2013
ARO
IN REVIEW

U.S. Army Research Laboratory (ARL)
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ARO IN REVIEW 2013

A summary of the U.S. Army Research Office (ARO) research programs for fiscal year 2013 (FY13), including program goals, management strategies, funding information, and accomplishments

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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 Laboratory - Army Research Office (ARL-ARO) for fiscal year 2013 (FY13; 1 Oct 2012 through 30 Sep 2013). 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, life sciences, materials science, mathematical sciences, mechanical sciences, network 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 large and small businesses. ARO also ensures that the results of these efforts are transitioned to the Army research and development community for the pursuit of long-term technological advances for the Army.

II. ARO STRATEGY AND FUNCTION

ARO's mission represents the most long-range Army view for changes in its technology, with system applications often 20-30 years away. ARO pursues a long-range investment strategy designed to maintain the Army's overmatch capability in the expanding range of present and future operational capabilities. ARO competitively selects and funds basic research proposals from educational institutions, nonprofit organizations, and private industry. ARO executes its mission through conduct of an aggressive basic science research program on behalf of the Army to create cutting-edge scientific discoveries and the general store of scientific knowledge that is required to develop and improve weapons systems for land force dominance. The ARO research portfolio consists principally of extramural academic research efforts consisting of single investigator efforts, university-affiliated research centers, and specially tailored outreach programs. Each program has its own objectives and set of advantages as described further in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

The ARO strategy and programs are formulated in consultation with the ARL Directorates, the Research, Development and Engineering Command's (RDECOM's) Research, Development and Engineering Centers (RDECs), the Army Medical Research and Materiel Command (MRMC), the Army Corps of Engineers, and the Army Research Institute for the Behavioral and Social Sciences. ARO programs and research areas are intimately aligned with, and fully supportive of, the research priorities set within 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) Army Capabilities Integration Center's

Integrated S&T Lines of Effort, the Assistant Secretary of the Army for Acquisition, Logistics, and Technology [ASA(ALT)] Special Focus Areas, and the ASA(ALT) Triennial Basic Research Review. In addition, ARO's parent organization, the Army Research Laboratory, has eight Science and Technology Campaigns, including an extramural basic research campaign that ARO leads. For the other seven campaigns, which include research from Human Sciences to Materials, ARO supports research that will increase our fundamental knowledge and understanding of the physical, engineering, environmental, and life sciences as they related to long-term national security needs and the ARL Campaigns.ARO serves the following functions in pursuit of 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 STRATEGY

ARO employs multiple programs, initiatives, and investment 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 ARO-managed OSD research programs 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) 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, the reader is 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).

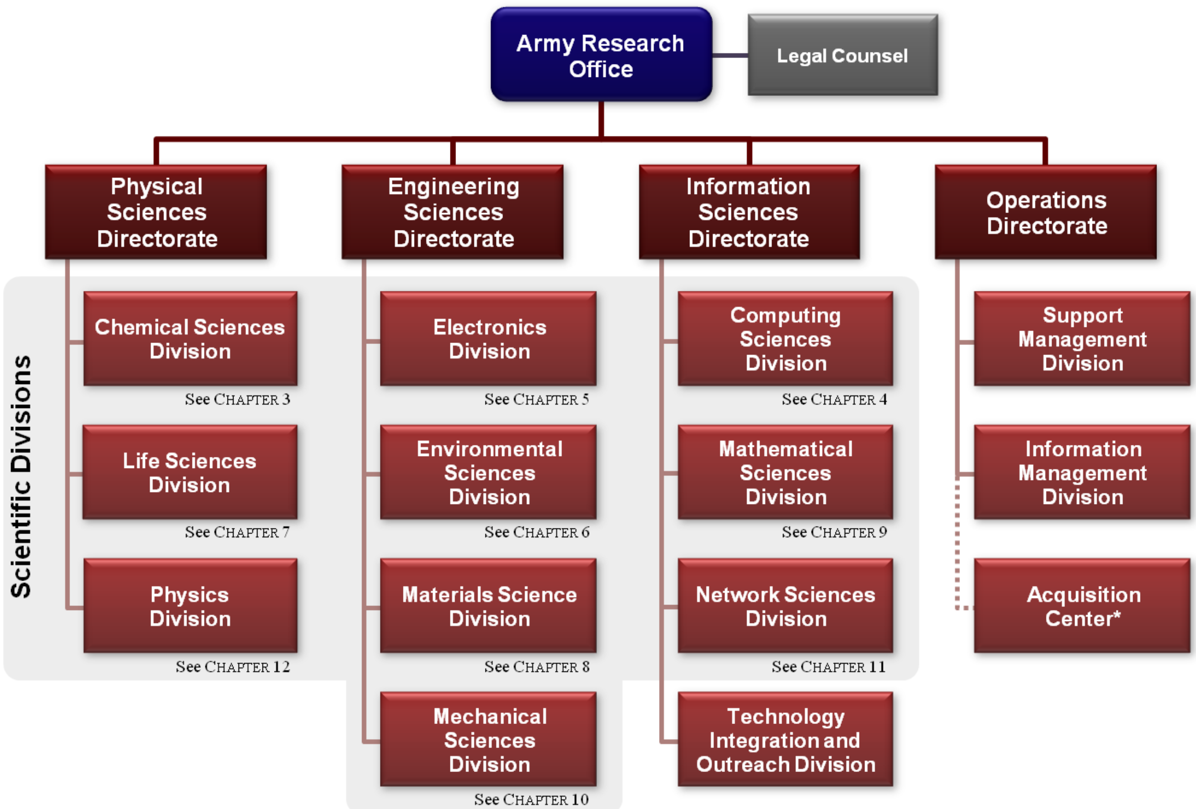

FIGURE 1

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 throughout 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, life sciences, materials science, mathematical sciences, mechanical sciences, network 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. It is noted that the ARO Divisions are not confined to only funding research in the departments that align with the Division names. The Divisions have the flexibility to find and fund the most promising research to advance their mission no matter what academic department it is in.

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. Army Funding

The Army funds the majority of the extramural basic research programs managed by ARO. 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)

ARO coordinates with the Office of the Secretary of Defense (OSD) in managing the URI programs and also manages the Army's Small Business Technology Transfer (STTR) program (see Section VIII).

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.

- 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). Each of these OSD-funded programs has a unique focus and/or a unique 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).

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]) to support a variety of external programs with specific research focuses. These joint programs have objectives consistent with the strategies of the corresponding ARO Program. Due to the unique nature of these cooperative efforts, each externally-funded effort is discussed within the chapter of the aligned scientific Division (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. ARO's Core (BH57) Research Program represents the principle mission of ARO and is where the majority of the Army funds are used. A summary of the 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 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 continuously-open, worldwide BAA solicitation. This program focuses on basic research efforts by one or two faculty members along with supporting graduate students and/or postdoctoral researchers and is typically a three-year grant.

B. Short Term Innovative Research (STIR) Program

The objective of the STIR Program is to explore high-risk initial proof-of-concept ideas 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 to Army-relevant research questions, to support their research, and to encourage their teaching and research careers. 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 meetings 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. In particular, workshops are a key mechanism ARO uses to identify new research areas with the greatest opportunities for scientific breakthroughs that will revolutionize future Army capabilities.

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 require a large and highly collaborative mutidisciplinary research effort.They are typically funded at $1.25 million per year for three years with an option for two additional 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 FY13. These projects are based on proposals submitted to the FY13 MURI topic BAA, which was released in late FY12. The new-start projects, lead investigators, and lead performing organizations 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.

- *Dynamic Artificial Cells Composed of Synthetic Bioorthogonal Membranes*; Professor Neal Devaraj, University of California - San Diego

  (Topic: *Artificial Cells for Novel Synthetic Biology Chassis;* Dr. Stephanie McElhinny, Life Sciences, and Dr. Jennifer Becker, Chemical Sciences)

- *Theory and Experiment of Co-crystals: Principles, Synthesis, and Properties;* Professor Adam Matzger, University of Michigan
  (Topic: *Molecular Co-Crystal Design and Synthesis;* Dr. James Parker, Chemical Sciences, and Dr. Chakrapani Varanasi, Materials Science)
- *Adversarial and Uncertain Reasoning for Adaptive Cyber Defense: Building the Scientific Foundation*; Professor Sushil Jajodia, George Mason University
  (Topic: *Reduced Cyber-system Signature Observability by Intelligent and Stochastic Adaptation*; Dr. Cliff Wang, Computing Sciences)
- *Fundamental Issues in Non-Equilibrium Dynamics;* Professor Cheng Chin, University of Chicago
  (Topic: *Non-equilibrium many-body dynamics;* Drs. Paul Baker and Marc Ulrich, Physics)
- *Materials with Extraordinary Spin/Heat Coupling;* Professor Roberto Myers, Ohio State University
  (Topic: *Materials with Spin Mediated Thermal Properties;* Dr. Pani Varanasi, Materials Science and Dr. Mark Spector, ONR)
- *Information Engines – Nanoscale Control, Computing, and Information Out of Equilibrium;* Professor James Crutchfield, University of California - Davis
  (Topic: *Transforming Information within Nonequilibrium Nanosystems*; Dr. Samuel Stanton, Mechanical Sciences)
- *Predicting and Controlling Systems of Interdependent Networks - Exploiting Interdependence for Control*; Professor Raissa D'Souza, University of California - Davis
  (Topic: *Controlling Collective Phenomena in Complex Networks*; Dr. Randy Zachery, Network Sciences and Dr. Samuel Stanton, Mechanical Sciences)
- No proposals were received for this MURI topic; therefore a selection could not be made.
  (Topic: *Physiochemical Determinants of Cognition and Decision Making;* Dr. Elmar Schmeisser, Life Sciences, and Dr. Janet Spoonamore, Mathematical Sciences)

The following topics were published in FY13 and constitute the ARO portion of the FY14 MURI BAA. The topic titles, topic author(s), and corresponding ARO Division(s) are listed below.

- *Attosecond Molecular Dynamics;* Dr. James Parker, Chemical Sciences and Dr. Richard Hammond, Physics
- *Force-Activated Synthetic Biology;* Dr. Stephanie McElhinny, Life Sciences, and Dr. David Stepp, Materials Science
- *Nonlinear Dynamics of Energy Hypersurfaces Governing Reaction Networks;* Dr. Ralph Anthenien, Mechanical Sciences, and Dr. Samuel Stanton, Mechanical Sciences
- *Strongly Linked Multiscale Models for Predicting Novel Functional Materials;* Dr. Joseph Myers, Mathematical Sciences, and Dr. Chakrapani Varanasi, Materials Science
- *Multistep Catalysis;* Dr. Robert Mantz, Chemical Sciences, and Dr. David Stepp, Materials Science
- *Innovation in Social Organisms;* Dr. Micheline Strand, Life Sciences, and Dr. John Lavery, Mathematical Sciences
- *Ultracold Molecular Ion Reactions;* Dr. Paul Baker, Physics, and Dr. James Parker, Chemical Sciences
- *The Skin-Microbe Interactome;* Dr. Virginia Pasour, Mathematical Sciences and Dr. Wallace Buchholz, Life 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 FY12 by ARO for consideration in the PECASE program, four investigators were selected in FY13 to receive PECASE awards. These awards began as "new start" projects in FY14 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.

- *Engineering Ferroic and Multiferroic Materials for Active Cooling Applications*,
  PI: Professor Lane Martin, University of Illinois - Urbana
  ARO PM: Dr. John Prater, Materials Science
- *Non-equilibrium Dynamics with Ultracold Atoms*
  PI: Professor David Weld, University of California - Santa Barbara
  ARO PM: Dr. Paul Baker, Physics
- *Complex Phenomena in Stochastic Filtering*
  PI: Professor Ramon van Handel, Princeton University
  ARO PM: Dr. Harry Chang, Mathematical Sciences
- *The Computational and Neural Basis of Reinforcement Learning in Multidimensional Environments*
  PI: Professor Yael Niv, Princeton University
  ARO PM: Dr. Virginia Pasour, Mathematical 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 FY13, the Army awarded 57 grants at $9,994,624 total, with an average award of $175K.

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 ASD(R&E) 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 the two UARCs listed below.

- 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. 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 basic 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 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 2-5 year projects dealing with effects of shifts in access to natural resources on civil conflict in different regions of the world, the relationship between social values and socio-political action, and the impact of property rights and ownership on social stability. ARO also provides scientific, technical, and managerial support to OSD in formulating the overall program.

The titles of ARO-managed Minerva projects that began in FY13 are listed below, followed by the name of the lead PI, the performing organization, and the award duration.

- *Forecasting Civil Conflict under Different Climate Change Scenarios,* PI: Professor Elisabeth Gilmore, University of Maryland - College Park, FY13-FY16
- *Homewonership and Societal Stability: Assessing Causal Effects in Central Eurasia,* PI: Professor Theodore Gerber, University of Wisconsin - Madison, FY13-FY16
- *The Human Geography of Resilience and Change: Land Rights and Political Stability in Latin American Indigenous Societies,* PI: Professor Jeremy Dobson, University of Kansas, FY13-FY16
- *Moral Schemas, Cultural Conflict, and Socio-Political Action*, PI: Professor Steven Hitlin, University of Iowa, FY13-FY14
- *Natural Resources and Armed Conflict,* PI: Professor James Walsh, University of North Carolina - Charlotte, FY13-FY16

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 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, 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 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 Phase II Enhancement, Fast Track (requires matching funds), or via the Commercialization Readiness Program (CRP).

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 FY13 SBIR and STTR Topics

The following SBIR and Chemical and Biological Defense SBIR (CBD-SBIR) topics were published in FY13 SBIR solicitations. The lead topic author and corresponding Division are listed following each topic title.

- *Responsive Sequestration Coatings*; Dr. Jennifer Becker, Chemical Sciences
- *Global Spatiotemporal Disease Surveillance System*; Dr. Jennifer Becker, Chemical Sciences
- *Wide Field-of-View Imaging System with Active Mitigation of Turbulence Effects for Tactical Applications*; Dr. Liyi Dai, Computing Sciences.

The following STTR topics were published in FY13 STTR solicitations. The lead topic author and corresponding Division are listed following each topic title.

- *Liquid Crystal-Based Sensors for Detection of Airborne Toxic Chemicals for Integration with Unmanned Robotic Systems*; Dr. Jennifer Becker, Chemical Sciences
- *Construction of 3D Terrain Models from BIG Data Set*; Dr. Michael Coyle, Computing Sciences
- *Solar-blind (Be,Mg)ZnO Photodetectors (260-285 nm wavelengths)*; Dr. Michael Gerhold, Electronics
- *New Approaches for Ammonia Synthesis*; Dr. Robert Mantz, Chemical Sciences
- *Non-Deteriorating Numerical Simulation of 3D Unsteady Wave Phenomena over Long Times*; Dr. Joseph Myers, Mathematical Sciences
- *Near Real-Time Quantification of Stochastic Model Parameters*; Dr. Joseph Myers, Mathematical Sciences
- *Additive Manufacturing of Multifunctional Nanocomposites*; Dr. Larry Russell, Mechanical Sciences
- *Chemical Analyzer System for In Situ and Real Time Surface Monitoring for Composition Control During Synthesis of Compound Semiconductor Films*; Dr. Pani Varanasi, Materials Science

D. ARO FY13 SBIR and STTR Phase II Awarded Topics

The following SBIR and CBD-SBIR topics were selected for a Phase II award in FY13. The lead topic author and corresponding Division are listed following each topic title.

