However, soldiers in combat situations often maneuver in ways that would be uncommon for a typical civilian user of wireless devices, and because the antennas for a soldier are likely placed in unconventional locations on the body the potential communication performance experienced in these channels are unique and relatively unexplored.

It is anticipated that in FY13, Professor Jensen will experimentally explore these channels for realistic combat-specific environments. Using the measured data, dynamic channel models will be created that abstract the actual channels in order to better understand the environmental effects on communications. Using these models and experimental data, Professor Jensen then plans on investigating multi-antenna communications techniques that are conducive to the dismounted combat environment. It is expected that a result of this basic research will be a fundamental understanding of the channel conditions that will facilitate the design of multi-antenna communications systems for the dismounted soldier.

D. Combinatorial and Scalable Initiation in Complex Networks
Professor Paolo Shakarian, U.S. Military Academy, Single Investigator Award

The aim of this research is to devise algorithms for computing combinatorial centrality measures that scale for extremely large data sets (i.e., networks with millions of nodes and edges). It is now a folk theorem that sets of elements which jointly optimize a function generally outperform sets of elements which do so individually in the majority of resource allocation problems. Unfortunately, as such combinatorial problems are often difficult to solve exactly (most being at least NP-hard), one often resorts to approximation algorithms in order to scale them to large datasets. The PI is addressing this problem for centrality measures on networks that are ideally suited for initiation of a diffusion process. In FY13, the PI will uncover the mathematical underpinnings of such problems, develop algorithms that scale for large networks, perform experiments on real-world data, and provide working prototype software. The PI will also leverage a multi-disciplinary approach embracing tools from computer science, mathematics, statistical physics, and theoretical biology. Initiation-type network problems of concern to the U.S. Army include information operations (identifying members of a social network that will jointly optimize the spread of a message in an IO campaign), counter-insurgency (identifying a set of villages that together optimize anti-insurgent influence over a large area), and negotiation (identifying a set of key influential individuals in a highly-decentralized organization whom it would be ideal to negotiate with). All of these initiation problems deal with identifying sets of nodes that jointly cause some phenomenon in the network to spread to a maximum extent.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Purush Iyer
Division Chief (Acting)
Program Manager, Intelligent Networks

Dr. Janet Spoonamore
Program Manager, Decision and Neuro-Sciences

Dr. Samuel Stanton
Program Manager (Acting), Multi-Agent Network Control

Dr. Robert Ulman
Program Manager, Communication and Human Networks

B. Directorate Scientists

Dr. Randy Zachery
Director, Information Sciences Directorate

Dr. Bruce West
Senior Scientist, Information Sciences Directorate

Dr. Ellen Segan
Science Advisor to the 18th Airborne Corps

Ms. Anna Mandulak
Contract Support

C. Administrative Staff

Ms. Debra Brown
Directorate Secretary

Ms. Diana Pescod
Administrative Support Assistant

CHAPTER 12: PHYSICS DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2012* is to provide information on the programs and basic research efforts supported by ARO in FY12, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Physics Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY12.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Physics Division supports research to discover and understand exotic quantum and extreme optical physics. The Division promotes basic research that explores the frontiers of physics where new regimes of physics promise unique function. Examples such as ultracold molecules, complex oxide heterostructures, attosecond light pulses, and quantum entanglement all represent areas where the scientific community's knowledge of physics must be expanded to enable an understanding of the governing phenomena. The results of these research efforts will stimulate future studies and help to keep the U.S. at the forefront of research in physics.

2. Potential Applications. Beyond advancing the world understanding of exotic quantum physics and extreme optics, the research efforts managed by the Physics Division will provide a scientific foundation upon which revolutionary future warfighter capabilities can be developed. The Division's research is focused on studies at energy levels suitable for the dismounted Soldier: the electron Volt and milli-electron Volt range. In the long term, the discoveries resulting from ARO physics research are anticipated to impact warfighter capabilities in the area of Command, Control, Communications, Computers, Intelligence, Surveillance, and Reconnaissance (C4ISR). Research advances in the Division can be readily visualized to impact sensor capabilities for increased battlespace awareness and Soldier protection, enhanced navigation, ultra-lightweight optical elements and low-power electronics for decreased Soldier load, and advanced computational capabilities for resource optimization and maximal logistical support.

3. Coordination with Other Divisions and Agencies. To meet the Division's scientific objectives and maximize the impact of discoveries, the Physics Division coordinates and leverages efforts within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multidisciplinary research topics, and evaluate the effectiveness of research approaches. For example, research co-funded with the Mathematical Sciences Division seeks coherent-feedback quantum control of collective hyperfine spin dynamics in cold atoms. Collaborative efforts with the Electronics Division are also underway with a goal of developing the science of magnetic materials and the engineering of agile radio frequency device concepts. The Physics Division coordinates efforts with AFOSR and DARPA in pursuit of forefront research advances in atomic and molecular physics, including ultracold molecules and optical lattices. The Division also coordinates certain projects with Intelligence Advanced Research Projects Activity (IARPA), the Joint Technology Office (JTO), and the Joint Improvised Explosive Device Defeat Organization (JIEDDO). These interactions promote a synergy among ARO Divisions and impact the goals and improve the quality of the Division's research areas.

B. Program Areas

To meet the long-term program goals described in the previous section, the Physics Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY12, the Division managed research efforts within these four Program Areas: (i) Atomic and Molecular Physics, (ii) Condensed Matter Physics, (iii) Optics and Fields, and (iv) Quantum Information Science. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Atomic and Molecular Physics. The goal of this Program Area is to study the quantum properties of atoms and molecules and advance a fundamental understanding of exotic quantum behavior. When a gas of atoms are cooled their quantum nature is dominate and their behavior becomes wave-like rather than a cloud of distinct particles. Accordingly experiments that were once the sole purview of optics are now possible with matter: interference, lasing, diffraction, and up/down-conversion, to name a few. This Program Area explores these concepts with an eye toward enabling new opportunities, such as novel quantum chemistry and atomic devices that exploit quantum behavior. The specific research Thrusts within this Program Area are: (i) State-dependant Quantum Chemistry, (ii) Atomtronics, and (iii) Non-equilibrium Many-body Dynamics. Ultracold gases can be trapped in a one, two or three dimensional standing optical waves enabling the exploration of novel physics, quantum phase transitions, and mechanisms operative in condensed matter. In optical lattices, one can also create a new "electronics" or atomtronics based on atoms and molecules, but with statistics, mass, charge, and many additional handles not available in conventional electronics. The State-dependent Quantum Chemistry Thrust is not focused on synthesis but rather on the underlying *mechanisms*, such as electronic transport, magnetic response, coherence properties (or their use in molecule formation/selection), and/or linear and nonlinear optical properties. While the notion of taking objects held at sub-Kelvin temperatures onto a battlefield may seem irrational, dilute atomic gases can be cooled to nano-Kelvin temperatures without cryogens (like liquid nitrogen or liquid helium). The cooling is accomplished with magnetic traps and lasers. The long-term applications of this research are broad and include ultra-sensitive detectors, time and frequency standards, novel sources, atom lasers and atom holography, along with breakthroughs in understanding strongly-correlated materials and our ability to design them from first principles.

2. Condensed Matter Physics. The objective of this Program Area is to discover and characterize novel quantum phases of matter at oxide-oxide interfaces and at the surfaces and interfaces of topological insulators. Recent studies have shown that interfaces can support quantum phases that are foreign to the bulk constituents. Furthermore the bond angles and bond lengths in complex oxides are controllable at interfaces. In general the interface provides a mechanism for potentially controlling lattice, orbital, spin and charge structure in ways that are not possible in bulk, single phase materials. If these degrees of freedom can be engineered in ways analogous to charge engineering in semiconductors, it will present new opportunities for the development of advanced technologies utilizing states beyond just charge. The foray into topological insulators began in FY11. Topological insulators represent a relatively recent discovery of a state of matter defined by the topology of the material's electronic band structure rather than a spontaneously broken symmetry. What is unique about this particular state is that unlike the quantum Hall state—which is also characterized by a topology—it can exist at ambient conditions: at room temperature and zero magnetic field. In general discovering, understanding, and experimentally demonstrating novel phases of matter in strongly correlated systems will lay a foundation for new technological paradigms. Nanometer-scale physics, often interpreted as a separate field, is also of interest as confined geometries and reduced dimensionality enhance interactions between electrons leading to unusual many-body effects. A critical component for gaining new insights is the development of unique instrumentation and this program supports the construction and demonstration of new methods for probing and *controlling* unique phenomena, especially in studies of novel quantum phases of matter.

3. Optics and Fields. The goal of this Program Area is to explore the novel manipulation of light and the formation of light in extreme conditions. Research is focused on physical regimes where the operational physics deviates dramatically from what is known. The specific research Thrusts within this Program Area are: (i) Negative Index Materials, (ii) Transformation Optics, and (iii) Extreme Light. Negative index materials (NIMs) are artificially fabricated materials whose collective response to light culminates in backward refraction. This program has a particular interest in the development of NIMs that are functional at visible wavelengths and some success has been achieved in this area. Advances have led to research in transformation optics, in which the index of refraction (both positive and negative) of optical materials, is a controllable function of position and possibly time. Possible applications include sub-wavelength imaging, flat or conformal optics, cloaking, and light collection. The Extreme Light Thrust involves investigations of ultra-high intensity light, light filamentation, and femtosecond/attosecond laser physics. High-energy ultrashort pulsed lasers have achieved intensities of 10^{22} W/cm^2. Theoretical and experimental research is needed to describe and understand how matter behaves under these conditions, including radiation reactions and spin effects, from single particle motion to the effects in materials, and how to generate these pulses and use them effectively. One consequence of ultra-high power lasers is light filamentation. Short, intense pulses self focus in the atmosphere until the intensity reaches the breakdown value where nitrogen and oxygen are ionized, creating a plasma. This new form of radiation creates a supercontinuum of coherent light across the visible spectrum. Ultra-short intense pulses can be utilized to develop attosecond pulses by combining them with high harmonic generation. Potential long-term applications of these pulses include imaging through opaque materials, laser pulse modulation, "observing" electron dynamics, and even controlling electron dynamics.