- *Narrowband Perfect Absorber using Metamaterials*; Dr. William Clark, Electronics
- *Artificial Vaccines Based on DNA Origami*; Dr. Stephanie McElhinny, Life Sciences
- *Multisensory Navigation and Communications System*; Dr. Fredrick Gregory, Life Sciences
- *Fabrication of High-Strength, Lightweight Metals for Armor and Structural Applications*; Dr. Suveen Mathaudhu, Materials Science
- *Plasmonic Nanosensors for Chemical Warfare Agents*; Dr. James Parker, Chemical Sciences
- *UV-enhanced Raman Sensors with High SNR and Spectral Selectivity*; Dr. Michael Gerhold, Electronics
- *Direct Ethanol Fuel Cell*; Dr. Robert Mantz, Chemical Sciences
- *High-Strength, Nanostructured Aluminum Alloys*; Dr. Suveen Mathaudhu, Materials Science
- *Solid Acid Electrolyte Fuel Cell*; Dr. Robert Mantz, Chemical Sciences
- *Dislocation reduction in LWIR HgCdTe Epitaxial Layers*; Dr. William Clark, Electronics

The following STTR topics were selected for a Phase II award in FY13. The lead topic author and corresponding Division are listed following each topic title.

- *MEMS Based Thermopile Infrared Detector Array for Chem-Bio Sensing*; Dr. William Clark, Electronics
- *Multi-input/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
- *A11a-T011 High Risk Rapid Ethnographic Assessment Tool*; Dr. Joseph Myers, Mathematical Sciences
- *Biomimetic Membranes for Direct Methanol Fuel Cells*; Dr. Robert Mantz, Chemical Sciences
- *High-capacity, 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 Acoustic Resonators for Low-Loss Radio Frequency Devices*; 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 Using DNA Origami*; Dr. Stephanie McElhinny, Life Sciences
- *On Demand Energy Activated Liquid Decontaminants and Cleaning Solutions*; Dr. Jennifer Becker, Chemical Sciences

E. ARO FY13 SBIR Phase III Awarded Topics

The following SBIR topics were awarded a Phase III award in FY13. The lead topic author and corresponding Division are listed following each topic title. Phase III revenues can be obtained from Government or private customers, but cannot be SBIR funds.

- *Advancement of Capabilities, Products, and Sensors in Chem/Bio Detection, Quantification, and Mitigation IDIQ*; Dr. Stephen Lee, Chemical Sciences
- *Research and Development Supporting New EW Capabilities*; Dr. James Harvey, Electronics
- *Self-Contained Automated Vehicle Washing System*; Dr. Jennifer Becker, Chemical Sciences

F. 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 FY13 and funded by the Army, CBD, OSD and other sources with FY13 or FY12 funding is shown in TABLE 2.

TABLE 2

Total Funding for ARO-managed SBIR and STTR contracts awarded in FY13. Total funding (FY13 and reallocated FY12 funds) 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	$2,199K	$2,996K
Phase II	$8,218K	$8,357K
Phase II Fast Track	$497K	
Phase II Enhancement	$707K	-
CRP	-	-
Phase III	-	$19,795K
TOTAL	**$11,621K**	**$31,148K**

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 FY13 totaled $25.9 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 about $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 through the ARO Core Program BAA. There were 39 agreements with HBCU/MI institutions receiving over $2.5 million in funding through the ARO Core Program during FY13, including the 9 new starts. Unlike prior volumes of *ARO in Review*, these figures represent total funding for HBCU/MIs through the core program, both awards relying on matching funds and those not utilizing matching funds.

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.

- *Low Energy Ion Scattering Studies of Topological Insulator Materials*, Professor Jory Yarmoff, University of California-Riverside; Dr. Marc Ulrich, Physics
- *Fast Chemical Dynamics of Energetic Materials at High Pressures and Temperatures*, Professor Mohammad Mahmood, Howard University; Dr. James Parker, Chemical Sciences
- *Electromagnetics, Microwaves, and Power: Advanced Antenna Measurement Processing*, Professor Ronald Pogorzelski, California State University - Northridge; Dr. James Harvey, Electronics
- *Development and Detection of Mobile Malware*, Professor Hongmei Chi, Florida A&M University; Dr. Cliff Wang, Computing Sciences
- *Cybersecurity Dynamics*, Professor Shouhuai Xu, University of Texas at San Antonio; Dr. Cliff Wang, Computing Sciences
- *Online Tuning of All-Analog Radio Interference Cancellation*, Professor Yingbo Hua, University of California - Riverside; Dr. Robert Ulman, Network Sciences
- *Scalable Algorithms Based on Abstraction for Adversarial Reasoning Under Uncertainty (STIR),* Professor Christopher Kiekintveld, University of Texas at El Paso; Dr. Purush Iyer, Network Sciences
- *Untangling the Reaction Mechanisms Involved in the Explosive Decomposition of Model Energetic Materials (STIR)*, Professor Ralf Kaiser, University of Hawaii; Dr. James Parker, Chemical Sciences
- *The Smallest Thermal Machines and Quantum-Thermodynamic Processes for Energy Harvesting (STIR)*, Professor Ilki Kim, North Carolina A&T State University; Dr. Robert Mantz, Chemical 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. Six institutions were funded under HSAP/URAP in FY13, totaling approximately $33K. 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. The program was reviewed in late FY13 and directed to increase collaboration between ARL and the university teams, emphasizing the interdependency of success of the research initiatives. In FY13, $2.4 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, Electronics
- *Bayesian Imaging and Advanced Signal Processing for Landmine and IED Detection Using GPR*
  Howard University, Washington, DC
  Co-CAM: Dr. James Harvey, Electronics
- *Extracting Social Meaning From Linguistic Structures in African Languages*
  Howard University, Washington, DC
  Co-CAM: Dr. John Lavery, Mathematical Sciences
- *Lower Atmospheric Research Using Lidar Remote Sensing*
  Hampton University, Hampton, VA
  Co-CAM: Dr. Gorden Videen, Environmental Sciences
- *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, Mathematical Sciences

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

ARO has administered programs on behalf of ASD(R&E) since 1992. REP aims to enhance research capabilities of HBCUs and MIs and to strengthen their education programs in science, technology, engineering, and mathematics (STEM) disciplines that are relevant to the defense mission. The FY13 BAA solicited proposals from single investigators for the acquisition of equipment and instrumentation to augment existing research and education capabilities and/or to develop new capabilities. Proposals were limited to two per eligible institution.

Under this program, qualifying institutions were able to submit proposals to compete for research equipment/instrumentation grants. In 3Q FY12, BAA W911NF-13-R-0008 was issued for the FY13 DoD REP for HBCU/MI. More than 85 proposals were determined to be eligible under the solicitation. In FY13, 63 grants totaling $21.7 million (funded through current and prior-year funds) were made to 47 different HBCU/MIs institutions (24 HBCUs and 23 MIs) under the solicitation *"Department of Defense (DoD) Research and Educational Program for Historically Black Colleges and Universities and Minority-Serving Institutions (HBCU/MI, Equipment/Instrumentation).*"

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

There was no instrumentation program for TCUs in FY13.

E. Other HBCU/MI Activities

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 $2.0 million and was awarded to Benedict College in Columbia, SC in 3Q FY11. A no-cost extension for this program is in effect through July 2014. In addition, the John H. Hopps Scholars Program at Morehouse College (funded in FY08) continued to serve eight scholars during FY13.

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 US 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 FY13, ARO selected 64 NDSEG Fellows from thirteen categories relevant to Army fundamental research priorities. These awardees began their fellowships in the fall of 2013. 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 roughly on the percentage of applicants who submitted topics in that category. The number of fellows chosen from each scientific discipline for the FY13 NDSEG program is shown in TABLE 3.

TABLE 3

FY13 NDSEG fellows by discipline. The table displays the number of NDSEG Fellows chosen in FY13, according to topic categories relevant to the designated Army research priorities.

Scientific Discipline	NDSEG Fellows Selected in FY13
Aeronautical and Astronautical Engineering	3
Biosciences	7
Chemical Engineering	3
Chemistry	6
Civil Engineering	6
Cognitive, Neural, and Behavioral Sciences	4
Computer and Computational Sciences	5
Electrical Engineering	5
Geosciences	4
Materials Science and Engineering	6
Mathematics	4
Mechanical Engineering	6
Physics	5
TOTAL	**64**

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 FY13, 170 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 FY13, 274 students engaged in research experiences in military laboratories through the Science and Engineering Apprentice Program (SEAP) and College Qualified Leaders (CQL) program, and 188 students participated in programs that offered enrichment classes in engineering at universities through the UNITE program. In FY13, 2,075 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 8,200 students participated 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 FY13, 101 apprentices were placed at 37 hosting universities throughout the U.S.

C. UNITE Program

The UNITE Program is an 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. The program provides stipends for participating students to offset costs associated with participating, which improve its ability to serve students who have previously encountered financial barriers to participation. Nine sites were funded in FY13 serving 188 students.

D. 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. The JSS program is a nationally-focused online program. The Army provides an online clearinghouse of JSS resources (*http://jrsolarsprint.org*), 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 was held, in which students from throughout the country uploaded images of their designs and conducted local time trials to compete for recognition on the Army's JSS website. Joint JSS and AEOP communication and marketing efforts were undertaken to registered and potential participants.

E. 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 FY13, HSAP/URAP awards provided 69 students with research experiences at 27 different universities. ARO invested approximately $284K in the FY13 effort.

F. 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 FY13, 104 high school students participated in SEAP at 11 sites and 170 college students participated in the CQL program at 12 sites.

G. 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 FY13, 2,075 students participated at GEMS programs held at 13 Army research laboratories spanning RDECOM, MRMC, and ERDC.

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

The YSCOA completed its third year of outreach efforts in FY13. 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, and JSS), 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 and evaluation 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:

- 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 major accomplishments in FY13 included a significant program evaluation and implementation of a number of changes, as listed below.

- Increased AEOP participants by 27%
- Conducted year-end program reviews with Individual Program Agents (IPAs), Cooperative Agreement Consortium Meeting and Army Cooperative Agreement and subject matter experts
- Completed FY14 Annual Program Plan prior to end of FY13
- AEOP Marketing Products included AEOP Brochures & Rack Cards, AEOP Brand Application Guide & Memo, AEOP Templates, AEOP Promotional Video, AEOP Pull-Up Banners, AEOP Social Media Cards, AEOP Tabletop Display Kits with branded tablecloths as well as AEOP Instructional Items
- Developed an AEOP Abstract Book
- Completed transition of GEMS, SEAP & CQL from George Washington University to the American Society for Engineering Education

XII. SCIENTIFIC SERVICES PROGRAM (SSP)

ARO established the SSP in 1957. This program provides a rapid means for the Army, DoD, OSD, 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 Eastern Science and Technology (BEST) Center located in Aberdeen, Maryland 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.

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 FY13, 59 new SSP tasks were awarded in addition to 356 modifications of the scope and/or funding of ongoing tasks on two SSP contracts. A summary of the agencies served under this program and the corresponding number of FY13 new SSP tasks is provided in TABLE 4.

TABLE 4
FY13 SSP tasks and sponsoring agencies.

Sponsoring Organization	SSP Tasks
Army Research, Development and Engineering Command (RDECOM)	
Army Research Laboratory (ARL)	9
Edgewood Chemical, Biological Center (ECBC)	2
Research, Development, and Engineering Centers (RDECs)	
Army Missile RDEC (AMRDEC)	1
Armaments RDEC (ARDEC)	1
Natick Soldier RDEC (NSRDEC)	4
Communications-Electronics RDEC (CERDEC)	1
Tank Automotive RDEC (TARDEC)	10
TOTAL: RDECOM	**28**
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	
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)	2
TOTAL: Other U.S. Army	**14**
Other DoD	
US Air Force	2
US Navy	5
Defense Human Resources Activity	1
Defense Logistics Agency	2
TOTAL: Other DoD	**10**
Department of Homeland Security (DHS)	
DHS Science & Technology Directorate	1
TOTAL: DHS	**1**
TOTAL FY13 SSP Tasks	**59**

XIII. SUMMARY OF PROGRAM FUNDING AND ACTIONS

A. FY13 Research Proposal Actions

The FY13 extramural basic research proposal actions for each ARO Division are summarized in TABLE 5, below.

TABLE 5

FY13 ARO Research Proposal Actions. The status of research proposals received within FY13 (*i.e.*, 1 Oct 2012 through 30 Sep 2013) is listed based on proposal actions reported through 20 May 2014. The table reports actions for extramural proposals in the 6.1 basic research categories: SI, STIR, YIP, HBCU/MI Core, MRI, MURI, PECASE, and DURIP. The proposals and actions for the FY13 DURIP competition are included, although most of these proposals were received late in FY12.

	Received	Accepted	Declined	Pending	Withdrawn
Chemical Sciences	101	50	37	13	1
Computing Sciences	51	25	13	13	0
Electronics	55	19	30	6	0
Environmental Sciences	23	11	10	1	1
Life Sciences	98	28	43	27	0
Materials Science	77	23	35	19	0
Mathematical Sciences	39	18	6	13	2
Mechanical Sciences	91	27	52	12	0
Network Sciences	61	23	23	12	3
Physics	69	24	32	13	0
TOTAL	**665**	**248**	**281**	**129**	**7**

B. Summary of ARO Core Program Budget

The ARO FY13 Core (BH57) Research Program budget is shown in TABLE 6, below.

TABLE 6

ARO Core (BH57) Program funding. The ARO Core Program FY13 Budget is listed according to each scientific discipline (Division) or special program; data source: 31 Jan 2014 Funding Status by Cost Center Report (scientific disciplines) and Status of Funds Report (special programs).

ARO Core (BH57) Program Type	Division or Program Title	FY13 Allotment
Scientific Disciplines	Chemical Sciences	$6,629,563
	Computing Sciences	$4,635,988
	Electronics	$5,879,678
	Environmental Sciences	$2,423,548
	Life Sciences	$6,603,069
	Materials Science	$6,147,682
	Mathematical Sciences	$4,392,300
	Mechanical Sciences	$6,037,051
	Network Sciences	$5,476,601
	Physics	$6,513,509
	SUBTOTAL: Core Program Funding by Scientific Discipline	**$54,738,988**
Special Programs	Senior Scientist Research Programs	$371,663
	ARL Fellows' Stipends	$75,000
	National Research Council (NRC) Associates Program	$455,369
	HBCU/MI Program[1,2]	$801,205
	HSAP/URAP	$152,717
	In-House Operations	$13,339,517
	SUBTOTAL: Core Program Funding to Special Programs	**$15,195,470**
TOTAL	**ARO Core (BH57) Program**	**$69,934,458**

[1] HBCU/MI Core Program funds are allocated at the Directorate level, and are matched with Division funds on a 1:1 basis, resulting in total FY13 HBCU/MI Core Program funding of $1.6M.

[2] This table does not include the additional funds provided from OSD for the HBCU/MI Program (see Table 9).

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

The FY13 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

FY13 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; data source: 31 Jan 2014 Status of Funds Report.

Other Army-funded Program	FY13 Allotment
Multidisciplinary University Research Initiative	$54,654,994
Presidential Early Career Award for Scientists and Engineers	$3,599,995
Defense University Research Instrumentation Program	$8,934,259
University Research Initiative Support	$2,078,752
MINERVA Program (Project V72)[1]	$2,975,000
Army Center of Excellence (Project H59)	$872,000
HBCU/MI – PIRT Centers (Project H04)	$2,494,000
Institute for Collaborative Biotechnologies (ICB; Project H05)	$10,834,000
Institute for Soldier Nanotechnologies (ISN; Project J12)	$9,287,000
Institute for Creative Technologies (ICT; Project J08)	$7,134,000
Army Education Outreach (Project J14)	$3,104,000
Board of Army Science and Technology (BAST; Project C18)	$669,279
Small Business Innovation Research (SBIR; Project M40)[1,2]	$7,011,837
Small Business Technology Transfer (STTR; Project 861)[1,3]	$10,310,268
SBIR/STTR Services / Contract Support (Project 720)	$1,265,000
Research In Ballistics (Project H43)	$1,061,000
TOTAL: Other Army-funded Programs	**$126,285,384**

[1] These amounts do not include the additional funds provided by OSD (see Table 9).
[2] Includes $5,213,184 of FY12 funds received in or reallocated for FY13
[3] Includes $1,131,016 of FY12 funds received in or reallocated for FY13

TABLE 8

FY13 allotment for externally-funded programs. FY13 funds received from sources other than Army or OSD are indicated below; data source: 31 Jan 2014 Status of Funds Report. The Other Agencies category includes funding from a range of sources, such as the Joint IED Defeat Organization (JIEDDO) and the Joint Project Manager, Nuclear, Biological, and Chemical (JPMNBC).

External Program	FY13 Allotment
Medical Research and Material Command (MRMC)	$18,151,490
Communications and Electronics RDEC (CERDEC)	$3,089,931
Scientific Services Program (SSP)[1]	$15,694,398
Other Army	$16,391,684
Air Force Research Laboratory (AFRL)	$5,320,407
Defense Advanced Research Projects Agency (DARPA)[2]	$112,656,512
Other Agencies (*e.g.*, JIEDDO and JPMNBC)[3]	$94,828,583
TOTAL: External Programs	**$266,133,004**

[1] Includes $3,656,091 of FY12 funds received in or reallocated for FY13
[2] Includes $46,019,448 of FY12 funds received in or reallocated for FY13
[3] Includes $13,783,100 of FY12 funds received in or reallocated for FY13

TABLE 9

OSD direct-funded programs. These funds were allocated directly from OSD to the indicated program; data source: 31 Jan 2014 Status of Funds Report.

OSD Direct-funded Programs	FY13 Allotment
STTR (Project 8Z5)[1,2]	$2,709,575
HBCU/MI and Research and Educational Program (REP)[3]	$15,311,000
Chemical and Biological Defense Programs (Project BP0)[4]	$9,510,102
MINERVA	$5,060,000
TOTAL: OSD Direct Funding	**$32,590,676**

[1] This amount does not include the additional Army funds provided for SBIR/STTR (see Table 7).
[2] Includes $832,967 of FY12 funds received in or reallocated for FY13
[3] This amount does not include the additional Army Core Program funds provided for the HBCU/MI Program (see Table 6).
[4] Includes $1,749,575 of FY12 funds received in or reallocated for FY13

D. Grand Total FY13 Allotment for ARO Managed or Co-managed Programs

TABLE 10

Summary of FY13 allotment for all ARO managed or co-managed programs. This table lists the subtotals from TABLES 6-9 and the grand total FY13 allotment for all ARO managed or co-managed programs, including any FY12 funds received in or allocated for FY13.

Program Category	FY13 Allotment
Core (BH57) Programs	$69,934,458
Other Army-funded Programs	$126,285,384
External Program Funds	$266,133,004
OSD Direct-funded Programs	$32,590,676
GRAND TOTAL: (all sources)	**$494,943, 522**

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 2013* is to provide information on the programs and basic research supported by ARO in FY13, 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 FY13.

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 research 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 its research portfolio 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 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

The Chemical Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. 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 FY13, 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 microstructure, architecture, functionality, and macroscopic properties. Research in this program may ultimately enable the design and synthesis of functional polymeric materials that give the Soldier new and improved protective and sensing capabilities as well as capabilities not yet imagined. This Program Area is divided into two research thrusts: (i) Precision Polymeric Materials and (ii) Responsive Polymeric Materials. Within these thrusts, high-risk, high payoff research efforts are identified and supported to pursue the program's long-term goal. Additionally, research efforts that connect innovative polymer chemistry with the comprehensive characterization of polymeric materials are of joint interest with the Mechanical Behavior of Materials Program in the ARO Materials Science Division. The Precision Polymeric Materials Thrust supports research aimed at developing new approaches for synthesizing polymers with precisely defined molecular weight, microstructure (monomer sequence and tacticity), branching, and functional group location, and on using self assembly to create precise, complex polymer structures with diverse functions and new properties. Areas of interest include new polymerization methodologies, the design and synthesis of new monomers with controlled reactivity, the design and synthesis of new catalysts that give precision control over polymer microstructure, and self-assembly of polymers into functional hierarchical nanostructures. The Responsive Polymeric Materials Thrust focuses on the design and synthesis of novel polymers that undergo predictable conformational and/or chemical changes in response to specific external stimuli. Of particular interest are research efforts in the areas of polymer mechanochemistry, self-immolative polymers, and reconfigurable materials.

These high-risk, high payoff research areas may lead to long-term applications for the Army such as 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) Molecular Dynamics and (ii) Quantitative Theoretical Methods. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high-payoff research efforts. The Molecular Dynamics Thrust broadly supports research on the study of energy transfer mechanisms in molecular systems (reactive and non-reactive). The Quantitative Theoretical Methods Thrust supports research to develop and validate theories for quantitatively describing and predicting the properties of chemical reactions and molecular phenomena.

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.

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 obtain a molecular level understanding of interfacial activity and of dynamic nanostructured and self-assembled chemical systems. High-risk basic research in this program is expected to lead to the design and synthesis of new chemical systems that will provide unprecedented hazardous materials management capabilities and soldier survivability. This Program Area is divided into two research Thrusts: (i) Interfacial Activity and (ii) Synthetic Molecular Systems. Within these Thrusts, high-risk, high-payoff research efforts are identified and supported to pursue the program's long-term goals. The Interfacial Activity Thrust supports research efforts on understanding the mechanisms of mass transport and reactivity on surfaces and at interfaces as well as how to control the structure and function of chemical and biological molecules on surfaces. Research in the Synthetic Molecular Systems Thrust is exploring novel methods for incorporation of multi-functionality and dynamic and responsive behavior into chemical systems. Specific areas of interest include the stabilization of nanostructured and self-assembled systems, incorporation of enhanced catalytic activity into chemical systems, and the design and synthesis of chemical systems that sense and respond to specific external stimuli.

This Program Area supports research that will likely lead to many long-term applications for the Army and the general public. Potential long-term applications include novel chemical sensing capabilities, selective membranes, multi-functional surfaces for self-repair and self-healing, and new approaches to hazardous waste management. Research in these areas may also lead to multi-functional and stimuli-responsive systems for "smart" materials that can sense and autonomously respond in unprecedented ways for soldier protection.

C. Research Investment

The total funds managed by the ARO Chemical Sciences Division for FY13 were $49.3 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY13 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 $10.9 million to projects managed by the Division. The Division also managed $5.4 million of Defense Threat Reduction Agency (DTRA) programs, $8.4 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 $3.0 million for contracts. The Institute for Soldier Nanotechnologies received $11.7 million. Finally, $2.9 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.3 million provided through the ARO Core (BH57) allotment, in addition to funding for 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 creation, leadership, and management of 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 FY13 (*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 FY13 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 FY13, the Division awarded 16 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to understand and control ultracold chemical reactions, to synthesize and characterize nanostructured protein-based hybrid biomolecular materials, and to develop computational frameworks for exploring the properties of polymer membranes at molecular-level resolution. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Elliot Bernstein, Colorado State University - Ft. Collins; *Time and Energy Resolved Studies of the Decomposition of Energetic and Model Molecules Following Electronic Excitation and Ionization*
- Professor Robin Côté, University of Connecticut - Storrs; *Investigating Ultracold Chemical Reactions and Methods for Control*
- Professor Venkat Ganesan, University of Texas - Austin; *Multiresolution Simulation Approaches For Elucidating the Morphology-Property Correlations in Block Copolymer Membranes*
- Professor Juliet Gerrard, University of Canterbury; *Proteins as Supramolecular Building blocks for Responsive Materials*
- Professor Jeffrey Gilman, National Institute of Standards and Technology; *Evaluation of Mechanophores as Super-Resolution Molecular Sensors in Nanocomposites*
- Professor Stephen Klippenstein, University of Chicago; *Effect of Dynamics in the van der Waals Region on the Chemical Kinetics of Nitrogen Containing Molecules*
- Professor Eric Kool, Stanford University; *Interaction of Bacterial Metabolites with Fluorescent Synthetic DNA*
- Professor Anna Krylov, University of Southern California; *Metastable Autoionizing States of Molecules and Radicals in Highly Energetic Environment*
- Professor Douglas Natelson, William Marsh Rice University; *Dissipation and Heating in Molecular-scale Junctions via Surface-enhanced Raman Spectroscopy*
- Professor Herschel Rabitz, Princeton University; *Exploring the Systematics of Controlling Quantum Phenomena*
- Professor Sankaran Thayumanavan, University of Massachusetts - Amherst; *Supramolecular Disassembly for Sensing with Amphiphilic Polymers*

- Professor Kenneth Wagener, University of Florida - Gainesville; *Extending Morphology Control to Sophisticated Precision Polymer Systems*
- Professor Karen Winey, University of Pennsylvania; *Rapid Screening of New Precise Copolymers: Morphology and Ionic Conductivity*
- Professor Ting Xu, University of California - *Berkeley; Nanostructured Protein-based Hybrid Biomolecular Materials for the Study of Molecular Level Synergistic Assemblies*
- Professor John Yates, University of Virginia; *Controlling the Efficiency of Semiconductor-*TiO_2
- Professor Richard Zare, Stanford University; *Coherent Preparation of Molecular Hydrogen in (v,J,M) Eigenstates for Reaction Dynamics Studies*

2. Short Term Innovative Research (STIR) Program. In FY13, the Division awarded five new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to characterize living polymerization reactions in real time at the single-molecule level and to characterize reaction mechanisms of energetic compound decomposition. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Adam Braunschweig, University of Miami - Coral Gables; *Donor-acceptor Superstructures with Emergent Stimuli Responses*
- Professor Peng Chen, Cornell University; Single-molecule *Visualization of Living Polymerization*
- Professor Thomas Glover, University of South Alabama; *Nanoscale Modification of Fibers via Reactive Dye Chemistry*
- Professor Ralf Kaiser, University of Hawaii - Hilo; *Untangling the Reaction Mechanisms Involved in the Explosive Decomposition of Energetic Compounds*
- Professor Ilki Kim, North Carolina A&T State University; *Exploring Non-equilibrium Thermodynamics of Dissipative Nanoscopic Systems*

3. Young Investigator Program (YIP). In FY13, the Division awarded three new YIP projects. These grants are driving fundamental research such as studies to characterize microstructures at ionic liquid/electrode interfaces and to explore the properties of new polymeric materials. The following PIs and corresponding organizations were recipients of new-start YIP awards.

- Professor Nandini Ananth, Cornell University; *Vibrationally Promoted Hot Electron Generation in Reactions at Metal Surfaces*
- Professor Kevin Noonan, Carnegie Mellon University; *New Polymeric Materials Incorporating Heteromatic Phosphabenzene Units*
- Professor Luke Haverhals, Bradley University; *Characterizing Microstructures at Ionic Liquid/Electrodes Interfaces*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY13 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Macromolecular Materials Gordon Research Conference*; Ventura, CA; 6-11 January 2013
- *Molecular Energy Transfer Gordon Research Conference*; Ventura, CA; 13-18 January 2013
- *Center for Electrochemistry Annual Workshop on Electrochemistry*; Austin, TX; 9-10 February
- *Advances in Proton Exchange Membranes for Fuel Cells*; Pacific Grove, CA; 17-20 February 2013
- *53th Sanibel Symposium*; St. Simons Island, GA; 17-22 February 2013
- *Adaptive Soft Materials Symposium at the Materials Research Society National Meeting*; San Francisco, CA; 1-2 April 2013
- *Workshop on Surface Plasmons, Metamaterials, and Catalysis*; Houston, TX; 20-22 May 2013
- *Workshop on Recent Developments in Electronic-Structure Theory*; Williamsburg, VA; 11-14 June 2013
- *Liquid Crystals Gordon Research Conference*; Biddeford, ME; 16-21 June 2013
- *2013Conference On the Dynamics of Molecular Collisions*; Granlibakken, CA; 7-12 July 2013

- *Energy Storage Materials Symposium at the 246th ACS National Meeting*; Indianapolis, IN; 8-12 September 2013

5. Special Programs. In FY13, 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. 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 project, which ended in FY13, was co-managed by the Chemical Sciences and Materials Science Divisions. This MURI explored 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 investigated 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 designed, synthesized, and characterized a revolutionary new class of mechano-responsive molecules, called mechanophores, which respond to mechanical stress with pre-designed chemical reactions. Based on 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.

2. 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 by the Materials Science and Chemical Sciences Divisions.

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.

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. This research is co-managed by the Chemical Sciences and Life Sciences Divisions.

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.

8. Theory and Experiment of Cocrystals: Principles, Synthesis and Properties. This MURI began in FY13 and was awarded to a team led by Professor Adam Matzger of the University of Michigan at Ann Arbor. This MURI team is investigating molecular co-crystal formation and the implications for controlling solid-state behavior. This research is co-managed by the Chemical Sciences and Materials Science Divisions.

The largely untapped potential for creating new molecular crystals with optimal properties is just beginning to be realized in the form of molecular co-crystallization. Co-crystallization has the potential to impact the macro-scale performance of many materials, ranging from energetic materials, to pharmaceuticals, to non-linear optics. Unfortunately, the dynamics of molecular co-crystal formation is poorly understood. Molecular co-crystals contain two or more neutral molecular components that rely on non-covalent interactions to form a regular arrangement in the solid state. Co-crystals are a unique form of matter, and are not simply the result of mixing

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

two solid phases. Organic binary co-crystals are the simplest type and often display dramatically different physical properties when compared with the pure 'parent' crystals. A significant amount of research on co-crystal design has been carried out by the pharmaceutical industry for the synthesis of pharmaceutical ingredients. However, co-crystal design has not been exploited in broader chemistry and materials science research areas. A recent breakthrough discovery demonstrates that co-crystallization can be used to generate novel solid forms of energetic materials.

The objective of this MURI is to develop a fundamental understanding of intermolecular interactions in the context of crystal packing, and to use the knowledge gained for the design of new co-crystalline molecular materials with targeted, optimized physical and chemical properties. In the long term, a better understanding and control of molecular co-crystallization has the potential to improve the properties of a variety of materials, including: energetic materials, pharmaceuticals, organic semiconductors, ferroelectrics, and non-linear optical materials.

9. Artificial Cells for Novel Synthetic Biology Chassis. This MURI began in FY13 and was awarded to a team led by Professor Neal Devaraj at the University of California - San Diego. The goal of this MURI is to understand how biological and biomimetic synthetic cellular elements can be integrated to create novel artificial cells with unprecedented spatial and temporal control of genetic circuits and biological pathways. This research is co-managed by the Life Sciences and Chemical Sciences Divisions.