4. Quantum Information Science. The objective of this Program Area is to understand, control, and exploit nonclassical, quantum phenomena for revolutionary advances in computation and in secure communications. Three major Thrusts are established within this program: (i) Foundational Studies, (ii) Quantum Computation and Communication, and (iii) Quantum Sensing and Metrology. Research in the Foundational Studies Thrust involves experimental investigations of the wave nature of matter, including coherence properties, decoherence mechanisms, decoherence mitigation, entanglement, nondestructive measurement, complex quantum state manipulation, and quantum feedback. The objective is to ascertain current limits in creating, controlling, and utilizing information encoded in quantum systems in the presence of noise. Of particular interest is the demonstration of the ability to manipulate quantum coherent states on time scales much faster than the decoherence time, especially in systems where scalability to many quantum bits and quantum operations is promising. Quantum computation entails experimental demonstrations of quantum logic performed on several quantum bits operating simultaneously. Demonstrations of quantum feedback and error correction for multiple quantum bit systems are also of interest. There is particular interest in developing quantum algorithms for solving NP-complete problems for use in resource optimization and in developing quantum algorithms to simulate complex physical systems. Research in the Quantum Computation and Communication Thrust involves studying the transmission of information through quantum entanglement, distributed between spatially separated quantum entities. Long-range quantum entanglement, entanglement transfer among different quantum systems, and long-term quantum memory are of interest. An emerging field of interest is quantum sensing and metrology using small entangled systems. Entanglement provides a means of exceeding classical limits in sensing and metrology and the goal is to demonstrate this experimentally.

C. Research Investment

The total funds managed by the ARO Physics Division for FY12 were $30.2 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY12 ARO Core (BH57) program funding allotment for this Division was $5.9 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $8.4 million to projects managed by the Division. The Division also managed $6.7 million of Defense Advanced Research Projects Agency (DARPA) programs, and $5.9 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $0.7 million for contracts. Finally, $2.6 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY12 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research projects. Research projects are developed by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts.

The following subsections summarize projects awarded in FY12 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY12, the Division awarded fourteen new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to create and explore a large multi-qubit state in entangled photon pairs, to understand the emission, photon-photon interaction, and the ultrafast dynamics in nanorod metamaterials, and to cool and trap the strongly polar SrF molecule and then study its collisional and chemical properties in the ultracold regime. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Kenneth Brown, Georgia Tech University; *Probing Molecular Ions With Laser-Cooled Atomic Ions*
- Professor Zenghu Chang, University of Central Florida; *High Flux Isolated Attosecond XUV Source*
- Professor Brian DeMarco, University of Illinois - Urbana; *Quantum Simulation of the Disordered Fermi-Hubbard Model*
- Professor David DeMille, Yale University; *Laser Cooling and Trapping of Diatomic Molecules*
- Professor Martha Greenblatt, Rutgers, The State University of New Jersey - New Brunswick; *New Quasi Low-Dimensional 4d and 5d Transition Metal Oxides with Correlated Electronic Properties*
- Professor John Howell, University of Rochester; *Weak Value Precision Measurements of Magnetic Field, Cross-deflection Modulation and Frequency*
- Professor Eric Hudson, University of California - Los Angeles; *Understanding Molecular Ion-Neutral Atom Collisions for the Production of Utracold Molecular Ions*
- Professor Prem Kumar, Northwestern University - Evanston Campus; *Creating and Manipulating High-Dimensional Photonic Entanglement*
- Professor Margaret Murnane, University of Colorado - Boulder; *Bright Coherent Optical Waveforms from the IR to the VUV*
- Professor Viktor Podolskiy, University of Massachusetts - Lowell; *Nonlocal Plasmonic Metamaterials for Ultrafast and Nonlinear Optics*
- Professor Ana Maria Rey, University of Colorado - Boulder; *Exploring New State of Matter with Ultra-cold Polar Molecules*

- Professor Subir Sachdev, Harvard University; *Dynamics of Quantum Matter with Long Range Entanglement*
- Professor Kyle Shen, Cornell University; *Momentum-resolved Inverse Photoemission Spectroscopy System For the Investigation of Complex Electronic Materials*
- Professor Chuanwei Zhang, University of Texas - Dallas; *Spin-orbit Coupled Ultra-cold Atomic Gases: Fundamentals and Applications*

2. Short Term Innovative Research (STIR) Program. In FY12, the Division awarded five new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to design an optical lattice using ^{7}Li which will improve the fundamental rate at which processes evolve in optical lattice experiments by a factor of 100, and to study the epitaxy of topological insulators on silicon and characterize film growth mechanisms. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor John Howell, University of Rochester; *Weak Value Cross-Phase Modulation*
- Professor Wolfgang Ketterle, Massachusetts Institute of Technology; *High Power Optical Lattices for a Lithium-7 Quantum Simulator*
- Professor Paul Kwiat, University of Illinois – Urbana; *Advanced Quantum Sensing*
- Professor Vito Scarola, Virginia Polytechnic Institute and State University; *Modeling the Stability of Topological Matter in Optical Lattices*
- Professor Chih-Kang Shih, University of Texas at Austin; *Influence of Surface Steps on Molecular Beam Epitaxy of Topological Insulators*

3. Young Investigator Program (YIP). In FY12, the Division awarded two new YIP projects. These grants are driving fundamental research, such as the exploration of methods to control the magnitude and spatial homogeneity of electronic bandwidth in oxide materials. The following PIs and corresponding organizations were recipients of the new-start YIP awards.

- Professor James Rondinelli, Drexel University; *Ab initio Design of Noncentrosymmetric Metals: Crystal Engineering in Oxide Heterostructures*
- Professor Steven May, Drexel University; *Symmetry Mismatched Heterostructures: New Routes to Bandwidth Control in Oxides*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY12 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *2nd International Conference on Quantum Error Correction*; Los Angeles, CA; 5-9 December 2011
- *Workshop on Chemical Sensing and Quantum Manipulation with Molecular Ions*; Atlanta, GA; 3-4 March 2012
- *Mechanical Systems in Quantum Regime Gordon Research Conference;* Galveston, TX; 4-9 March 2012
- *Workshop on Linear and Nonlinear Optical Interactions in Metamaterials and Plasmonic Nanostructures*; Huntsville, AL; 23-24 April 2012
- *7th International Conference on Semiconductor Quantum Dots*; Santa Fe, NM; 13-18 May 2012
- *Multiphoton Processes Gordon Research Conference*; South Hadley, MA; 3-8 June 2012
- *43rd Annual Meeting of the American Physical Society Division of Atomic, Molecular, and Optical Physics*; Orange County, CA; 4-8 June 2012
- *Workshop on Recent Developments in Electronic Structure Theory*; Winston-Salem, NC; 5-8 June 2012
- *Plasmonics Gordon Research Conference*; Waterville, ME; 10-15 June 2012
- *Workshop on Linear and Nonlinear Optical Interactions in Metamaterials and Plasmonic Nanostructures*; Huntsville, AL; 20-22 June 2012
- *Correlated Electron Systems Gordon Research Conference*; South Hadley, MA; 24-29 June 2012
- *Workshop on Oxide Interfaces by Design*; Newport, RI: 9-10 July 2012
- *21st International Laser Physics Workshop*; Calgary, Alberta, Canada; 23-27 July 2012

- *Workshop on Complex Oxide Heterostructures*; Cambridge, MA; 7-8 August 2012
- *Kavli Institute for Theoretical Physics, Dynamics and Thermodynamics in Isolated Quantum Systems Symposium*; Santa Barbara, CA; 20-24 August 2012
- *Optical Society of America, Cavity Optomechanics Incubator Symposium*; Washington, DC; 30 September - 2 October 2012

5. Special Programs. In FY12, ARO Core Research Program funds provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded three new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Record-fast Laser Pulses for New Studies in Physics. This MURI began in FY07 and was awarded to a team led by Professor Zenghu Chang at Kansas State University; however, Professor Shuting Lei is now the lead PI with Professor Chang as co-PI, due to Professor Chang's transition to the University of Central Florida. The objective of this research is to investigate methods for generating extremely short laser pulses.

Attosecond (one quintillionth of a second or 10^{-18} s) laser pulses are a new regime and are expected to revolutionize physics and technology just as the femtosecond (one billionth-billionth of a second, or 10^{-15} s) era did. Just as the previous epoch ushered in a new generation of physics and engineering, attosecond science is expected to provide the foundation for unprecedented achievements, ranging from precision laser surgery to quantum molecular control. Such short pulse generation is now possible due to the recent attainment of record high laser intensities (10^{22} W/cm^2) coupled with breakthroughs in chirped-envelope phase control. The researchers are attempting to develop attosecond pulses that approach the atomic timescale (~25 attoseconds), which will provide the first opportunity to monitor, understand, and eventually control the molecular electronics underlying any physical, chemical and biological system. Potential future Army-relevant applications include gas-phase reaction studies (*i.e.*, combustion), molecular electronics in nanoparticles (*e.g.*, nanotubes, nanorods, quantum dots), and electronic coherence studies in solids (*e.g.*, for building faster electronic devices). The vast spectrum in the Fourier decomposition of these ultrashort pulses demonstrates that they contain components above the plasma frequency for any substance and will, therefore, propagate through solid materials. This property provides the basis for a new kind of imaging, with applications ranging from weapon detection to uncovering defects in materials.

2. Conversion of Quantum Information among Platforms. This MURI began in FY09 and was awarded to a team led by Professor Christopher Monroe at the University of Maryland. The objective of this MURI is to explore the conversion of quantum information from one form to another.

Since the inception of research in quantum information, a number of platforms have been explored to implement quantum information: trapped ions, ultracold atomic gases, semiconductor quantum dots, superconductors, and others. Each of these systems has a unique advantage while also suffering disadvantages in other areas. For example, trapped ions are relatively easy to manipulate and are readily isolated from the environment. However they cannot be readily scaled up to the size necessary for practical applications. Semiconductors are perfect for that, but the quantum information is too quickly lost to the surrounding material for a practical computation to occur. To address these matters, the MURI is considering the potential for converting quantum information from one platform to the other without losing the quantum nature of the information. In particular the intra-conversion of information between atomic systems, solid state systems, and optical systems will be explored. If the best of each platform can be combined and the detrimental problems avoided, then the development of quantum information capabilities will be accelerated. The advent of a quantum computer will provide solutions to problems that are computationally intractable on conventional computers, impacting resource optimization and improved logistical support.