The field of synthetic biology aims to achieve design-based engineering of biological systems. Toward this goal, researchers in the field are identifying and characterizing standardized biological parts for use in specific biological organisms. These organisms serve as chassis for the engineered biological systems and devices. While single-celled organisms (e.g., bacteria, yeast) are typically used as synthetic biology chassis, the complexity of even these relatively simple organisms presents significant challenges for achieving robust and predictable engineered systems. A potential solution is the development of minimal cells which contain only those genes and biomolecular machinery necessary for basic life. Concurrent with recent advances toward minimal biological cells, advances have also been made in biomimetic chemical and material systems, including synthetic enzymes, artificial cytoplasm, and composite microparticles with stable internal compartments. These advances provide the scientific opportunity to explore the integration of biological and biomimetic elements to generate an artificial hybrid cell that for the first time combines the specificity and complexity of biology with the stability and control of synthetic chemistry.

The objective of this MURI is to integrate artificial bioorthogonal membranes with biological elements to create hybrid artificial cells capable of mimicking the form and function of natural cells but with improved control, stability, and simplicity. If successful, these artificial cells will provide a robust and predictable chassis for engineered biological systems, addressing a current challenge in the field of synthetic biology that may ultimately enable sense-and-respond systems, drug-delivery platforms, and the cost-effective production of high-value molecules that are toxic to living cells (e.g., alternative fuels, antimicrobial agents).

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

Research through the SBIR program has 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 FY13, the Division managed 13 new-start SBIR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of six Phase I contracts, three Phase II contracts, one Phase III contract, and three Phase I Chemical and Biological Defense SBIR (CBD-SBIR) contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications, such as the development of a broad-spectrum reactive nanocomposite gel to sequester chemical agents, plasmonic nanosensors for detecting warfare agents, and a direct ethanol fuel cell system.

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 FY13, the Division managed five new-start STTR contracts, in addition to active projects continuing from prior years. These contracts consisted of four Phase I projects and one Phase II STTR project. These new-start projects aim to bridge fundamental discoveries with potential applications, such as the development of a nondestructive concrete characterization system and nonlinear laser wave mixing for trace detection of explosives.

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 FY13, the Division awarded three new ARO (Core) HBCU/MI projects and 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 FY13.

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 FY13, 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 metal oxide surfaces and molecular quantum states.

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 FY13, the ISN supported 42 faculty, 60 graduate students, and 26 postdoctoral fellows across 12 departments at MIT. The ISN program is unique in that it currently has 15 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 $11.7 million of program funds was allocated to the ISN in FY13, which was the first year of a contract that was renewed in FY12 for a five-year period. Of these FY13 funds, $9.7 million was allocated for 6.1-basic research and $2.0 million was allocated for five applied-research projects, including one new project.

I. DARPA Biofuels Alternative Feedstocks

The Biofuels Alternative Feedstocks program is developing affordable alternatives to petroleum-derived JP-8 without using algae and cellulosic biomass. The Division's Electrochemistry Program aids in the management of this this DARPA program. 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

DARPA is developing revolutionary new approaches to portable energy sources. The Division's Electrochemistry Program aids in the management of this this DARPA program. 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.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. Stimuli Responsive Amphiphilic Colloidal Assemblies

Professor Sankaran Thayumanavan, University of Massachusetts - Amherst, Single Investigator Award

The goal of this research is to design and synthesize responsive nanostructures with multiple, specific stimuli-responsive mechanisms. In FY13, the research team combined nanoassemblies that independently responded to different stimuli. Amphiphilic micelles that respond to changes in pH were made with block copolymers containing poly(2-(diisopropylamino)ethylmethacrylate and 2-aminoethylmethacrylate hydrochloride. In solution, these micelles encapsulate a pyrene dye. Nanogel materials composed of random copolymers, poly(oligoethyleneglycolmonomethylethermethacrylate-*co*-glycidylmethacrylate-*co*-pyridyldisulfide ethylmethacrylate) encapsulate a carbocyanine based fluorescent dye and are responsive to changes in oxidation. Surface reactions between the micelles and nanogels led to composite nanoassemblies which could be controlled by varying the amount of each component in the starting material. The dynamic assembly and disassembly of the composite was characterized using transmission electron microscopy (TEM) and dynamic light scattering (see FIGURE 1).

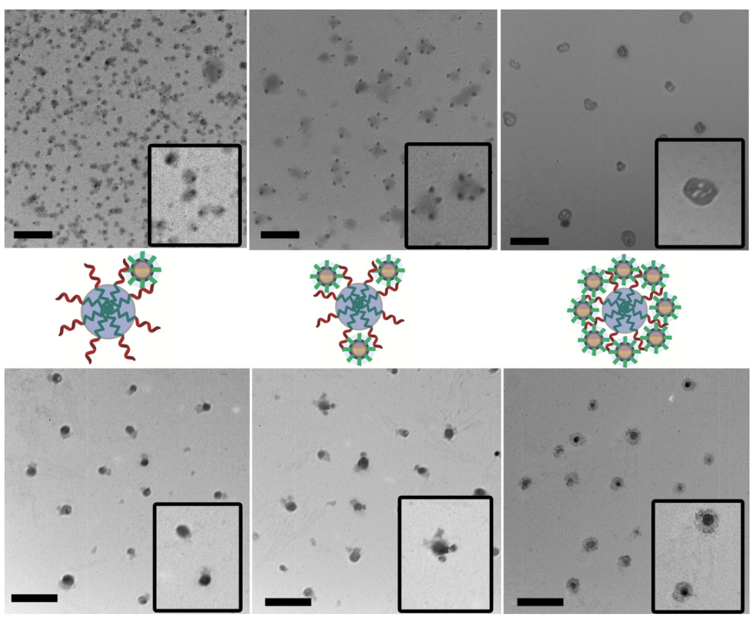

FIGURE 1

Responsive nanoassemblies. TEM of composite nanostructures assembled from poly(2-(diisopropylamino) ethylmethacrylate-*b*-2-aminoethylmethacrylate hydrochloride) block copolymer and poly(oligoethyleneglycolmonomethylethermethacrylate-*co*-glycidylmethacrylate-*co*-pyridyldisulfide ethylmethaccrylate) nanogel.

Experimental results demonstrated that the guest molecules could be independently released in the presence of their respective triggers (see FIGURE 2). Pyrene was released from the pH responsive micelle component upon a decrease in pH from 7.4 to 6.5 but was fully retained with addition of an oxidant, glutathione. Likewise, the nanogel demonstrated concentration-dependent, responsive behavior when exposed to glutathione, releasing the carbocyanine based dye, but remained unaffected by pH variations. This demonstrated the selective and sequential release of dye from individual components within a hybrid system. Future work will continue to probe the how these responsive systems can be used to modify surface properties of materials.

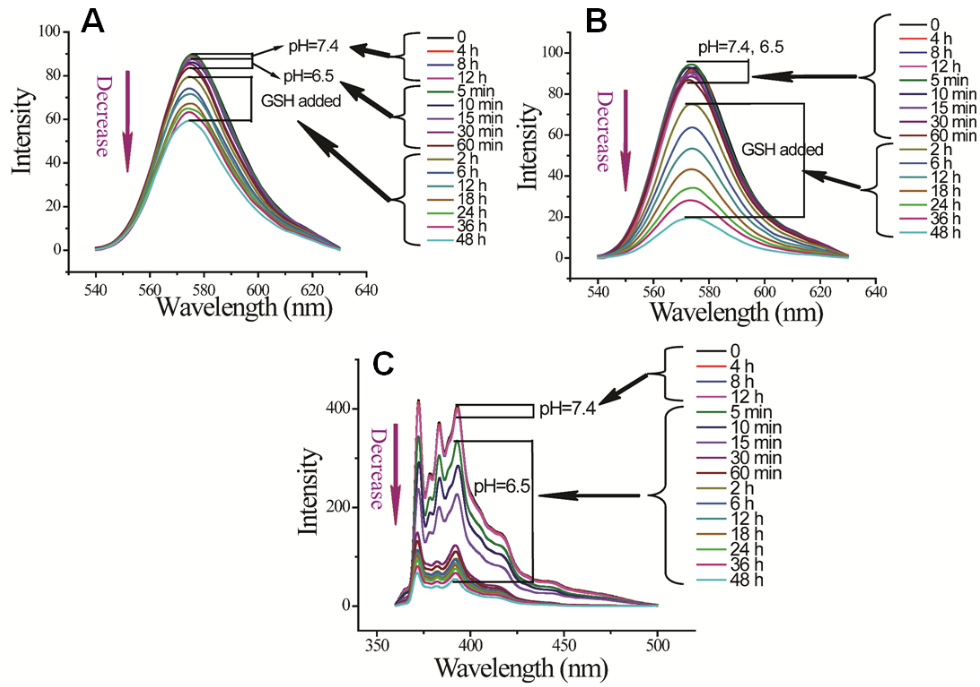

FIGURE 2

Independent release of guest molecules. Fluorescence spectra trace release of carbocyanine based dye from the composite nanostructure in response to (**A**) 0.1 mM glutathione; (**B**) 70 mM glutathione; and (**C**) release of pyrene in response to pH.

B. 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 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 was used to conduct site-specific labeling of two specific sites in organophosphorus hydrolase (OPH) with FRET labels. Non-natural amino acids were incorporated at the Lys 175A and Lys175B positions and labeled with electroflor dyes using click chemistry (See FIGURE 3).

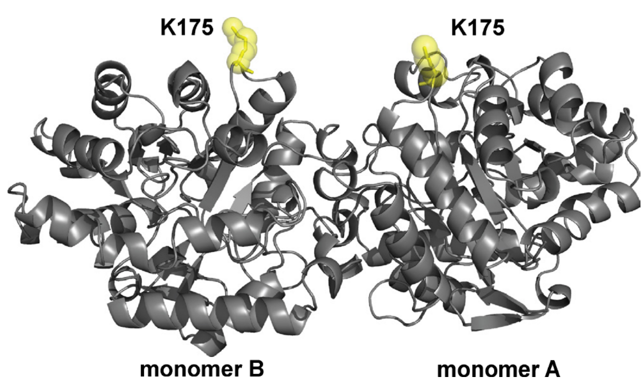

FIGURE 3

Structure of OPH showing the position of site-specific donor and acceptor labeling.

Single molecule Total Internal Reflection Fluorescence Microscopy was then used to monitor single enzyme folding dynamics on a fused silica surface. The fluorescence intensity of individual enzyme molecules was monitored over time and from this the relative distance of the labeled sites was determined. The team's analysis of > 30,000 individual trajectories enabled the observation of heterogeneities in the kinetics of surface-induced

OPH unfolding with unprecedented resolution. The sample molecular trajectories and the distribution of relative fluorophore distance of OPH on a fused silica surface are plotted in FIGURE 4. Experimental work demonstrated that while in solution, protein molecules remain folded; however, they readily denature upon absorption to the surface and subsequently desorb, indicating adsorption of unfolded protein is reversible and highly dynamic. In addition, kinetic analysis revealed two distinct pathways for enzyme unfolding on surfaces. The majority of molecules (85 ± 5%) unfolded with a time scale of 0.10 seconds, while the reminder unfolded more slowly with a time scale of 0.7 seconds. These studies enable the characterization of enzyme folding at the single-molecule level and will provide unprecedented insight into enzyme stability on surfaces and biofouling mechanisms. Based on these initial findings, Professor Kaar will continue to investigate this new single-molecule method with other surfaces and proteins.

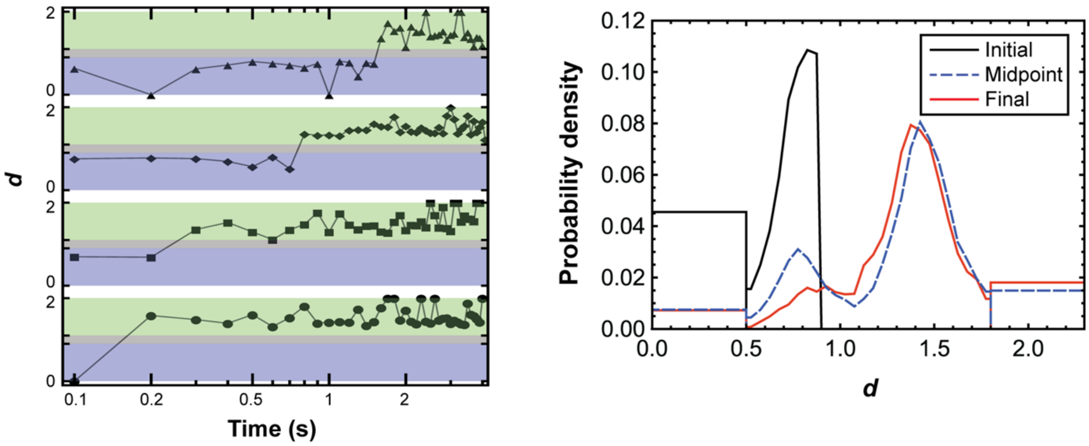

FIGURE 4

Sample molecular trajectories and the distribution of relative fluorophore distance of OPH. The panels show the sample molecular trajectories (left) and distribution of relative fluorophore-to-fluorophore distance of OPH (right) on fused silica surfaces at different stages.

C. Magnesium Solvation and Electrochemistry in Ionic Liquids

Professor Daniel Buttry, Arizona State University, Single Investigator Award

Professor Buttry and colleagues have been studying the solvation environment for Mg^{2+} in ionic liqud electrolyte systems and correlating the spectroscopic measurements with electrochemical investigative results of Mg/Mg^{2+} redox couple, focusing particularly on the kinetics of the electrodeposition and dissolution of Mg. In FY13, the research team investigated magnesium's surface passivation and electrochemical irreversibility (see FIGURE 5).

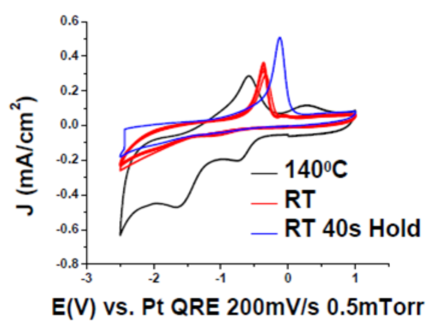

FIGURE 5

Magnesium electrodeposition. Comparison of Mg under potential deposition at room temperature on Pt at room temperature and 140°C. Blue scan was held at -2.5V for 40s at room temperature.

To understand the complexities of the situation deeper, Raman spectroscopy was used to probe the nature of the Mg^{2+} solvation environment. The results show that Mg^{2+} exists ag $Mg(TFSI)^{3-}$. This is undesirable because prevents Mg^{2+} for participating in conduction making delivery to the electrode difficult. FIGURE 6 shows Raman data taken for $Mg(TFSI)_2$/BMPTFSI solutions as well as other dissolved Mg^{2+} salts in the same IL. Based on the results from Professor Buttry's laboratory, $Mg(TFSI)_2$ showed the greatest miscibility, being soluble up to a 50% molar ratio with respect to BMPTFSI. The Raman spectrum for BMPTFSI from 87-2000cm^{-1} is shown in FIGURE 6A. FIGURE 6B shows the raw data being fit by two Voigt curves fixed at 40% Gaussian and 60% Lorentzian with line widths between 9 and 11 for the 742 peak and 8-9 for the 752 peak. These Voigt profiles resulted in the best overall fit of the data, are consistent with profiles used in LiTFSI studies, and are justifiable due to the highly viscous nature of the liquids. The areas under the fitted curves were used to quantify relative polulations of TFSI states. FIGURE 6C displays the fraction of coordinated TFSI- anions as a function of the $Mg(TFSI)_2$ molar concentration, using $[Mg(TFSI)_2]_x[BMPTFSI]_{1-x}$ to express the material composition (a common notation throughout the LiTFSI literature and thus used here for comparison). It is clear from this plot that TFSI coordinates with Mg^{2+} as a three-fold ligand. In FIGURE 6D, the data for other MgX_2 salts (X=ClO_4^-, I^-, Br^-, Cl^-) plotted alongside $Mg(TFSI)_2$.

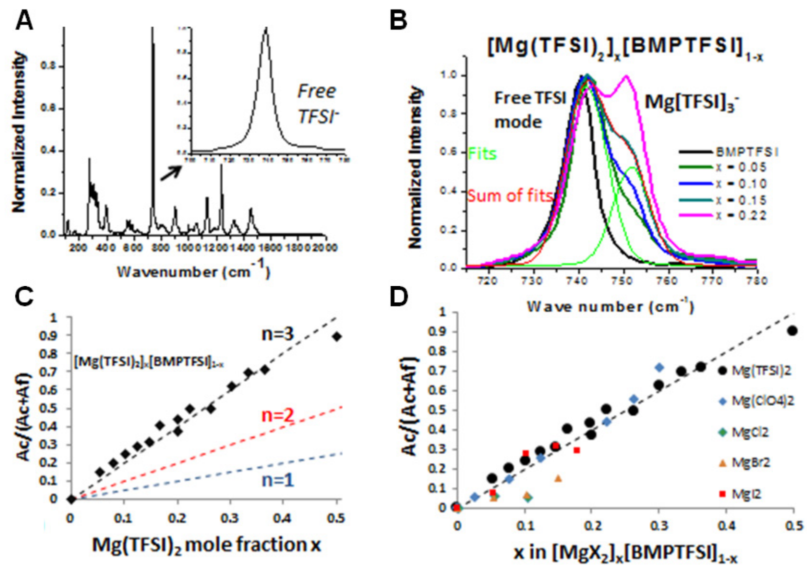

FIGURE 6

Magnesium Raman Data. (**A**) BMPTFSI Raman spectrum from 87-2000cm^{-1}; the inset displays 742cm^{-1} free TFSI peak at 742cm^{-1}. The inset displays the ~742cm^{-1} peak which has been attributed to "free" $TFSI^-$ anions ($TFSI^-$ anions not coordinating with the metal cation). (**B**) Spectra acquired over range of concentrations for $Mg(TFSI)_2$/BMPTFSI with Voigt curve fits. (**C**) Measured fraction Mg-TFSI/total TFSI. (**D**) Data for other MgX_2 salts (X=ClO_4^-, I^-, Br^-, Cl^-) plotted alongside $Mg(TFSI)_2$.

Professor Buttry determined that in TFSI based ionic liquids coordination of the magnesium will need to be controlled to enable reversible electrodeoposition and stripping necessary for future magnesium based batteries. Magnesium batteries have the potential to provide an alternative storage medium that has several advantages over current technologies on the market, including much higher gravimetric and volumetric energy densities as well as safer production and use.

D. Nitric Oxide Production in Nitroalkyl Radicals that Circumvents Nitro-nitrite Isomerization

Professor Laurie Butler, University of Chicago, Single Investigator Award

The fundamental reaction mechanisms important in the explosion of energetic materials involve highly reactive radical intermediates whose reactions propagate the combustion process. The role of the radical intermediates in the overall mechanism has been traditionally difficult to characterize due to their transient nature. The approach of the PI to revealing the key elementary reactions of these radical intermediates is to generate them with the high vibrational energies that drive their unimolecular decomposition reactions, but in a collision-free environment where the product branching from each radical can be probed directly. The experiments are complementary to studies that use time-dependent spectroscopic methods to detect the transient radical species, but they are specifically designed to be able to probe the product channel branching. Chain propagating radicals are generated from a specific highly vibrationally excited radical-intermediate from a halogenated photolytic precursor molecule, and then the reaction dynamics are probed as the radical accesses the energetically allowed product channels. The internal energy distribution of the radical reactant is characterized, using momentum and energy conservation, by measuring the velocity distribution of the halogen co-fragment. This allows one to access a broad range of energies for the branching ratio studies, energies that are relevant to high-temperature, high-pressure explosive processes.

In FY13, Professor Butler's laboratory tracked the decomposition of the 2-nitro-2-propyl radical ($CH_3C(NO_2)CH_3$). This radical structurally mimics the energetic material (EM) TNAZ (1,3,3-trinitroazetidine), and it has been chosen for study in order to better understand the chemistry of energetic materials whose molecules have germinal dinitro functional groups (see FIGURE 7).

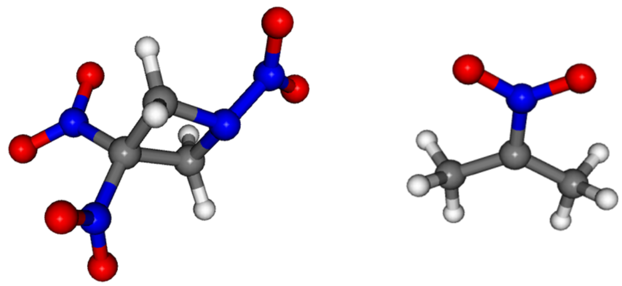
TNAZ (1,3,3-trinitroazetidine) 2-nitro-2-propyl

FIGURE 7

Molecular structures of TNAZ and 2-nitro-2-propyl radical. The radical is formed from laser-photolytic cleaveage of 2-bromo-2-nitropropane with 193 nm photons.

In addition, the research team found that the NO product is formed promptly upon generation of the nitroproply radical (see FIGURE 8). The scientists used high level *ab initio* calculations to model their experimental results. They concluded that a newly discovered mechanism for NO production, that is substantially lower in energy than the traditional NO-producing mechanism, is at work in the decomposition of this radical. The new mechanism involves passage through a low-energy transition state (~35 kcal/mol) and then immediate production of acetone and the NO fragment. This mechanism has never been observed previously in decomposition of energetic molecules. The investigators hypothesize that the reason for the new mechanism is simply that a radical center exists at the carbon atom to which is bound the NO group. No such analogy is possible in the EM molecules. The existence of the radical center has the effect of dramatically lowering the transition state energy and leads to prompt production of NO product. This contrasts with the traditional chemical mechanism which involves nitro-nitrite isomerization, followed by NO elimination. Such detailed mechanistic information as has been uncovered here is critically important to understanding the chemistry, properties, and behavior of energetic materials.

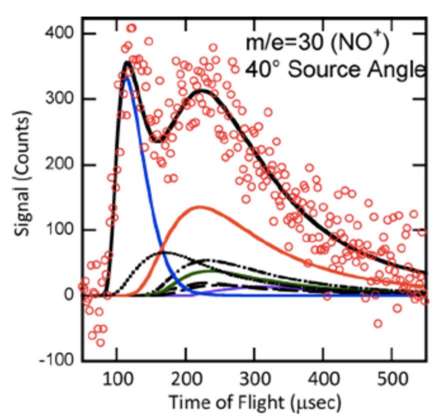

FIGURE 8

Time-of-flight spectrum taken at m/e = 30, NO^+ at source angle and 40°. The blue fit represents the contribution of NO fragments from the dissociation of $CH_3C(NO_2)CH_3$ to NO + $CH_3C(O)CH_3$.

E. Quasi-classical Trajectory Study of CH_3NO_2 Decompostion via Roaming-Mediated Isomerization

Professor Joel Bowman, Emory University, Single Investigator Award

The objective of this research is to develop quantitative potential energy surfaces for small molecules which are considered models for energetic materials, and to perform trajectory studies to determine the principal chemical decomposition pathways that are allowed. In this study, the PI has developed a global potential energy surface (PES) for CH_3NO_2 from 114,000 UB3LYP/6-311+G(d,p) electronic energies. This PES was then used in quasi-classical trajectory calculations on CH_3NO_2 dissociation to investigate dissociative pathways in this system (see FIGURE 9). A sample trajectory is shown in FIGURE 10.

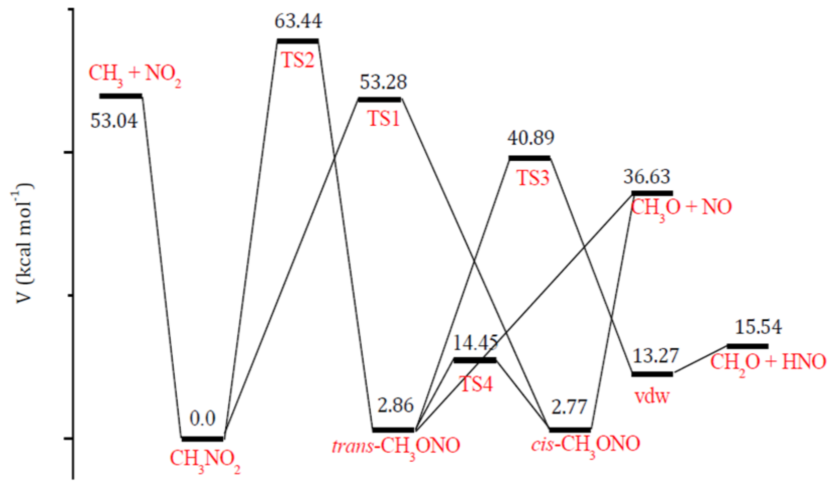

FIGURE 9
Stationary states on the PES for CH_3NO_2.

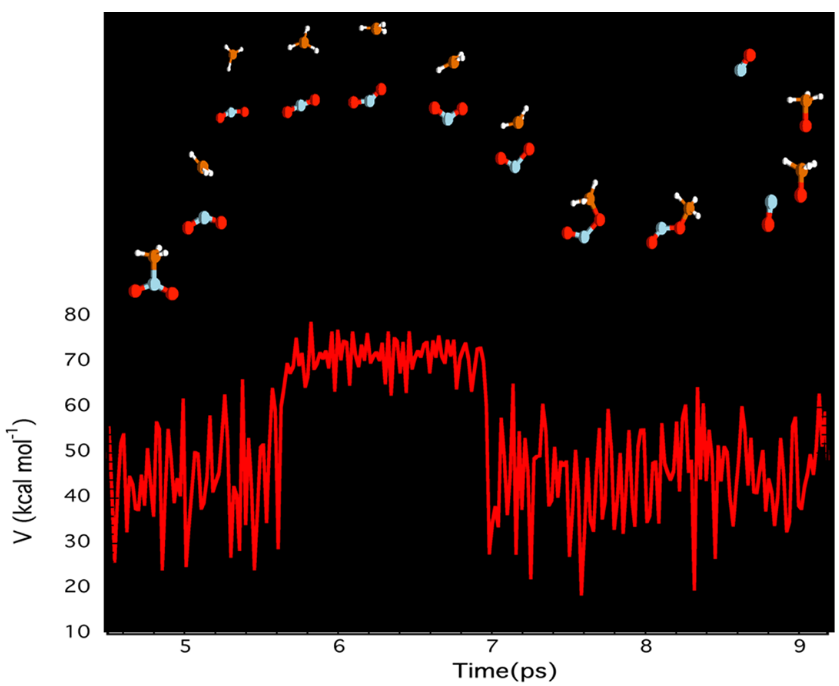

FIGURE 10
Sample trajectory of CH_3NO_2 dissociation. Potential energy relative to the CH_3NO_2 global minimum and several frames for a sample trajectory of energy 53.2 kcal/mol.

The investigators found that in this trajectory, the excited molecule undergoes vibrational motion until a time such that the excess energy has pooled in the C-N bond. This occurs near 6 picoseconds, and then the bond ruptures and the NO_2 fragment stays trapped within the potential field of the CH_3 moiety. They orbit each other until the CH_3 group abstracts an O atom from the NO_2 unit. Interestingly, the NO and CH_3O moieties can continue to orbit one another until a H atom is abstracted from CH_3O, forming CH_2O (ketone) and HNO as final products. This trajectory observes very unique dynamics: the orbiting of one molecular fragment with respect to another has been termed 'roaming', and there are significant consequences. Specifically, roaming allows the chemical systems to stray away from regions that are saddle points and find alternative pathways to products. This can alter the expected branching fraction of products in a reaction from what standard theories would predict. The phenomenon of roaming is especially important in energy regimes where the internal energy of the system is approximately the same as that of a bond energy. The branching ratio as a function of energy dependence is shown in FIGURE 11.

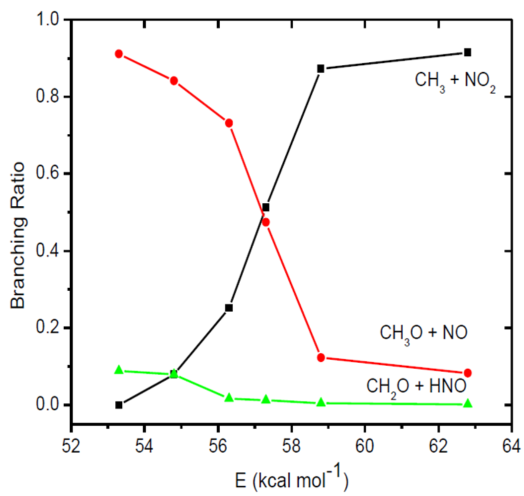

FIGURE 11

Energy dependence of roaming for CH_3NO_2. At threshold, essentially all of the products of the reaction are CH_3O + NO. As the internal energy of the system increases, the propensity for roaming decreases and the dominant products become CH_3 and NO_2 at energies that exceed 57 kcal/mol. The channel forming CH_3 and NO_2 is the reaction channel predicted by standard chemical reaction theories. The channel producing CH_3O and NO was known previously from experimental observation, but the details of the dynamics (*i.e.*, the 'roaming' mechanism) were hidden prior to these findings.

F. Robust Nanoparticles

Professors Todd Emrick and Alfred Crosby, University of Massachusetts - Amherst, Single Investigator Award

Professors Emrick and Crosby's research aims to assemble nanoscale building blocks, with novel optical and electronic properties, into macroscopic, complex hierarchical structures with exceptional flexibility and mechanical integrity. Using flow coating techniques, the research team has successfully developed a facile, evaporative deposition method to direct the assembly of dissolved solutes, such as nanoparticles or polymers, into organized structures over multiple length scales. Furthermore, tailoring the chemistry of the nanoparticle ligands, using polymerizable ligands or pre-made polymer ligands, has provided a route to transform these nanoparticle assemblies into robust materials with tunable structure and functionality.

In FY13, the research team discovered that hybrid nanoparticle/polymer ribbon assemblies, fabricated by flow coating, will spontaneously form helical structures when placed into a volume of liquid, such as water (see FIGURE 12). The driving force for this spontaneous helical formation is the reduction of surface area, which is made possible by the asymmetric (*i.e.*, non-rectangular) cross-sectional shape obtained by flow coating. As the ribbon bends, it compresses one surface while stretching the other, which allows for a preferred bending direction in order to form helices. The fabricated helices are 2-3 orders of magnitude larger in contour length than radius, and similarly larger in radius than thickness, naturally affording high flexibility and extensibility. The generality of this geometry-driven helix formation mechanism opens new frontiers for making nano- and micro-helical structures from virtually any material, ranging from commodity materials to highly tailored chemical components. This, combined with the ability to produce such materials in a scalable and robust process, presents a considerable advantage in novel designs and fabrication of hierarchical materials. Thus, these nanoparticle/polymer helices have great potential in the design of wearable electronics and sensors, as well as novel nano-scale mechanical reinforcements in soft elastomers and gels.