3. Harnessing Electronic Phenomena at Oxide Interfaces. This MURI began in FY09 and was awarded to a team led by Professor Susanne Stemmer at the University of California - Santa Barbara. The objective of this research is to investigate the unexpected electronic effects found to exist at the interfaces of certain crystalline oxides.

Recent studies have shown that carefully designed and grown interfaces between different crystalline oxides can lead to electronic phenomena at that interface that are foreign to the oxides that form it. These studies have suggested the potential for a new type of electronics technology; therefore this new MURI aims to determine if these effects can be designed and controlled. The research focuses on the Mott transition: a metal-to-insulator transition that results from electron-electron repulsion. The objective is to design and control the oxide-oxide interface as a new approach to understanding, predicting and controlling the Mott metal-insulator transition and the associated electronic phenomena. The electronic energy states that determine the character of the material are tied to the metal-oxygen atom distance in the crystal and the crystal symmetries. Accordingly the team will construct alternating layers of a material containing a known Mott metal-insulator transition with an insulator that will affect the bonding distances and symmetry of the adjacent Mott material. The ability to control this transition may lead to new options for enhancing logic, memory and other technologies important for advanced computational capabilities.

4. Transformation Optics - Exploring New Frontiers in Optics. This MURI began in FY09 and was awarded to a team led by Professor David Smith at Duke University. The objective of this research is to explore new frontiers in optics made possible by the discovery of negative-index materials (NIMs).

In current optics technology, light refracts (bends) as it passes from one material to another. By curving a surface, such as a lens, refraction is used to focus light. Unfortunately this process loses some of the information contained within the light. As a result, current lenses, such as those used in a microscope, essentially prevent the user from viewing objects smaller than the wavelength of visible light (*i.e.*, limited to about 0.5 micrometers). NIMs can be designed through the use of metamaterials (*i.e.*, artificial materials engineered to provide specific properties not available in naturally-made structures) or by the construction of photonic crystals.

A prior MURI award (FY06-FY11) that was managed by the ARO Physics Division and led by Professor Vlad Shalaev at Purdue University, pioneered many early discoveries and advances in NIMs that in turn manifested a new field in optics termed transformation optics. By combining the negative refraction of NIMs with an index of refraction that varies spatially and temporally, optical materials can be designed to have properties not possible with conventional optics. This MURI team, which includes Professor Shalaev as a co-investigator, is exploring this new frontier in physics. The researchers are investigating methods of controlling light by design, routing it where conventional optics cannot. For example, with transformation optics, light of a particular wavelength can be bent around an object rendering the object invisible at that wavelength. This has already been demonstrated in the microwave band but has not yet been shown at the wavelengths of visible light. The second objective is the development of a flat hyperlens: a lens that is flat on both sides and not only magnifies but also resolves nanometer-scale features. This lens could provide a resolution at least an order of magnitude beyond the diffraction limit of conventional optics. Not only can transformation optics be used to bend light around an object but it can also be used to bend light toward an object. The third major objective is to design materials accordingly such that light from all directions is concentrated on a single detector. These concentrators could revolutionize optical sensors and solar energy collection as its omnidirectional nature eliminates the requirement of moving parts.

5. Atomtronics: an Atom-Analog of Electronics. This MURI began in FY10 and was awarded to a team led by Professor Ian Spielman of the University of Maryland. The objective of this MURI is to explore and understand the concepts of atom-based physics, beginning with the rich and fundamental physics discoveries already revealed with cold atoms systems and to investigate the concepts required for future device applications.

Atom-based physics studies (atomtronics) are analogous to, but will go beyond, the fundamental twentieth century studies regarding the properties of electrons (*i.e.*, electronics) that enabled the electronics revolution. Solid-state electronics, heralded by the transistor, transformed both civilian and military culture within a generation. Yet there is only a single kind of electron: its mass, charge and spin (and thus quantum statistics as well) are unalterable. Atoms on the other hand, come with different masses, can have multiple charge states, and have a variety of spin and other internal quantum states. Accordingly studies in atomtronics aim to understand an atom-based physics rather than electron-based device physics. Breakthroughs in cold atom physics and degenerate quantum gases presage this new kind of device physics. That cold atom science has resulted in atomic analogies to other technologies, such as optics and lasers, suggests that the same may be repeated with electronics. Very good analogies of solids and junctions can be made with trapped atoms. It is now well-known how one, two and three dimensional structures with essentially any lattice geometry can be formed in cold, trapped atoms. Presently a few theory papers are pointing the way to simple devices.

The most apparent, but not necessarily the only approach to atomtronics, is through optical lattices, where Bloch's theorem holds. Band structure is the first basis on which physicists understand traditional (electronic) metal, insulator, and semiconductor behavior. Interaction and disorder modify this and exploration of Mott-like and Anderson-like insulators and transitions are envisioned as well. Doping can be mimicked by modifying atoms in certain wells or by locally modifying the lattice potential, which can be done with additional optical fields. Such defects could be deeper or shallower wells, or missing, or could be additional sites. Recent breakthroughs involving three dimensional optical lattices and the loading of atoms into lattices with reasonably long lifetimes have set the stage for atomtronics.

Atomtronics researchers are focused on two key themes devices and connections. The envisioned analogs to devices can be described as those that perform actions under external control and those that are cascadable. The researchers will explore spin-orbit coupling in atomic systems in an effort to exploit new degrees of freedom in "spintomic" devices as well as novel reversible logic via cascadable spintomic gates. In addition researchers will investigate far from equilibrium regimes, which is not possible in condensed matter systems due to the residual phonon interactions at finite temperatures. The second theme centers on connections and is split between analogs to electronics and novel interfacing. The research team will use the superfluid properties of ultracold atoms confined in rings to create circuits. These small circuits will interact with lasers to demonstrate an analogous SQUID device. Finally the researchers will explore novel interfacing by trapping atoms with evanescent waves along ultrathin optical fibers. It is hoped that this technique will allow several devices to be coupled while remaining isolated from the environment.

6. Multi-Qubit Enhanced Sensing and Metrology. This MURI began in FY11 and was awarded to a team led by Professor Paola Cappellaro at the Massachusetts Institute of Technology. The objective of this research is to explore and demonstrate imaging, sensing and metrology beyond the classical and standard quantum limits by exploiting entangled multi-qubit systems.

Precision measurements are among the most important applications of quantum physics. Concepts derived from quantum information science, such as quantum entanglement, have been explored for the past decade to enhance precision measurements in atomic systems with important potential applications such as atomic clocks and inertial navigation sensors. Quantum information science has also enabled the development of new types of controlled quantum systems for the realization of solid-state qubits. These systems could potentially be used as quantum measurement devices such as magnetic sensors with a unique combination of sensitivity and spatial resolution. However, progress towards real-world applications of such techniques is currently limited by the fragile nature of quantum superposition states and difficulties in preparation, control and readout of useful quantum states. The power of entangled and squeezed states for quantum sensing lies in their sensitivity to the external parameter to be measured.

This MURI effort aims to overcome three major obstacles to practical quantum sensor operation: the difficulty to experimentally create desired entangled many-qubit input states to the sensing device, the fragility of the states during signal acquisition, and low fidelity of the readout process. The results of this research may ultimately lead to dramatic improvements in imaging, sensing, and metrology.

7. Light Filamentation. This MURI began in FY11 and was awarded to a team led by Professor Martin Richardson at the University of Central Florida. The objective of this research is to establish the underlying qualitative and quantitative understanding of the physical phenomena associated with light filaments in order to create and control the filaments and their associated unique properties.

A light filament is a novel form of propagating energy that is a combination of a laser beam and plasma. A light filament has three characteristics that make it unlike any other form of energy, and also make it ideal for remote detection of trace materials. Like laser light, a light filament is coherent. However, unlike laser light, as the beam propagates it undergoes wavelength dispersion, creating a coherent beam with wavelengths across the entire visible spectrum. Since the beam contains laser radiation at every wavelength, it is sometimes called a super-continuum or white laser. The continuum has a high UV content, which makes it of interest for remote chemical spectroscopy. Finally, by beating the diffraction limit, a light filament does not diverge in space. Unlike any other form of energy propagation, a light filament can be as small at a distant target as it was when it was created. Light filaments are formed when intense laser pulses are focused down, due to the nonlinearity of the air (the Kerr effect), to about 100 microns. At this point, the intense field ionizes the nitrogen and oxygen, creating a plasma. The plasma stops the self-focusing and equilibrium is reached. The complex interaction of the plasma and electromagnetic field creates these unique properties of light filaments. Although light filaments are extremely rich in phenomena for potential applications, the complex interaction of optical, plasma, and electromagnetic behaviors is poorly understood.

The research team is attempting to create light filaments and understand and predict light filament propagation characteristics, length, interactions with matter, and electromagnetic interactions. If successful, this research could ultimately lead to controllable light filaments that would revolutionize remote detection and imaging through clouds, creating a new ability in standoff spectroscopic detection.

8. Surface States with Interactions Mediated by Bulk Properties, Defects and Surface Chemistry. This MURI began in FY12 and was awarded to a team led by Professor Robert Cava at Princeton University. This project is exploring the recently-discovered class of materials known as topological insulators.

A topological insulator is a material that behaves as a bulk insulator with a metallic surface (permitting the movement of charges on its surface). The concept of topological insulators is a recent development in condensed matter physics which heralds a regime in which as-yet-undiscovered physics is playing a role.

The objective of this research is to advance the discovery, growth, and fabrication of new bulk- and thin-film-based topologically-stabilized electronic states in which electron-electron interactions play a significant role. The research team is bringing strong materials science, chemistry and surface science approaches to bear on the study of the novel properties of topological insulators. Research in topological insulators is an area with great potential for long-term benefits for the Army, such as electronically-controlled magnetic memory and low-power electronics.

C. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY12.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY12, the Division managed one new-start Phase II STTR contract, in addition to active projects continuing from prior years. This new-start contract aims to bridge fundamental discoveries with potential applications by designing and fabricating an innovative device for laser-beam switching, deflection, and frequency shifting to address qubits for quantum computing applications.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY12, the Division managed one new REP award, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY12.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY12, the Physics Division managed seven new DURIP projects, totaling $1.5 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including the microscopic analysis of light filaments in air, and research to study topological insulators.

H. DARPA Information in a Photon (InPho) Program

The goal of this program, co-managed by the Physics Division, is to pursue the basic science and the associated unifying physical and mathematical principles that govern the information capacity of optical photons, exploiting all relevant physical degrees of freedom. Important outcomes of this program include (i) the rigorous quantification of photon information content for communications and imaging applications in both the classical and quantum domains, (ii) novel methodologies to maximize the scene information that can be extracted from received photons in next-generation imaging/sensing platforms, and (iii) novel methodologies to maximize the information content of transmitted/received photons in next-generation communication systems. This program builds upon ARO-supported advances in quantum information and optics and is expected to further advance the fields while also exploring opportunities for applications in sensing and communications.

I. DARPA Optical Lattice Emulator (OLE) Program

The goal of this program, co-managed by the Physics Division, is to develop methods to exploit the control of, and universal properties of, ultracold atoms confined in optical lattices to simulate the quantum properties of bulk materials. A better understanding of the properties of novel artificial materials can be made possible using exquisite control of the microscopic state and interactions of the atoms. Furthermore, specific phase transitions can be simulated to complete our understanding of the fundamental processes that governs high-temperature superconductivity. This program was motivated in large part by the Physics Division and compliments many ARO-supported research efforts in ultracold gases, providing theoretical and experimental synergy to the Core BH57 Program.

J. DARPA Quantum Assisted Sensing and Readout (QuASAR) Program

The goal of this program, co-managed by the Physics Division, is to bring state-of-the-art science of metrology and sensing and combine them with today's technological developments. The program goal is to bridge the gap between the best scientific performance and the appropriate packaging for fielding high-performance working sensors that are relevant to the DoD. This program was motivated in large part by the Physics Division and compliments many ARO-supported research efforts in ultracold gases, providing theoretical and experimental synergy to the Core program.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Physics Division.

A. Electrostatic Doping of a Metal-Insulator Transition Without Ionic Liquids

Professor Susanne Stemmer, University of California - Santa Barbara, MURI Award

The MURI team led by Professor Stemmer is investigating methods for the control of Mott metal-insulator transitions (MIT) at complex metal oxide interfaces, with the ultimate goal of predicting, understanding, and controlling the unique potential capabilities associated with Mott MITs. In FY12, the research team reported[1] tuning of a Mott MIT by electrostatic doping, revealing that the insulating state involves correlations beyond the pure Mott physics.

A Mott insulator is a correlated state in which Coulomb repulsion between electrons opens a band gap (insulating behavior) in what would otherwise be a partially-filled band (metallic behavior) of electronic states. In a material that exhibits a Mott MIT, there is a metallic state at high temperatures and as the temperature is reduced, the Mott insulating state arises below some transition temperature. According to pure Mott physics, doping a Mott insulator should modify the band structure leading to a metallic state. However, many Mott insulators involve additional correlations that make the insulating nature at low temperatures robust against doping. Accordingly, a host of other states such as magnetic phases and superconductivity are related to the Mott insulator state. In general, the Mott MIT is one of the deepest unsolved problems in condensed matter physics. An understanding of these properties could ultimately enable a new revolution akin to the discovery of the integrated circuit. To understand these materials and probe the nature of the insulating state, doping to levels of $\sim 10^{21}$ cm^{-3} is an essential experimental capability. This doping level cannot be achieved with standard metallic gates. Chemical doping has been the standard route, but this modifies the structure of the material and thus, potentially, the relevant physics. Lately, electrostatic doping with ionic liquids has been a promising and widely adopted approach because it can provide the necessary doping levels. Yet ionic liquid doping is prone to electrochemical changes (*i.e.*, reduction) of the metal oxide also changing the relevant physics. Interestingly, Professor Stemmer has devised a way to use another complex oxide to provide large doping densities.

Lanthanum doping of $SrTiO_3$ can readily achieve bulk electron density levels of 10^{21} cm^{-3} and juxtapositioning a Mott insulator such as $NdNiO_3$ next to heavily-doped La:$SrTiO_3$ can provide a source of charges for the Mott insulator, as recently demonstrated by Professor Stemmer's laboratory. The band alignment between these two materials was shown to result in electron transfer from the La:$SrTiO_3$ to the $NdNiO_3$. On an insulating substrate, 5 nm of La:$SrTiO_3$ was grown by molecular beam epitaxy followed by an ultrathin layer of $NdNiO_3$. For 2.5 nm thick $NdNiO_3$ films, La doping levels of the $SrTiO_3$ of zero, 10^{19}, 10^{20}, and 10^{21} cm^{-3} were investigated. At the highest La doping level, enough electrons were transferred to the $NdNiO_3$ Mott insulator to cause an average of a 6% change in the carrier concentration throughout the film.

If the $NdNiO_3$ were a pure Mott insulator, this doping level would destroy the insulating state and cause the film to become metallic. However, a metallic state was not recovered for any doping level. Instead, the transition temperature to the insulating state merely shifted from ~150 K to ~120 K (see FIGURE 1). These results suggest that the phase diagram of $NdNiO_3$ is very rich and that series of detailed studies will be necessary to elucidate the phases of the doped Mott insulator. Thus, Professor Stemmer's team has demonstrated a method for doping in a Mott insulator without introducing a concomitant change in the material. While it is possible that an oxide used to provide the charges may modify the symmetry or strain state of a material, judicious choices of the doping oxide can minimize or eliminate this potential effect. The approach demonstrated by Professor Stemmer's laboratory may become a standard method within the field of complex oxide studies.

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[1] Son J, Jalan B, Kajdos A, Balents L, et al. (2011) Probing the metal-insulator transition of $NdNiO_3$ by electrostatic doping. *Appl. Phys. Lett.* 99:192107.

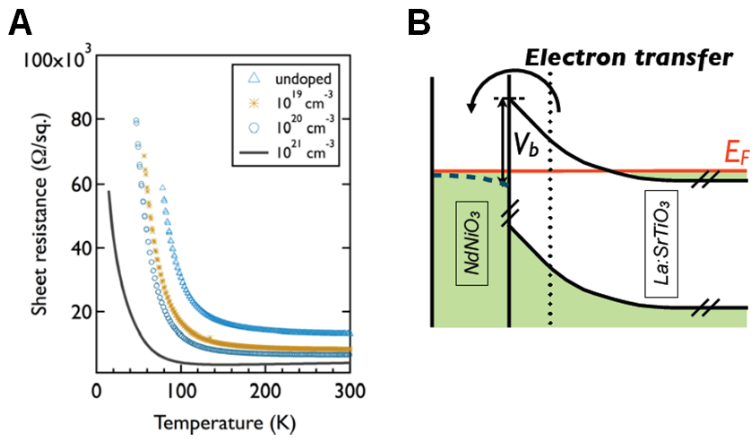

FIGURE 1

Change in temperature-dependent sheet resistance of La-doped $NdNiO_3$ films. (A) The sheet resistance of epitaxial, 2.5-nm thick $NdNiO_3$ thin films on La-doped $SrTiO_3$ changed as a function of La-dopant concentration in $SrTiO_3$. (B) A schematic of the expected band lineup at the interface between metallic $NdNiO_3$ and La:$SrTiO_3$ illustrates electron transfer La:$SrTiO_3$, decreasing sheet resistance of $NdNiO_3$. The dashed lines indicate the position of a half filled d-band for an ideal Mott insulator. *[Son, et al. 2011]*

B. Probing the Dirac Spectrum of a Topological Insulator

Professor Nai Phuan Ong, Princeton University, Single Investigator Award

A topological insulator is an insulator in which the typical ordering of electronic bands in an insulator has been flipped, typically by spin-orbit coupling. This re-ordering is such that when it is brought into contact with an insulator with the typical arrangement (even such as vacuum or air) that the required connectivity between bands of like parity forces electronic states to cross the Fermi level. The consequence is a metallic state at the interface, or in the case of the normal insulator being vacuum, at the surface. Because the metallicity is due to the topology of the electronic structure, it is robust against disorder. Since x-ray spectroscopy confirmed the existence of these theoretically states, this topic has become most verdant in condensed matter physics. Its importance can hardly be overstated. In the 1980s, the discovery of the quantum Hall effect ushered in a new era in which the old paradigm of new phases being the result of a broken symmetry no longer applied. Now topology can provide new phases without breaking symmetry. The quantum Hall effect and its related physics all exist at ultralow temperatures and high magnetic fields. The topological insulator states, however, are the first topological state that can exist at ambient conditions; magnetic fields and low temperatures are not necessary. Since the advent of the spectroscopic confirmation of the topological states, the aspiration of researchers has been to demonstrate the topological nature of the topologically-protected states using the most sensitive of electronic probes: electronic transport. FIGURE 2 shows a topological insulator prepared for such studies and the spectroscopy that reveals the topological states.

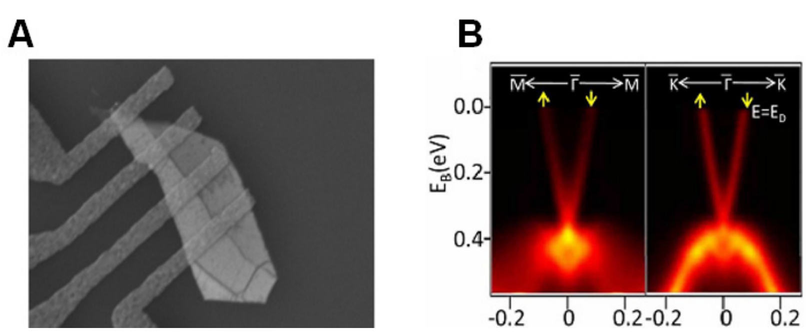

FIGURE 2

Topological insulator. (A) A flake of exfoliated Bi_2Te_2Se prepared with electrodes for transport studies. (B) Angle-resolved photoelectron spectroscopy of Bi_2Te_2Se clearly revealing the topologically protected states. The thin lines denoted by the yellow arrows are the topological states. The Dirac point—the point where the topological states cross—occurs very close to the bulk valence band readily observed at ~0.4 eV.