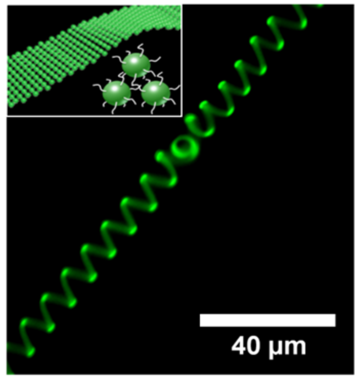

FIGURE 12

Hybrid nanoparticle/polymer ribbon assemblies that form helical structures. Fluorescent microscope image of functional quantum dots forming mesoscale helices in water. Inset: Schematic of helix-forming cross-linked nanoparticle ribbon nanostructure.

F. Understanding Impact of Plasmons on Graphene Properties

Professors Tomás Palacios and Marin Soljacic, Massachusetts Institute of Technology, ISN (UARC)

Professors Palacios and Soljacic are seeking to understand the impact of plamsons on the mid-IR photoresponse of graphene, including: (i) near-field control of thermal radiation transfer by plasmons; (ii) plasmonic losses; (iii) the properties of plasmons on the surface of one-atom thick metals; and (iv) the properties of 2D photonic (graphene) crystals exhibiting flat surface bands pinned between two Dirac points. In FY13, the team's analysis of the dependence of near-field heat exchange on doping and electron relaxation time in the infrared led to the discovery that plasmon-polariton modes strongly mediate, enhance and tune the near-field radiation transfer between closely separated graphene sheets; such control arises from either inter- or intraband mechanisms, with maximum thermal radiation transfer predicted at low doping and for plasmons in two sheets of graphene at resonance (*e.g.*, enhancements up to 1000 over the far-field limit at sheet separations of 10 nm).[2] These predictions are expected to be verified using an experimental setup that mimics an AFM (see FIGURE 13).[3] This research may enable future applications such as including externally controllable thermal switches, tunable plasmonic emitters and high efficiency, high-power density, near-field thermophotovoltaic systems.[4] Considerable efforts were also made to understand the different loss mechanisms of confined plasmonic modes in graphene due to competing many-body effects such as electron-phonon interactions, electron-electron interactions and impurity scattering. Strong interband losses (that is, those where plasmons decay to create electron-hole pairs) were shown to only occur above a threshold frequency that is a function of the doping level in the graphene sheet; electrostatic gating can be used to eliminate these losses for frequencies in the THz and IR regime and have been demonstrated to yield photocurrents in the near-IR (see FIGURE 14). The interaction between plasmons and optical phonons was discovered to become the dominant loss mechanism at intermediate frequencies, leading to sharp increases in relaxation times and potentially enhanced photocurrent signal response time (see FIGURE 14A-B). The research team also compared graphene to metallic mono-atomic layers. Using the Drude model, it was shown that the plasmon wavelength of silver layers is decreased by two orders of magnitude

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[2] Ilic O, Jablan M, Joannopoulos JD, et al. (2012). Near-field thermal radiation transfer controlled by plasmons in grapheme. *Phys. Rev. B*. 85:155422.

[3] Shen S, Narayanaswamy A, and Chen G. (2009). Surface phonon polaritons mediated energy transfer between nanoscale gaps. *Nano Letters*. 9:2909-2913.

[4] Ilic O, Jablan M, Joannopoulos JD, et al. (2012). Overcoming the black body limit in plasmonic and graphene near-field thermophotovoltaic systems. *Optics Express*. 20:A366.

to a wavelength comparable to that observed in graphene. While plasmons in such metallic layers have an abundance of free carriers far in excess of graphene, such metallic layers lack the mechanical stability of suspended graphene, which will be a major advantage for graphene based devices. Finally, it was theoretically demonstrated that flat surface bands can be engineered within a Dirac pseudogap for 2D photonic crystals that could lead to slow light dispersion and a large density of states.

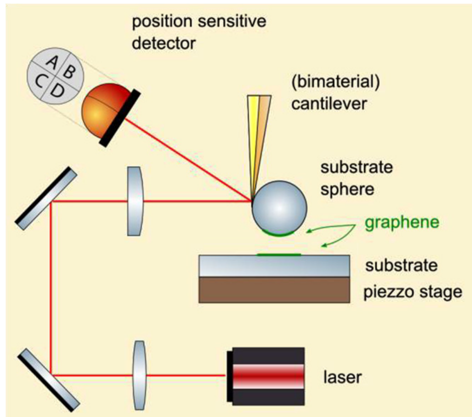


FIGURE 13

Schematic of the proposed experiment to measure the contribution of graphene plasmons to near-field thermal radiation transfer. In this experiment, CVD graphene is transferred onto both the sphere and the planar substrate and its properties are characterized using Raman spectroscopy. As the distance between the sphere and the substrate is reduced (using nm-precision piezo stage), the increase in the thermal energy transfer coefficient results in the bending of the cantilever. The amount of bending is measured using a position sensitive detector. Thermal energy exchange due to convection is suppressed by operating in vacuum

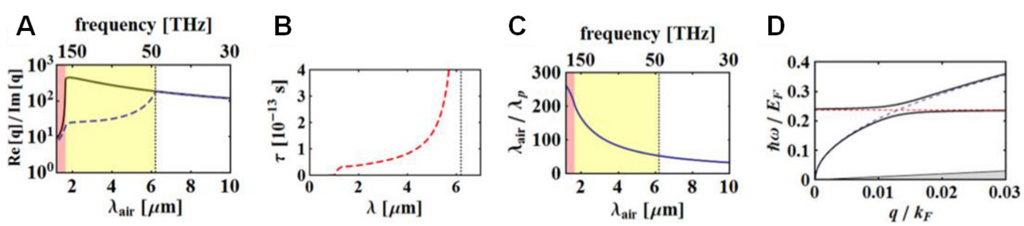


FIGURE 14

Plasmon properties of the plasmon-phonon coupled modes. These data are (**A**) plasmon losses quantified as Re(q)/Im(q), (**B**) relaxation time due to interaction with optical phonons, (**C**) localization of graphene plasmons quantified as λair/λp, and (**D**) hybridized plasmon-phonon dispersion curve for the unconventional mixing of plasmon and optical phonon polarization.

Having established a fundamental understanding of how plasmonic effects impact infrared detection by graphene, experiments were then conducted to characterize prototype, graphene thermo-electric pixel elements in the mid IR range (λ = 10 μm). Infrared photo-voltage characterization of graphene pixels was completed as shown in FIGURE 15. As the physical detection mechanisms have a tremendous impact on the performance of the pixel, initial experiments focused primarily on an electrostatic PN junction formed in the graphene; the physical detection mechanisms present inside the graphene pixel could be discerned by controlling the carrier type of the graphene as well as the direction of the built in field. The PN junctions were observed to exhibit photocurrents in the near-IR (λ = 850nm), attributed primarily to hot carrier mechanisms. In order to study these mechanisms at longer wavelengths (λ = 10 μm), high quality chemically vapor grown (CVD) graphene was necessary to fabricate electrostatically controlled PN junctions due to the longer optical length scales. Moreover, at low energies (~ 125 meV), optical phonon scattering was suppressed and is predicted to lead to increased carrier lifetimes and enhanced photo-response. Using electrostatic gating, the absorption mechanisms in graphene were studied by selecting between conventional photovoltaic effects and photo-thermoelectric effects; the measurements show a clear signature that thermo-electric effects dominate the detection mechanism over photovoltaic effects (see FIGURE 16). Experiments suggested that the photocurrent signal is enhanced by electrostatic gating near the Dirac peak and reduced disorder in the graphene sample.

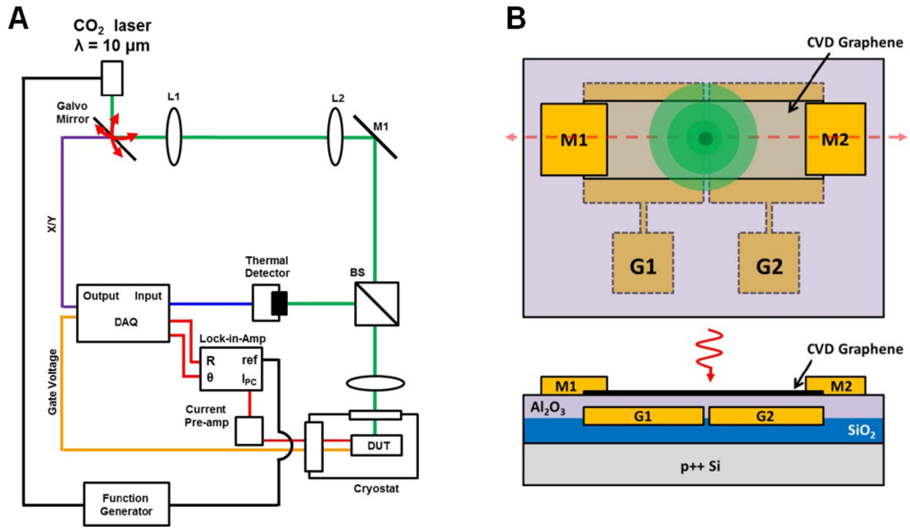


FIGURE 15

Infrared characterization experiment. The experiment was configured with (**A**) a confocal CO_2 laser scanning system and an (**B**) electrostatic PN junction for thermo-electric versus photovoltaic measurements.

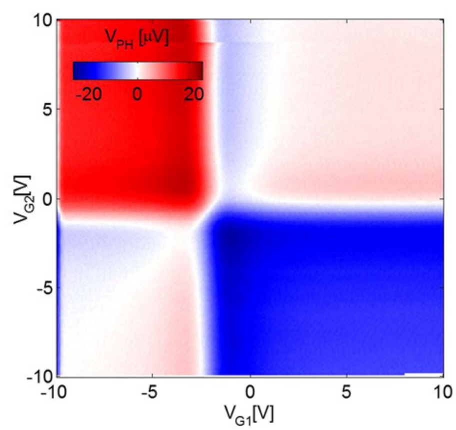


FIGURE 16

Variable gate photovoltages maps from graphene devices. The six fold regions are a signature of the curvature of the Seebeck Coefficient of graphene.

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. Mechanically-Active Polymer Composites

Investigator: Professor Stephen Craig, Duke University, MURI Award
Recipient: Bridgestone Corp.

As part of their research in the "Mechanochemically-Active Polymer Composites" MURI, Professor Craig's research team has focused on designing stress-responsive mechanophores that sense local stress and trigger a chemical remolding at the "at-risk" segments. This research has led to the discovery of mechanically active gem-dihalocyclopropanes that (i) act as an "energy sponge," capturing mechanical energy through the activation of chemical reactions in a manner reminiscent of the toughening observed in TRIP ceramics and (ii) once mechanically activated, are susceptible to nucleophilic substitution reactions that can create new, stress-bearing cross-links in response to localized forces of tension, causing the polymers to become stronger in response to a typically destructive mechanical environment (see FIGURE 17). The research team has successfully incorporated large quantities of these mechanophores into polybutadiene, representing the first demonstration of multiple mechanochemical reactions in a single polymer chain. The stress-relieving and stress-strengthening behavior demonstrated by these materials has resulted in a transition and collaboration with Bridgestone Corp. which seeks to match mechanochemical functionality with polymer composition criteria for selected applications of rubbery polymers.

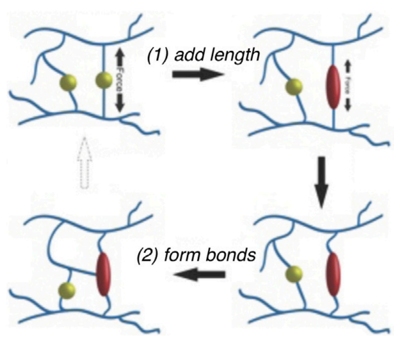


FIGURE 17

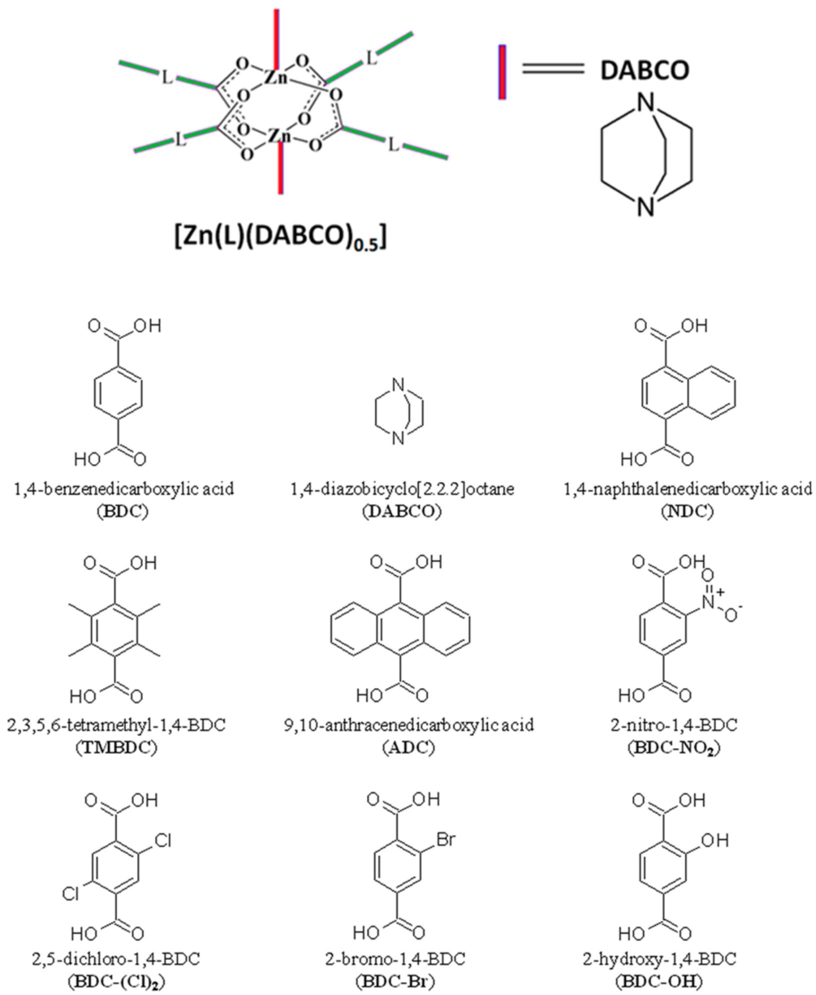
Schematic of mechanochemical remodeling of synthetic polymers. Localized forces in polymer networks trigger covalent reactions that (1) release stored length and (2) form new, stress-bearing bonds; a strategy being developed for high-performance rubbery materials.

B. Multifunctional Nanostructures for Adsorption of Toxic Materials

Investigator: Professor Krista Walton, Georgia Institute of Technology, PECASE Award
Recipient: U.S. Army Edgewood Chemical Biological Center (ECBC)

The objective of this research, led by Professor Walton, is to develop a rational design approach for creating functional, porous inorganic-organic hybrid materials. Professor Walton has been focusing on designing metal-organic framework based materials for the adsorption of ammonia under dry and humid conditions. In FY13, the Walton group made progress in increasing MOF stability toward water. The research team conducted a systematic study to evaluate the affect of ligand functionalization on the water stability of a family of metal-organic frameworks, DMOF-X (where X = ADC, NDC, TM, Br, Cl_2, NO_2, OH), as shown in FIGURE 18.

Analysis of nonpolar and polar functional groups demonstrated that nonpolar groups enhance the stability of the MOF compared to the parent MOF by shielding the Zn-O bond from hydrolysis, while polar groups destabilize the MOF. After exposure to 90% relative humidity, surface area losses range from 97-100% for the parent MOF and those with polar groups; however, for the nonpolar functionalized ligands, surface area losses are minimized to only 4-32%. In addition, increasing steric bulk also increased water stability. In FY13, materials with enhanced water stability transferred to the ECBC CBR Filtration team where enhanced ammonia adsorption under humid conditions has been demonstrated. Future work at ECBC will continue to evaluate these materials with enhanced stability for inclusion into mixed filter beds.



1. $[Zn(NDC)(DABCO)_{0.5}]$ or DMOF-N
2. $[Zn(BDC)_{0.5}(TMBDC)_{0.5}(DABCO)_{0.5}]$ or DMOF-TM1
3. $[Zn(TMBDC)(DABCO)_{0.5}]$ or DMOF-TM2
4. $[Zn(ADC)(DABCO)_{0.5}]$ or DMOF-A
5. $[Zn(BDC\text{-}NO_2)(DABCO)_{0.5}]$ or DMOF-N
6. $[Zn(BDC\text{-}(Cl)_2)(DABCO)_{0.5}]$ or DMOF-Cl_2
7. $[Zn(BDC\text{-}Br)(DABCO)_{0.5}]$ or DMOF-Br
8. $[Zn(BDC\text{-}OH)(DABCO)_{0.5}]$ or DMOF-OH

FIGURE 18

DMOF ligand functionalization. The structure of parent DMOF is shown at the top; ligands used to synthesized isostructural DMOFs (DMOF-X) are shown in the bottom panel.

C. Parallel Large-scale Semi-definite Programming for Strong Electron Correlation
Investigator: Professor David Mazziotti, University of Chicago, Single Investigator Award
Recipient: U.S. Army Research Laboratory - Weapons Materials Research Directorate (ARL-WMRD)

Two-electron reduced density matrix (2-RDM) methods represent all of the electrons in any molecule or material with only two electrons by replacing the wave function by the 2-RDM as the basic variable for quantum many-electron theory. Until now, the 2-RDM method has been only a theoretical concept with respect to computational chemistry modeling, since a key piece of information known as the representability conditions were missing. In breakthrough research sponsored by ARO, the PI found all the necessary representability conditions in order to make this method work, which had been a problem in theoretical physics for over sixty years. The PI constructed an easy-to-use software program which relies on semidefinite programming and the 2-RDM concept to model the electronic structure of atoms and molecules. The 2-RDM method has already been shown to exceed the performance of the gold standard ab initio method CCSD(T) in capturing non-dynamical correlation energy, and moreover the 2-RDM method scaling is lower by more than a factor of ten. In FY13, this code transitioned to scientists at ARL-WMRD who are evaluating it for use in energetic materials chemistry research. In addition, the PI has distributed the code to several university laboratories across the U.S.

D. Niobium/niobium Oxide Metal-insulator Bilayers
Investigator: Professor Ryan O'Hayre, Colorado School of Mines, PECASE
Recipients: Natick Soldier Research, Development and Engineering Center (NSRDEC);
Army Research Laboratory - Sensors and Electron Devices Directorate (ARL-SEDD)

The material Nb/Nb_2O_5 has been identified as a promising component for metal-insulator-metal (MIM) devices for solar energy conversion. Its properties include low turn on voltage, high asymmetry, and high non-linearity, all of which are attractive metrics for MIM rectification purposes. Professor Ryan O'Hayre has developed a novel synthesis technique to synthesize Nb/Nb_2 bilayers. Professor O'Hayre fabricated and characterized a set of Nb/Nb_2O_5 bilayer samples on insulating substrates. Nb metal films were deposited on oxidized Si wafer substrates by DC magnetron sputtering and then subsequently treated by anodic oxidation to produce a highly-reproducible Nb_2O_5 oxide film of tunable thickness (see FIGURE 19). In FY13, a series of samples with tunable oxide thicknesses were produced and transitioned to NSRDEC and ARL-SEDD for evaluation.

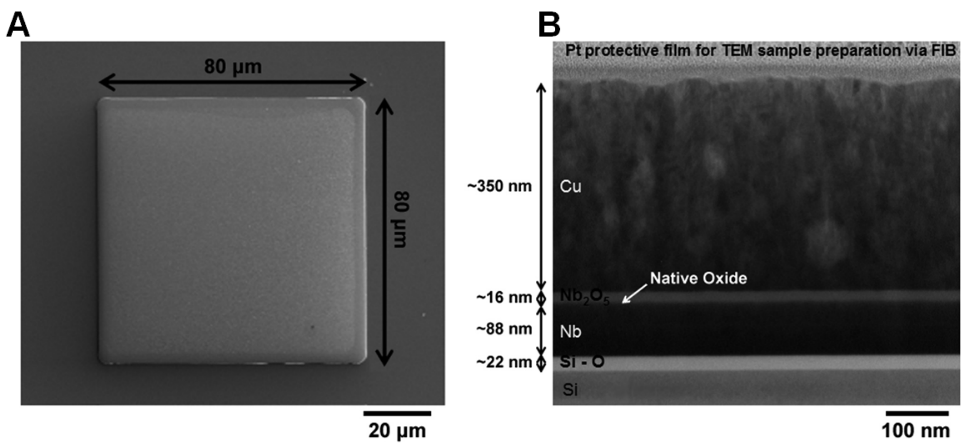


FIGURE 19

Niobium/niobium oxide metal-insulator bilayer samples. (A) SEM image of a completed 80 lm by 80 lm $Nb/Nb_2O_5/Cu$ diode after the lift-off procedure and (B) a TEM cross-sectional image showing the individual layers. Both the interfaces (Nb/Nb_2O_5) and (Nb_2O_5/Cu) are smooth and continuous, illustrating the quality of the deposited layers and the fabrication route.

Researchers and NSRDEC and ARL evaluated the materials with six different top electrode metals: Ag, Au, Cu, Ni, Nb, and Pt. It was found that these materials possessed asymmetric properties with the highest performing devices in each of those material systems surpassing the minimum desired figure-of-merit asymmetry and nonlinearity. The $Nb/Nb_2O_5/Pt$ material system possessed the most desirable performance values and characteristics for use as a potential rectifier.

V. ANTICIPATED ACCOMPLISHMENTS

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

A. New Microstructures for Old Monomers: Synthesis of Gradient Pi-Conjugated Copolymers

Professor Anne McNeil, University of Michigan - Ann Arbor, PECASE

Professor McNeil's research aims to generate a novel class of π-conjugated materials with unique and tunable properties, including phase-compatibilizing abilities in polymer blends. To accomplish this goal, the research team will synthesize a comprehensive library of gradient copolymers to provide fundamental insight into the role of copolymer microstructure on properties. It is anticipated that these novel copolymers will exhibit tunable optical, electronic and physical properties based on the comonomer identity, copolymer sequence, molar composition, and molecular weight (see FIGURE 20).

In FY13, the research team prepared and characterized a "third-generation" gradient copolymer, wherein a poly(thiophene) backbone is functionalized with a gradient distribution of fullerene molecules. Preliminary results excitingly demonstrated that even with only 10%-loading of fullerene, the gradient copolymer stabilized a physical blend of P3HT and fullerene. Thus, it is anticipated that in FY14 the team will determine the impact of percent composition, sequence distribution, and copolymer molecular weight on P3HT/fullerene compatibilization, as well as the resulting impact on solar cell efficiencies. If successful, these studies will make a substantial impact on the field by providing a route to controlled, nanostructured thin films and lead to an improved understanding of the relationship between film structure and solar cell efficiency.

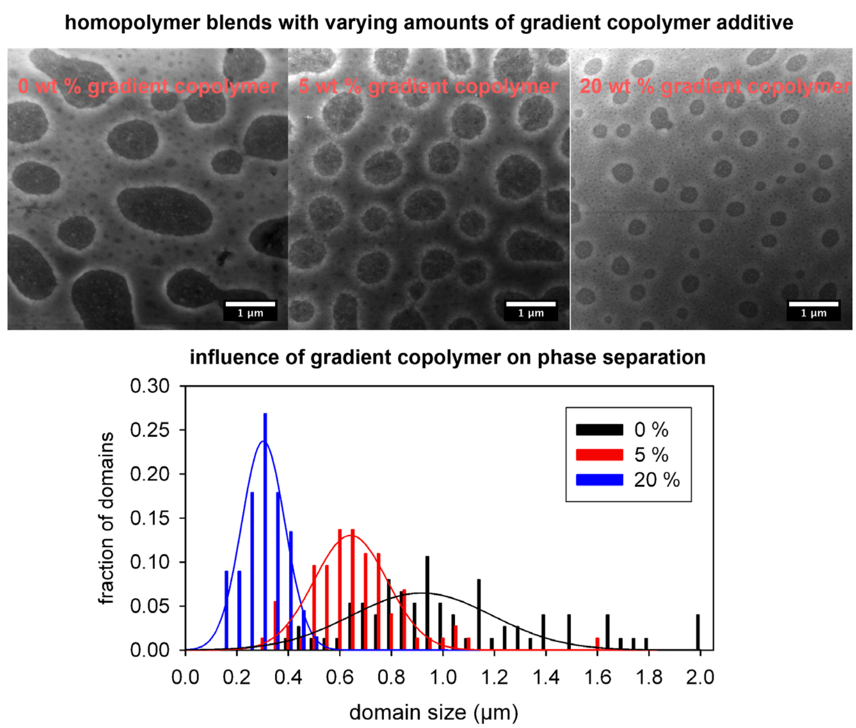


FIGURE 20

Influence of gradient copolymer additive on phase separation. (Top) SEM/HAADF images showing the impact of the PI's "second-generation" gradient copolymers on phase separation in polymer blends. (Bottom) Histogram showing that the domain size decreases with increasing weight percent of gradient copolymer additive.

B. Characterizing Microstructures at Ionic Liquid/electrodes Interfaces
Professor Luke Haverhals, Bradley University, YIP Award

Professor Haverhals and colleagues are studying interfacial structure and dynamics between ionic liquids and conductive or semiconductor electrodes. In the past decade, ionic liquids (ILs) have been targeted as electrolytes for a wide variety of electrochemical applications. However, there is presently a knowledge gap with respect to characterizations of the interfaces between electrodes and IL-based systems. In ionic liquids the medium is composed solely of ions so that there are no molecular species (to solvate ions). In place of a diffuse layer, there exist 'structured' layers of alternating ions that vary as a function of distance from the electrode (see FIGURE 21).

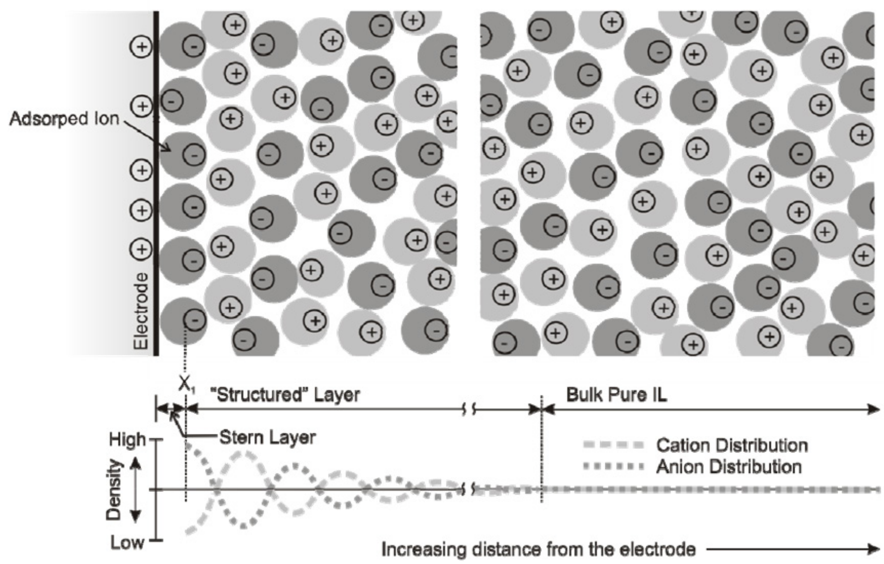


FIGURE 21

Double layer structure. This illustration loosely depicts the interface between a positively charged electrode and a pure IL electrolyte. X1 is the inner Helmholtz plane for adsorbed ion; however, given there is no solvated ions (by molecular species), there is no outer Helmholtz plane (X2). Also note that, for ILs, ions are often not symmetric.

In FY14, it is anticipated that Professor Haverhals will utilize infrared reflection-absorption spectroscopy (IRRAS) and surface enhanced infrared absorption (SEIRA) spectroscopy techniques to characterize the geometric arrangement of electrolyte and redox media near electrode surfaces while under controlled polarization conditions. Electrode polarization type (waveforms) and measured current responses will differentiate critical charge transfer and transport fundamental properties.

C. Interaction of Bacterial Metabolites with Fluorescent Synthetic DNA
Professor Eric Kool, Stanford University, Single Investigator Award

The objective of this research, which is being co-funded with the Life Sciences Division, Microbiology Program, is to investigate the behavior of DNA-polyfluorophore assemblies in the presence of organic vapor-phase molecules. This research will study how short, synthetic fluorescent modified DNAs, oligodeoxyfluorosides (ODFs), interact with organic vapors including those released by bacterial colonies. It is anticipated that in FY14, the researchers will focus on synthesizing structural variations of ODFs and investigate how these structural variations affect electronic and photophysical interactions with other molecules. Monomer length, alternating dye units, and blocking groups will be incorporated in the ODFs and their responses to analyte vapors such as vapor phase bacterial metabolites, will be tested. Dyes will include pyrene and perylene and blocking groups will include terphenyl and adenine deoxyribosides (see FIGURE 22).

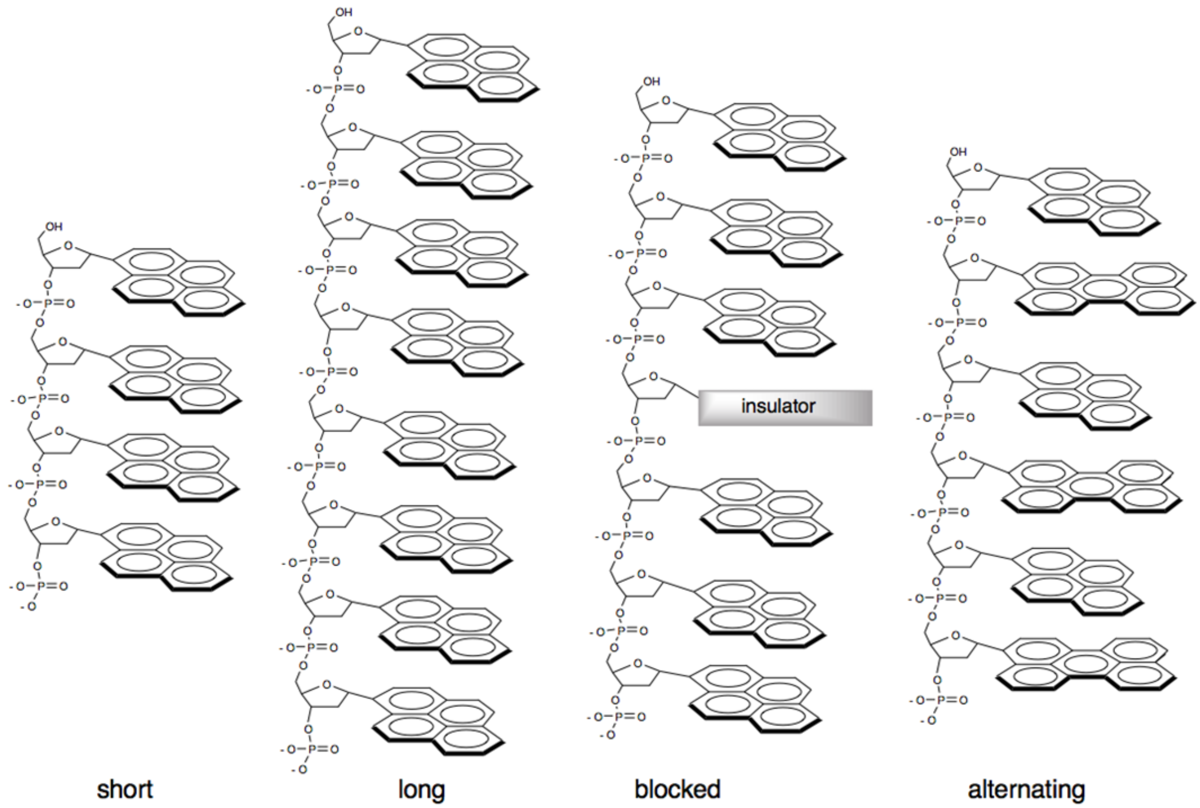


FIGURE 22

Examples of systematic structural variations to be examined. Pyrene and perylene dyes are shown, but over a dozen different fluorophores could be used in this configurations.