Since the discovery of topological insulators only a few years ago, no one has been able to definitely demonstrate electronic transport in a topological insulator that is governed unambiguously by the topological states. The challenge is due to bulk defects which provide an alternate conduction path which obscures conduction through the topologically-protected states. Every known topological insulator is prone to electrically-active point defects. The highest quality topological insulators to date are Bi_2Se_3 and Bi_2Te_2Se and the lowest defect levels observed are on the order of 10^{16} cm^{-3}; sufficiently high to obscure the topological physics.

To overcome this problem, Professor Ong employed two tricks: magnetotransport to distinguish two-dimensional from three-dimensional conduction and gating to deplete carriers from the bulk. In magnetotransport, the conductivity oscillates with applied magnetic field. The magnetic field quantizes the electronic energy levels into bands (Landau levels) that pass through the Fermi level as the magnetic field is varied giving rise to what are called Shubnikov-de Haas or quantum oscillations. The nature of these oscillations can be used to not only distinguish between 2D and 3D conduction but also between typical parabolic band dispersion and a linear dispersion. A linear dispersion, referred to as a Dirac spectrum, is a hallmark of topological states. The presence of bulk carriers, however, increases the magnetic field required to observe the important oscillations when electrons only occupy the lowest Landau levels. To access these levels, Professor Ong's team utilized ionic liquid gating while carefully guarding against the detrimental electrochemistry to which the method is susceptible. FIGURE 3 shows the quantum oscillations for two samples with various gate biases. For sample 2, the shift of the oscillations toward lower magnetic field is readily noticeable. The hallmark of a topological surface state in magnetotransport is that inverse of the magnetic field, 1/B, is proportional to the Landau level filling, n, plus ½. This additional ½ comes from the lowest Landau level being populated with both holes and electrons and is what distinguishes it as a Dirac spectrum.

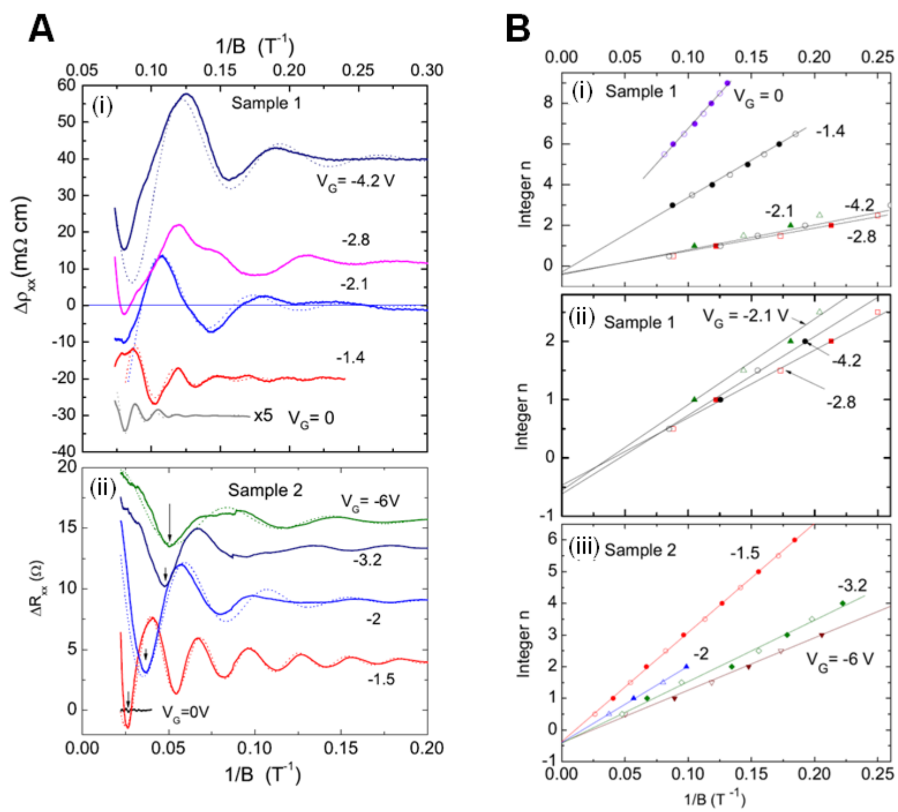

FIGURE 3

Quantum oscillations of a topological state. (A) Quantum oscillations of the conductance as a function of the inverse of the magnetic field for two samples with varying gate voltages. Note that with increasing magnitude of bias the oscillations shift to lower field. (B) The relationship between the Landau levels and the magnetic field strength. Filled circles indicate oscillation maxima, corresponding to an integer number of filled Landau levels. Open circles indicate oscillation minima, corresponding to a half-integer number of filled Landau levels. Note that filling lower Landau levels is only possible with a gate voltage > 0. Intercepts converge on -1/2.

While the lowest Landau level occupied is n = 1, the data cleanly extrapolates to -½. These results are the most effective signature of topologically-protected states in transport measurement published to date. Given that the studies involve large magnetic fields, the community awaits evidence of the topological states from transport measurements conducted at ambient conditions.

C. Spin-optics in Metamaterials

Professor Natalia Litchinitser, The State University of New York (SUNY), Single Investigator Award

The goal of this project is to investigate fundamental optical phenomena at the interface of singular optics ("structured light") and metamaterials ("structured media"). This research, led by Professors Natalia Litchinitser (PI) and Alexander Cartwright (co-PI) at the University at Buffalo, SUNY, and by Professor Grover Swartzlander (co-PI) at the Rochester Institute of Technology, is providing some of the first detailed, theoretical and experimental studies of linear and nonlinear light-matter interactions of vector and singular optical beams in metamaterials. Understanding the physics of the interaction of complex beams with nanostructured "engineered" matter is likely to bring new dimensions to the science and applications of complex light, including novel regimes of spin-orbit interaction, extraordinary possibilities for dispersion engineering, novel possibilities for nonlinear singular optics, trapping and optomechanical micromanipulation, as well as significant potential for applications in optical signal processing.

In FY12, the research team developed numerical models and an experimental method to generate and characterize cylindrical vector beams and vortices in nanostructured engineered optical metamaterials, designed to control the propagation and polarization properties of light. The team fabricated optical fiber based components for experimental realization of radially-polarized optical vortices and fiber-based magnetic metamaterials (see FIGURE 4).

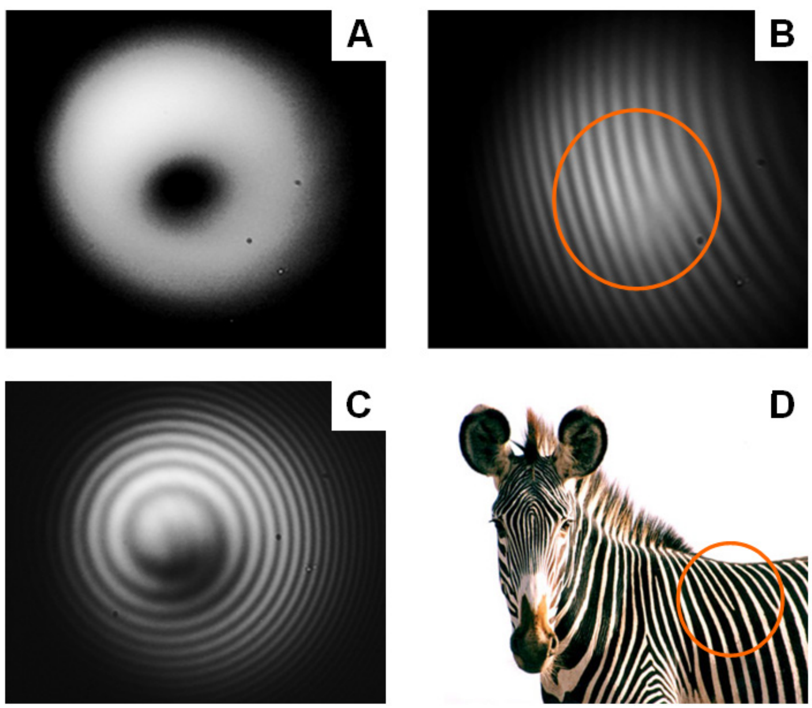

FIGURE 4

Experimentally-generated radially-polarized vortex beam. The beam has a characteristic (**A**) intensity profile, (**B**) fork interference pattern produced by interfering the vortex beam with a plane wave similar to a zebra pattern in (**D**), and (**C**) fork interference pattern produced by interfering the vortex beam with a spherical wave.

The team also performed a detailed characterization and numerical modeling of generated vortex beams and their interaction with magnetic metamaterials (see FIGURE 5). The changes in the polarization state of the beam after its propagation through the metamaterial were analyzed by inserting an additional rotating polarizer. These results revealed that (i) in the off-resonance case, the metamaterial structure acts mainly as a strongly anisotropic grating polarizer resulting into a 2-lobe pattern with a major dark line remaining in the same direction independent of the position of an analyzer (an additional linear polarizer), and (ii) in an on-resonance case, the pattern evolves from a 2-lobe one to a nearly donut shaped pattern with a major dark line rotating with the analyzer. Detailed theoretical studies of the changes in the polarization state in the latter case are in progress. In summary, the researchers successfully designed an all-fiber based radially polarized vortex-metamaterial system, and conducted detailed investigation of the interactions of such vortices with magnetic metamaterials was performed. These studies suggest that the propagation of vector vortex beams in magnetic metamaterial structures results in a complex evolution of the polarization state of the beam on magnetic resonance, while the orbital angular momentum remains intact.

In addition, the researchers investigated the theoretical interactions of singular beams with negative index metamaterials and performed initial studies of vortex-based second harmonic generation in NIMs. These studies indicate that magnetic metamaterials could be used to manipulate complex polarization states, while negative index materials could be used to engineer phase front of singular beams. Moreover, these initial theoretical studies predict that vortex-based nonlinear optical processes, such as second harmonic generation or parametric amplification that rely on phase matching, will also be strongly modified in negative index materials. This is due to the fact that for vortices the Poynting vector is not collinear with the direction of the beam as it has an azimuthal component while phase and energy velocities are antiparallel in NIMs. These results could ultimately enable multidimensional information encoding for secure communications. The experimental methods and results from this research are described in more detail in the research team's recent publications [2-3]

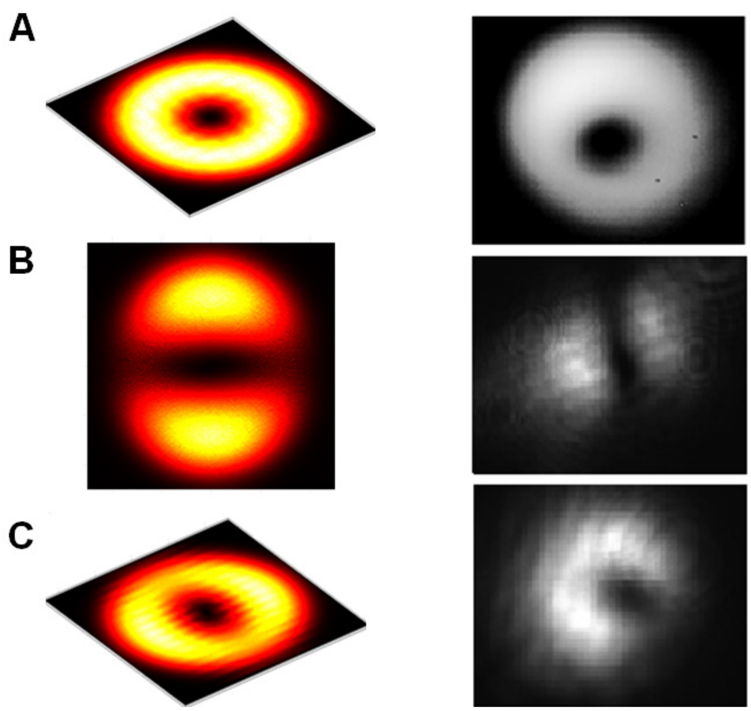

FIGURE 5

Theoretical predictions versus experimental results for radially polarized vortex-magnetic metamaterial interactions. The panels show the calculated intensity profiles (left column) and experimental intensity distributions (right column) for the cases of a radially polarized vortex beam propagation in (**A**) free space, (**B**) in magnetic metamaterial off-resonance, and (**C**) in magnetic metamaterial on-resonance.

[2] Wang X, Venugopal G, Zeng J, et al. (2011). Optical fiber metamagnetics. *Opt. Express* 19:19813-21.

[3] Litchinitser NM. (2012). Structured light meets structured matter. *Science* 337:1054-5.

D. Low Power Quantum Illumination

Professor Jeffrey Shapiro, Massachusetts Institute of Technology (MIT), Single Investigator Award

Quantum illumination (QI) is a novel technique for achieving an advantage over classical-state illumination in target detection in a high loss and high noise environment. The goal of this project is to theoretically and experimentally quantum entanglement based measurements. In FY12, the research team successfully implemented a table-top QI experiment (see FIGURE 6). For this experiment, multi-temporal-mode entangled signal and idler beams were generated by spontaneous parametric downconversion (SPDC) in a 4-cm-long periodically poled magnesium oxide-doped lithium niobate (MgO:PPLN) crystal. PPLN is highly nonlinear and its copolarized frequency-nondegenerate outputs at the signal and idler wavelengths of 1638 nm and 1500 nm, respectively, can be easily separated with a nearly lossless dichroic mirror (DM). The signal photon number per mode N_s is much less than unity and the number of temporal modes was estimated to be about 1012 per second. The signal beam was phase modulated with a square-wave π-phase modulation depth at 16 kHz for clean detection in an audio spectral region that was free of significant technical noise. The signal was attenuated to simulate the loss expected in a target detection scenario. Noise from a broadband diode laser was added to the attenuated signal to simulate the high noise environment, with a noise photon number per mode N_B in the range of 40–100 . The returned signal with noise was then combined with the continuous-wave pump and the retained idler beam for phase-sensitive detection using a low-gain optical parametric amplifier (OPA) as the joint quantum receiver. The OPA output at the idler wave-length was directly detected using an InGaAs avalanche photodiode and an ultralow-noise transimpedance amplifier. The observed signal was then measured using an audio spectrum analyzer (see FIGURE 7).

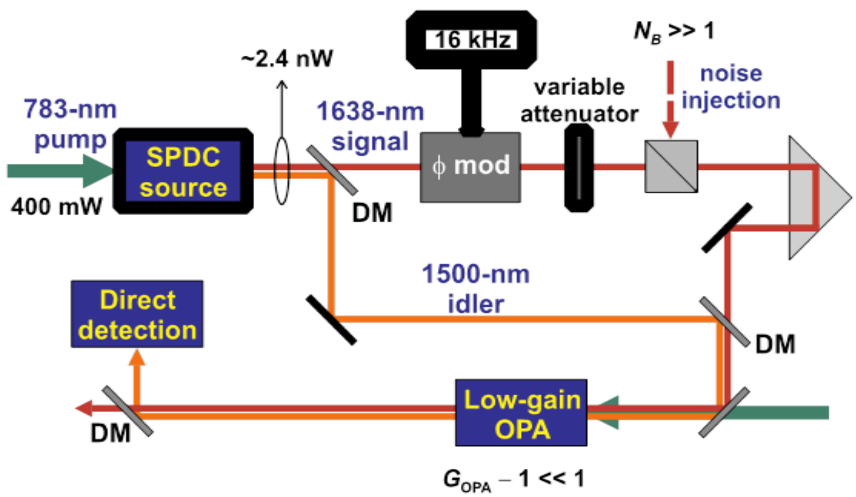

FIGURE 6

Table-top quantum illumination experiment. The schematic illustrates the experimental setup for QI-based target detection under high-loss and high-noise conditions (SPDC, spontaneous parametric downconversion; DM, dichroic mirror; OPA, optical parametric amplifier).

The OPA receiver output shown in FIGURE 7 was made with a SPDC pump power of 400 mW at 783 nm yielding approximately 2.4 nW of signal and idler outputs, with a corresponding photon-pair number per temporal mode of 0.007. The higher pump power, relative to previous experiments, was derived from a tapered amplifier chip that boosted the available power from 100 mW to 400 mW. The overall attenuation for signal and idler were 95% and 20%, respectively. Injected noise N_B averaged 50 photons per mode, which is much larger than that of the photon-pair number per mode N_S. As shown in FIGURE 7A, a high signal-to-noise ratio (SNR) of over 50 dB in a 1-Hz bandwidth was detected despite the high loss and high noise operating conditions. As shown in FIGURE 7B, the measured signal the signal beam from the SPDC was blocked as if the target were absent, demonstrating that in the absence of the target, the noise photons and the retained idler did not generate any measurable signal at the OPA receiver.

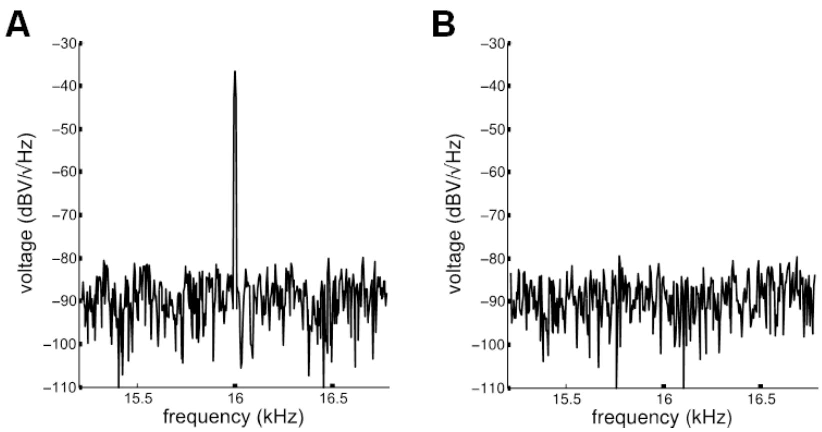

FIGURE 7

OPA receiver output displayed on an audio spectrum analyzer. The spectra of OPA output is shown in the (A) prescence and (B) absence of the target. SPDC signal beam was modulated at 16 kHz to yield high SNR of over 50 dB in a 1-Hz bandwidth.

E. Quantum Devices Using InAs Nanowires Operated in the Few-Electron Regime

Professor Jason Petta, Princeton University, PECASE Award

The goal of this project is to develop indium-arsenide (InAs) nanowire quantum dots for coherent control of single spins using all electrical techniques. In FY12, the researchers developed a MOCVD reactor that allows the growth of high quality, defect free, InAs nanowires to fabricate bottom-gated devices. Although technically more challenging, the bottom-gate configuration was chosen because of difficulties with the top-gated approach in previous experiments. In the bottom gate approach, narrow depletion gates were defined directly on an oxidized silicon substrate prior to the introduction of nanowires, and a thin silicon nitride dielectric was deposited on top of these gates. A suspension of nanowires was then deposited directly on large arrays of these gates, and individual nanowires fell out of suspension into random locations on the chip (see Figure 8). Nanowires which fell across a gate pattern were located using optical microscopy. Finally, contacts to the nanowire and the gate electrodes were defined in a single step of electron beam lithography. As shown in Figure 8, a typical bottom-gated sample was achieved and the results demonstrated that the few-electron regime could be reached and Pauli blockade observed. Pauli blockade is a necessary ingredient for readout of the spin state in double quantum dot type devices.

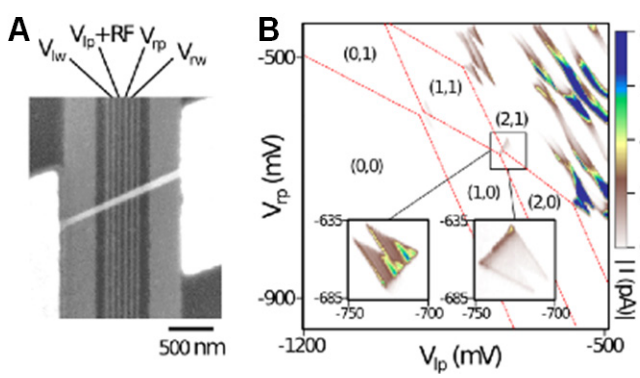

FIGURE 8

Fabrication of bottom-gated devices and demonstration of Pauli blockade. (A) The bottom-gated InAs nanowire DQD was approximately 55 nm in diameter and the depletion gates were approximately 30 nm in width, with a 60 nm pitch. The two large 'sidegates' are used to optimize the transparency of the nanowire leads. (B) The measured DQD charge stability diagram revealed that the few electron regime with nanowires of diameter 50-60 nm could be routinely attained. Pauli blockade allows for spin state readout.

Utilizing these devices, single spin rotations driven by electric dipole spin resonance were demonstrated. Previously, only continuous wave electric dipole spin resonance was detected. The investigators also demonstrated spin-orbit driven Rabi oscillations by combining voltage pulses on depletion gates with synchronized bursts of microwave excitation (see FIGURE 9). These results revealed that the spin-orbit interaction can be used to drive efficient single spin rotations, with spin selectivity provided by local electric fields and g-factor anisotropy.

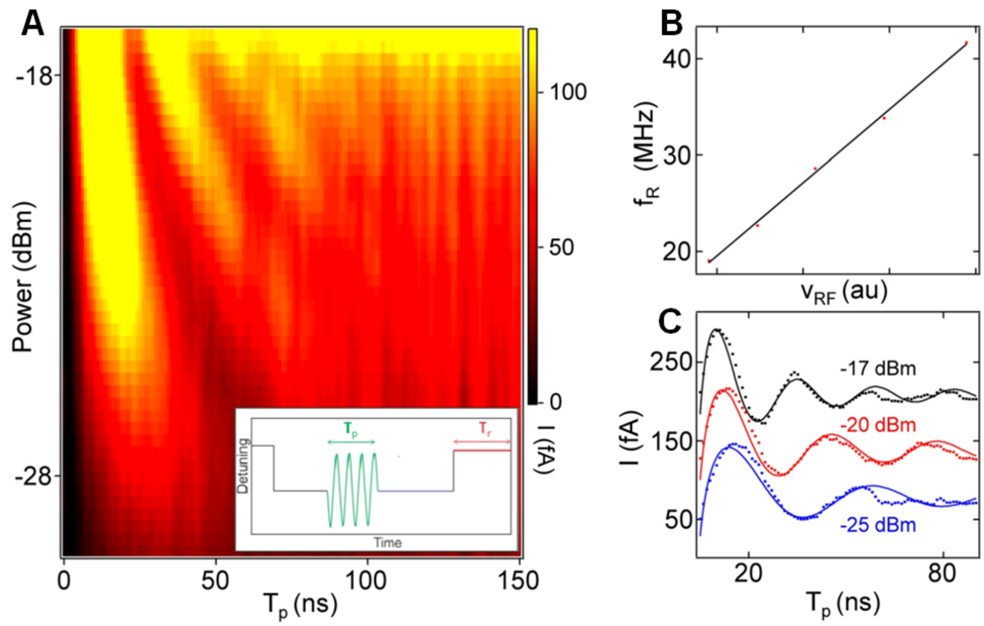

FIGURE 9

Demonstration of driven Rabi oscillations. The panels show (A) driven Rabi oscillations were measured in a single InAs nanowire double quantum dot, (B) Rabi frequency as a function of driving amplitude, and (C) cuts through the experimental data from (A).

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. First Superradiant Laser: Toward mHZ Linewidth Lasers

Investigator: Professor James Thompson, University of Colorado, STIR Award
Recipient: DARPA

The goal of this recently-completed STIR award was to investigate the prior theoretical predictions of Meiser, Holland, and Ye using a highly flexible test bed consisting of laser-cooled Rb atom in an optical cavity. The advantage of the test system chosen was that many key parameters could easily be varied, including the excited state linewidth, the atom number, the repumping rate, and cavity resonance frequencies. The immediate goal was not to realize a mHz laser source, but rather to explore the underlying physics, verify many of the key predictions, motivate extensions of the theory, and inform future efforts to build an ultra-narrow laser source for future study. In FY12, research by the Thompson laboratory, JILA, and NIST demonstrated the first superradiant laser that can control the wavelength of emitted light with a precision over ten thousand times better than conventional lasers, which may ultimately provide improved accuracy in navigation and sensing devices. This remarkable discovery was made possible through an ARL-ARO funded STIR award, a short-term award given to explore some of the highest-risk and potentially highest-payoff research.

The wavelength and coherence of a conventional laser is determined by the length of the cavity, as photons are reflected back and forth between the mirrors many times before exiting. However, minute fluctuations in the cavity length, due in part to temperature or mechanical vibration of the cavity mirrors, lead to a variation in the wavelength of the emitted light (see FIGURE 10).

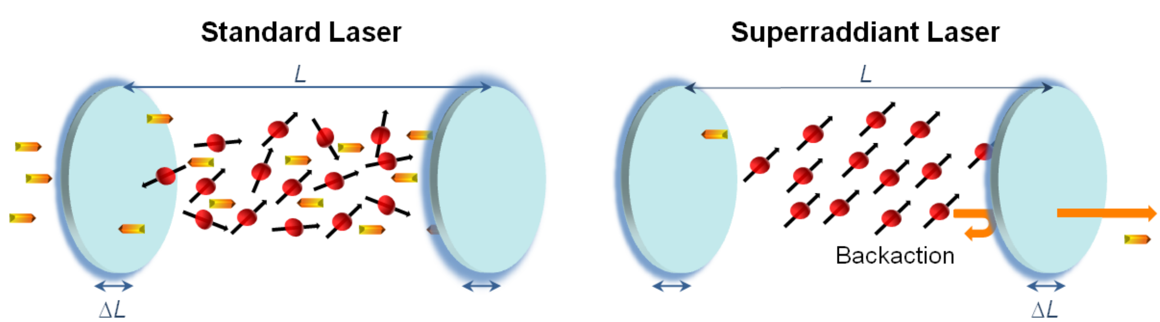

FIGURE 10

Standard laser versus superradiant laser. In a standard laser (top), an atomic medium is used to generate the laser light, but the phase of light is scrambled slightly due to vibrations in the mirrors, which in turn cause fluctuations (imprecision) in the frequency of light emitted. In contrast, in a superradiant laser (bottom) the laser frequency depends only very weakly on the distance between the mirrors. (Thermal Fluctuations = ΔL; Cavity length = L)

To create the superradiant laser, the investigators used ultracold atoms that were made to be coherent (i.e., superradiant) independent of mirrors (see FIGURE 11). This fundamental difference provides unprecedentedly small linewidths of 1 mHz or less—a factor of 2 to 3 orders of magnitude better than state-of-the-art (see FIGURE 12). In addition to instantly improving frequency and phase stability of the best clocks, the coherence length of such light would cover Earth-Sun distances, making it an attractive tool for very long baseline optical interferometry. The experimental methods and results from this research are described in more detail in the research team's recent publication.[4]

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[4] Bohnet JG, Chen Z, Weiner JM, et al. (2012). A steady-state superradiant laser with less than one intracavity photon. *Nature*. 484:78-81.

These results recently to DARPA for investigation of potential applications of this new type of laser, such as integration into atomic clocks for improved precision in timekeeping, precise navigation, and improved communication and sensing devices (*e.g.*, ultra-precise gradiometers).

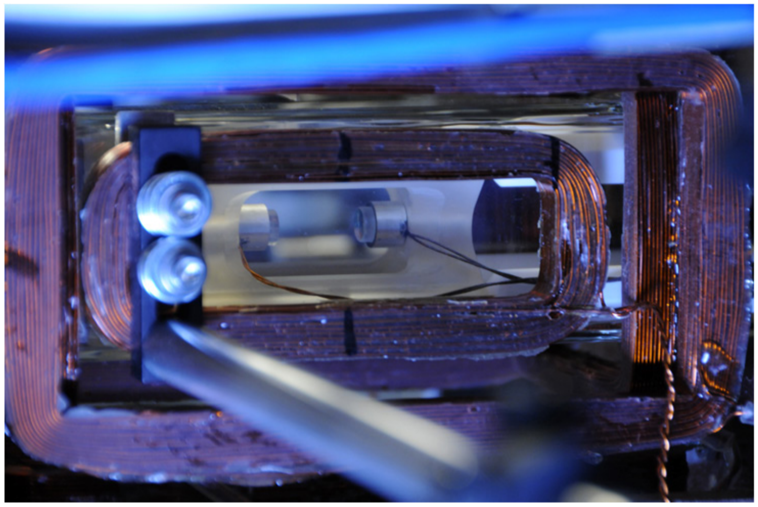

FIGURE 11

Superradiant laser cavity. The superradiant laser traps 1 million rubidium atoms between two mirrors, in a space of about 2 cm (center of image). The ultracold atoms, having synchronized their internal oscillations, are superradiant and will emit coherent laser light.

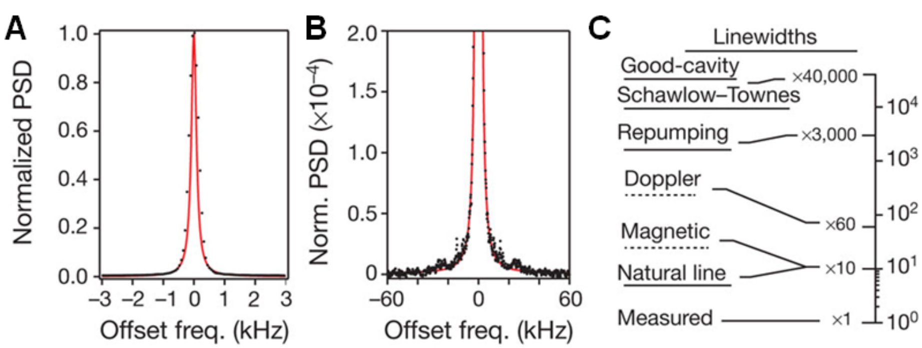

FIGURE 12

Beyond good-cavity, optical laser stability. The panels display (A) the power spectrum (PSD) with measured Gaussian FWHM, 350(25)Hz, four orders of magnitude smaller than the Schawlow-Townes linewidth limit, (B) A Lorentzian fit that excludes offset frequencies of less than 4 kHz yields a FWHM of 4.5(5) Hz, still larger than the 10(2)mHz linewidth predicted, and (C) a linewidth scale comparison. *[Bohnet et al. 2012]*

B. Nanoparticle-enhanced Liquid Crystal Phase Shifter

Investigator: Professor Zbigniew Celinski, University of Colorado - Colorado Springs, MURI Award
Recipients: Communications-Electronics Research, Development and Engineering Center (CERDEC), Industry

During the latter stages of a 2004 MURI on the physics of the interaction of GHz frequency electromagnetic fields with magnetic materials, Dr. Celinski and his team investigated new birefringent liquid crystals with embedded nanoparticles and demonstrated how these could be utilized in delay lines and phase shifters. In close collaboration with former CERDEC Scientist Dr. John Kosinski, Dr. Celinski and his colleagues pursued this technological concept and recently were awarded a patent on the device concept. The liquid crystal phase shifter concept is not new. By applying an electric field across a liquid crystal infused delay line, the re-orientation of the liquid crystal molecules changes the dielectric permittivity and thus changes the propagation velocity of the radio frequency (RF) electromagnetic field. This approach is limited, however, in the amount of phase shift that can be induced per length of delay line, and the size of these delay lines may be prohibitive for certain applications.

In their patent, Dr. Celinski and his colleagues described incorporating ferroelectric nanoparticles with shape anisotropy along with the liquid crystal. The shape of the nanoparticles ensures a permanent electric dipole and also a handle by which the liquid crystal molecules can rotate the nanoparticles when an electric field is applied or turned off. Because ferroelectrics have a larger dipole than liquid crystals, the overall permittivity is increased, enhancing the change in the RF electromagnetic field velocity. Dr. Celinski's team indicated a phase shift per applied voltage could be roughly twice that of liquid crystals without ferroelectric nanoparticles. This development increases the application space available to liquid crystal phase shifters, providing engineers with more opportunities for advanced RF technologies. Recently, industrial partners have shown interest in considering the approach for several RF applications.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Manipulating an Oxide's Electronic Bandwidth Through Structural Control

Professor Steven May, Drexel University, YIP Award

One of the major emerging themes in the study of complex oxides is the exploitation of the recent discovery that the rotation angles of BO_6 octahedra in an ABO_3 perovskite can be controlled by juxtapositioning the perovskite with another with different structural parameters. In the not-so-distant past, the conventional wisdom borne out of experience with semiconductors has been that strain induced in an overlayer by a substrate with a different lattice constant causes a unit cell volume conserving tetragonal distortion in the overlayer. In perovskites, however, the rotational freedom of the BO_6 octahedron in each perovskite unit cell provides an alternative pathway to accommodate the non-bulk-like in-plane structure forced upon it by a substrate or other nearby oxides (see FIGURE 13). In addition to strain due to lattice constant mis-match, complex oxides come in a variety of crystalline symmetries. Exploiting these differences through heteroepitaxial growth—that of one complex oxide on another—allows one to force an oxide thin film into crystalline structures that are foreign to the oxide in bulk. This opportunity provides new vistas for novel materials and for fundamental studies of many-electron phenomena in oxides.

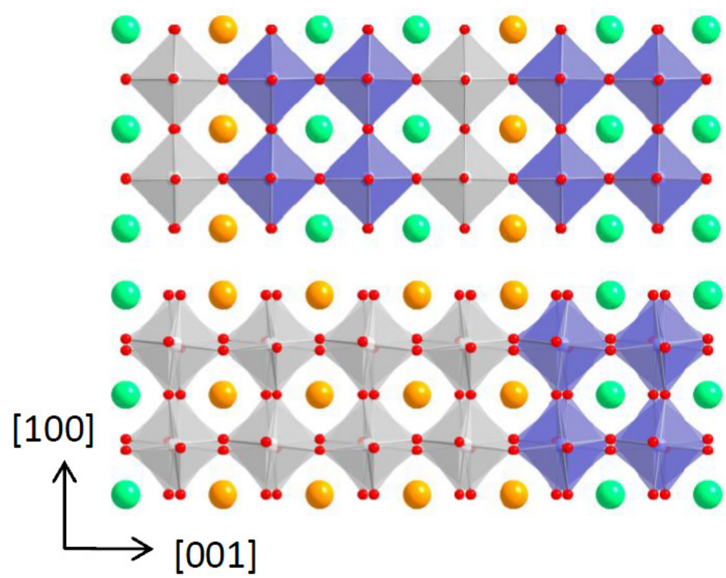

FIGURE 13

Example of controlling octahedral rotations. In the top image, $(LaNiO_3)_1(SrMnO_3)_2$ superlattices in which the cubic $SrMnO_3$ (blue/darker octahedra) dominates the $LaNiO_3$ (grey/lighter octahedra) which in bulk prefer to be rotated. In the bottom image, a superlattice with more $LaNiO_3$ layers than $SrMnO_3$ layers shows the nickelate dominating over the manganite such that the normally cubic $SrMnO_3$ is forced to follow the rotational pattern of $LaNiO_3$. *[May, et al., 2011]*

Professor May and his research team at Drexel University are employing this strategy with two goals and anticipated accomplishments in mind. First, the team is seeking to separate the effects due to induced crystalline symmetry and those due to lattice mis-match. Second, the team plans to use heterostructures of perovskites to induce octahedral rotational patterns that measurably modify the electronic bandwidth of the oxide. The bandwidth is the energetic extent of the bands near the Fermi level and is directly related to the B-O-B bond angles between octahedra. Modifying the octahedral rotations at will thus provides a mechanism for manipulating the bandwidth. Professor May is utilizing molecular beam epitaxy of perovskite manganites and ferrites in this study. Structural, chemical and electronic characterization will employ x-ray diffraction and spectroscopies and transport measurements. It is anticipated that bandwidth control will enable a new realm of electronic control in oxides paving the way for new concepts in advanced electronic materials and technologies.

B. Bright Coherent Optical Waveforms from the IR to VUV
Professor Margaret Murnane, University of Colorado - Boulder, Single Investigator Award

The goal of this project is to harness mid-IR lasers to create and characterize quasi-continuum waveforms spanning photon energies in the UV and VUV regions of the spectrum. It is anticipated that in FY13, this research will lead to the development of tunable, shaped, broadband light spanning the visible and deep-UV regions of the spectrum, with sufficient pulse energy (microjoules) to pursue applications of interest to DoD and the Army. A light source such as this, when coupled with advanced pulse shaping and learning algorithm technologies, would be would be of great interest for chemical and biological sensing, allowing new approaches to be developed that have potentially very high sensitivity.

The ultimate goal of these experiments is to learn how to manipulate the electrons that control localized chemical bonds between two atoms in a molecule. Chemical physics will benefit tremendously from the ability to excite shaped "electronic wave packets" in deep-UV absorbing molecules. Excitation of electrons in this wavelength regime might be used to weaken some bonds while strengthening others, driving a systematic rearrangement of a molecule's structure. This type of experiment would go far beyond present-generation control experiments. The resulting spectroscopy will also be a powerful tool for understanding molecular dynamics; for example, to directly probe the coupling between electrons in localized molecular bonds. The advanced laser technology and pulse shaping that will be used in this research may also have a significant impact on a broad range of topics in ultrafast science, including chemical sensing.

C. Low Power Quantum Illumination
Professor Jeffrey Shapiro, Massachusetts Institute of Technology (MIT), Single Investigator Award

Quantum illumination (QI) is a novel technique for achieving an advantage over classical-state illumination in target detection in a high loss and high noise environment. The goal of this project is to theoretically and experimentally quantum entanglement based measurements. Recent results from this project, led by the Shapiro laboratory, were described earlier in Section III.

It is anticipated that in FY13, further experiments will elucidate the advantages of quantum illumination versus classical illumination. Theory and experiments will be pursued in the use of optimal receivers for quantum illumination. The use of homodyne reception instead of an optical parametric amplifier will be studied. The final phase of the project will seek to conclusively demonstrate the performance advantage provided by quantum illumination over classical, coherent-state operation.

D. Quantum Devices Using InAs Nanowires Operated in the Few-Electron Regime
Professor Jason Petta, Princeton University, PECASE Award

The goal of this project is to develop indium-arsenide (InAs) nanowire quantum dots for coherent control of single spins using all electrical techniques. Recent results from this project, led by the Shapiro laboratory, were described earlier in Section III.

It is anticipated that in FY13, further experiments will demonstrate single-shot spin readout in the nanowire devices. This accomplishment would be a critical demonstration and capability for quantum information science experiments. In addition, the investigator will explore quantum control techniques to improve the coherence time of the electron spin state, and also techniques to transfer the electron spin state to nuclear spin. The coherence time of the nuclear spin is anticipated to be significantly better than for the electron spin and could serve as a quantum memory.

E. Quantum Computing and Control, and Quantized Non-Linear Optics with Superconducting Circuits
Professor Andrew Houck, Princeton University, PECASE Award

The objective of this project is to explore the strong coupling regime of a superconducting qubit and a microwave cavity. The tunable coupling qubit (TCQ) has been a key development in superconducting quantum devices. The TCQ has the potential for a new method of quantum non-demolition readout. In FY13, the Houck laboratory will explore methods to achieve high fidelity in the TCQ. Because the qubit has a V-like energy level spectrum, the extra level can be used for a cycling measurement, similar to the measurement used in ion traps. In principle this can achieve measurement fidelities in excess of 90%, without changing the following amplifier. This fidelity gain can be combined with recent gains from other groups in low noise amplifiers to achieve still higher fidelity. This high fidelity is important for any feedback control experiments. The TCQ can serve not only as a qubit, but also as a control element in more complex quantum circuits. In particular, the TCQ can act as a mechanism for tunable inter-cavity coupling with high on/off ratio, allowing each cavity to function as an isolated unit that can be coupled at will. The TCQ can also work to control photon-photon interactions, allowing a new control knob in quantum simulation experiments.

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