This research will provide a fundamental understanding of how fluorophores arranged on DNA interact and communicate with one another. In addition, this research provides a unique fluorescence-based identification for complex vapor mixtures from bacterial respiration and metabolism. This unique approach to pattern-based sensing could provide a revolutionary, rapid, simple, and low cost detection platform to identify the presence of harmful biological agents and monitor Soldier health.

D. Photoelectron Spectroscopy of Energetic Materials and Catalytic Clusters

Professor Elliot Bernstein, Colorado State University, DURIP and Single Investigator Awards

The goals of this research are to (i) to determine the low energy (less than 26.5 eV) ion states of energetic materials and their model systems and discover their structure, reactivity, and fragmentation behavior through time-of-flight mass spectrometry (TOFMS), extreme ultraviolet photoelectron spectroscopy (PES), and then (ii) to transition this new PES gained data and knowledge for the synthesis and generation of better, more application-specific energetic materials.

With regard to energetic materials of all varieties, very little is known or even researched, concerning their ion states and the part played by ions in the overall decomposition (release of their stored energy) of energetic species. The planned PES studies of these states and their behavior are novel and will open a completely new area for study of their behavior and properties. The techniques that the PI has employed in the past allow access to both neutral and ion properties of energetic materials and their model systems, and the new direction of PES studies will focus on the ionic states specifically. In FY14, the PI will address the issue of the importance of ionic states for the behavior of energetic materials directly and uniquely through UV and EUV TOFMS and PES.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Jennifer Becker
Division Chief
Program Manager, Reactive Chemical Systems

Dr. Robert Mantz
Program Manager, Electrochemistry
Program Manager (Acting), Polymer Chemistry

Dr. James Parker
Program Manager, Molecular Structure and Dynamics

Dr. Dawanne Poree
Contract Support, Polymer Chemistry

Ms. Wendy Mills
Contract Support, Reactive Chemical Systems

B. Directorate Scientists and Technical Staff

Dr. Douglas Kiserow
Director, Physical Sciences Directorate

Dr. Peter Reynolds
Senior Scientist, Physical Sciences Directorate

Dr. Robert Kokoska
Program Manager, Institute for Soldier Nanotechnologies and Institute for Collaborative Biotechnologies

Dr. Kelby Kizer
Special Assistant to the Directorate Director

Mr. John McConville
Technology Transfer Officer, Institute for Soldier Nanotechnologies

Dr. Daniel Colombo
Contract Support, Institute for Soldier Nanotechnologies and Institute for Collaborative Biotechnologies

C. Administrative Staff

Ms. Monica Byrd-Williams
Administrative Specialist

Ms. Jennifer Eaton
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 2013* is to provide information on the programs and basic research supported by ARO in FY13, 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 FY13.

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, for extracting critical information and actionable intelligence, for improved decision making, and to achieve information dominance to enhance the warfighters' situation awareness. Toward this end, the Division supports research 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 efforts will stimulate future studies and help 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. 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. For this reason, computing science is a key technology underpinning future Army operations.

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 organizations. The Division's 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 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 scientific solutions to the near-term needs of the warfighter.

B. Program Areas

The Computing Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY13, the Division managed research 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. This research supports 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 cyber information 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 to ensure their trustworthiness. The Resilient and Robust Information Infrastructure Thrust promotes research on cyber situation awareness theories and frameworks that combines intrusion prevention, detection, response, and recovery to establish 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-offs such as performance, resiliency, and, survivability. The Highly Assured Tactical Information Thrust may lead to the development of novel situation awareness theories and techniques that 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 Sciences Division for FY13 were $41.3 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY13 ARO Core (BH57) program funding allotment for this Division was $3.5 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 $6.0 million to projects managed by the Division. The Division also managed $7.9 million of National Security Agency (NSA) programs, and $2.9 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.6 million for contracts. The Institute for Creative Technologies (ICT) received $14.5 million for combined basic (6.1) and applied research (6.2 and 6.3). Finally, $5.1 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.2 million provided through the ARO Core (BH57) allotment, in addition to funding for 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 creation, leadership, and management of 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 FY13 (*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 FY13 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 FY13, the Division awarded 15 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to establish the foundation and guiding principles for creating secure, resilient, and trustworthy computing systems, to determine new techniques for implementing approximation in computer systems to achieve improved energy efficiency, to create new methods and theories for improved detection of subsurface objects through multimodal data fusion, and to establish data mining methodologies to detect, validate, and predict entities and events from heterogeneous social media sources. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Yingying Chen, Stevens Institute of Technology; *Making Inferences of Physical Properties*
- Professor Hichem Frigui, University of Louisville; *Multiple Instance Learning*
- Professor Paul Gader, University of Florida; *Spatial, Temporal, and Frequency Analysis of Wideband, Ground Penetrating Sensor Data*
- Professor Jiawei Han, University of Illinois - Urbana; *Mining Suspicious Tiny Sub-Networks in a Massive Social Network*
- Professor Alexander Hauptmann, Carnegie Mellon University; *Semantic Descriptions of Events Based on Detected Objects, Attributes and Actions*
- Professor Dominic Ho, University of Missouri - Columbia; *Sensor Array Processing for Subsurface Object Detection*
- Professor Marwan Krunz, University of Arizona; *Blinding Eve: Methods for Concealing Wireless Communications in Mobile Coalitions*
- Professor David Nicol, University of Illinois - Urbana; *Resiliency, Security, and Trust in Complex Engineered Systems*
- Professor Mark Oskin, University of Washington; *Disciplined Approximate Computing for Energy Efficiency and Resilience*
- Professor Martin Ribarsky, University of North Carolina - Charlotte; *Analyzing and Depicting Social Media through Signal Metrics*
- Professor Michael Saunders, Stanford University; *Scalable Matrix Algorithms for Interactive Analytics of Very Large Informatics Graphs*

- Professor William Scherlis, Carnegie Mellon University; *Science of Security Lablet - Scalability and Usability*
- Professor Peter Torrione, Duke University; *Information Aggregation for IED Identification with GPR, Video, and EM Induction: Within Sensor Processing, Multi Sensor Fusion, and Large-Scale Learning*
- Professor Laurie Williams, North Carolina State University; *Science of Security*
- Professor Suya You, University of Southern California; *3D Modeling of Urban Sites from Point Clouds*

2. Short Term Innovative Research (STIR) Program. In FY13, the Division awarded four new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to create the scientific foundation for cybersecurity dynamics, determine new methods for 3D shape descriptions and classifications, and explore algorithms for noise reduction in Big Data obtained from social media. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Hongmei Chi, Florida A&M University; *Development and Detection of Mobile Malware*
- Professor Yun Fu, Northeastern University; *Manifold Learning for 3D Shape Description and Classification*
- Professor Shouhuai Xu, University of Texas at San Antonio; *Cybersecurity Dynamics*
- Professor Guoliang Xue, Arizona State University; *Computational Exploration of Noise in Social Media*

3. Young Investigator Program (YIP).

No new starts were initiated in FY13.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY13 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *2012 IEEE International Conference on Image Processing*; Orlando, FL; 30 September - 3 October 2012
- *19th ACM Conference on Computer and Communications Security*; Raleigh, NC; 16-18 October 2012
- *Workshop on Human-Centric Computing with Collective Intelligence: Challenges and Research Directions*; Tempe, AZ; 30-31 October 2012
- *TransCyber: Workshop on Security and Dependability for Next Generation Automotive and other Cyber Transportation Systems*; College Park, MD; 8 November 2012
- *Workshop on Counterfeit Electronics*; Storrs, CT; 28-29 January 2013
- *Workshop on Cloud Security;* Fairfax, VA; 11-12 March 2013
- *2013 International Conference on Social Computing, Behavioral-Cultural Modeling, and Prediction*; Washington, DC; 2-5 April 2013
- *Workshop on Sensing and Analysis of High-Dimensional Data;* Durham, NC; 23-25 July 2013

5. Special Programs. In FY13, 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 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 led 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 MURIs 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.

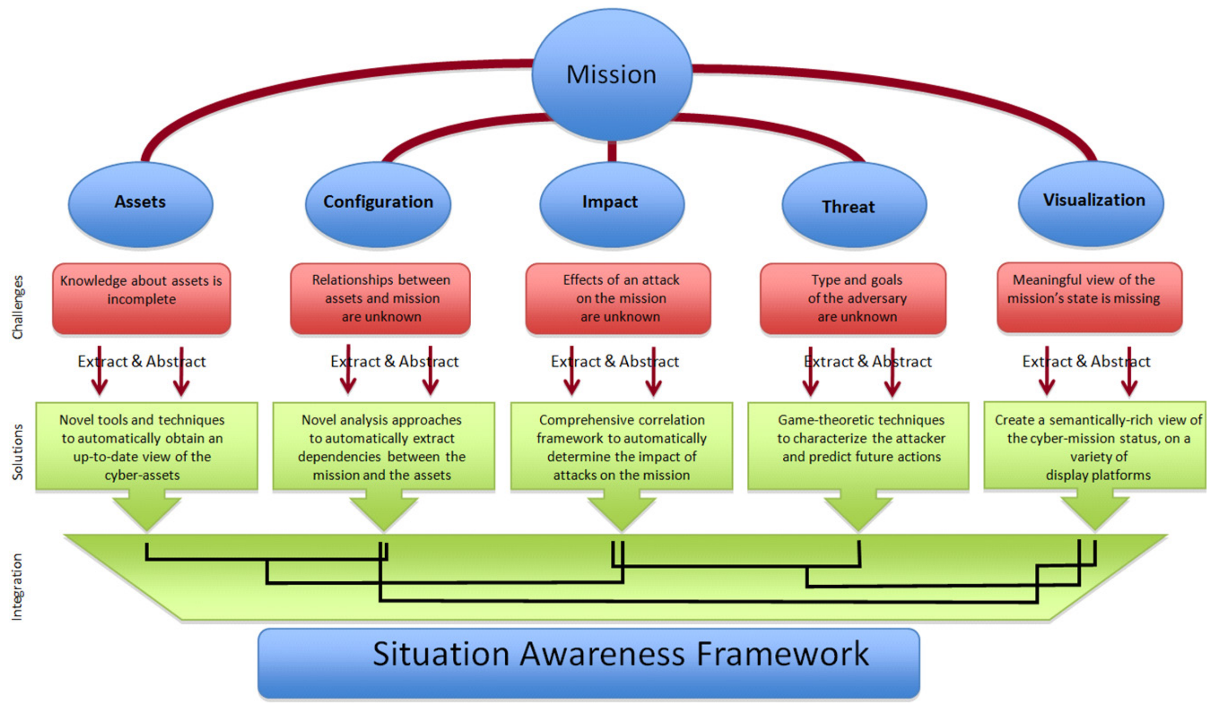


FIGURE 1

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 led 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 research 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 led 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.

This 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.

7. Adversarial and Uncertain Reasoning for Adaptive Cyber Defense: Building the Scientific Foundation. This MURI began in FY13 and was awarded to a team led by Professor Sushil Jajodia of George Mason University. Adaptive defense mechanisms are essential to protect our nation's critical infrastructure (computing, communication, and control) from sophisticated adversaries who may stealthily observe defense systems and dynamically adapt their attack strategies. This research aims to create a unified scientific foundation to enable the design of adaptive defense mechanisms that will maximize the protection of cyber infrastructure while minimizing the capabilities of adversaries.

The research will leverage recent advances in security modeling, network science, game theory, control theory, software system and network protocol security to create the scientific foundation, which may include general models for defense mechanisms and the systems they protect as well as irrational and rational adversaries. This research will develop a new class of technologies called Adaptive Cyber Defense (ACD) that will force adversaries to continually re-assess, re-engineer and re-launch their cyber attacks. ACD presents adversaries with optimized dynamically-changing attack surfaces and system configurations, thereby significantly increasing the attacker's workloads and decreasing their probabilities of success.

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

Research through the SBIR program has 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 FY13, the Division managed three new-start SBIR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of three Phase I contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications, including the development of a passive imaging capability for visualizing scenes through strong turbulence, a decision support tool using canonical representations and algorithms for data fusion and information delivery, and an innovative wide field-of-view imaging system with opto-electronic active mitigation of atmospheric turbulence effects for tactical scenarios.

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 FY13, the Division managed 6 new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of three Phase I contracts and three Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications, including the development of tools for cyber situational awareness for human-in-the-loop systems to capture knowledge representation used by experts to perform complex tasks, acoustic simulation tools capable of handling large-scale dynamic environments by exploiting multi-core CPUs and GPUs, and a portable multi-band compressive imaging sensor that is dynamically programmable to support adaptive data acquisition for improving object detection and classification.

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 FY13, the Division managed 11 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 FY13.

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 FY13, the Division managed five new DURIP projects, totaling $0.9 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of MIMO radar and distributed fusion based on value of information, cybersecurity, wireless network-on-chip architectures for multi-core systems, and behavior control of large groups of autonomous agents over a sensor network.

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 FY13, the ICT supported 15 faculty, 42 graduate and undergraduate students, 7 postdoctoral fellows, and 75 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 $14.5 million of program funds were awarded to the ICT in FY13, with $7.3 million allocated for 6.1 basic research, $5.2 million allocated for 6.2 applied research, and $2.0 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. FY13 was the final year of support for the Cylab; 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. FY13 was the final year of support for the consortium; 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. FY13 was the final year of support for the SOSI; research efforts were carried out under a no cost extension.

L. Joint NSA/ARO Advanced Computing Initiative (ACI)

The Advanced Computing Initiative (ACI) is a new NSA/ARO joint venture on energy efficient computing. Energy efficiency is now a primary constraint in designing new supercomputers. In order to provide robust performance, future systems will need to be able to dynamically trade off energy efficiency, performance, and reliability. The ACI is a four-year program that began in FY13 and is meant to support research for enabling these tradeoffs. NSA will supply all of the funding while ARO will assume the program management and contracting responsibilities. The ACI program has a close relationship to ARL's High Performance Computing efforts that offer potential cost savings and reliability benefits for the Army. The costs associated with consuming megawatts of electricity both directly and for the elaborate cooling systems to deal with the excessive heat supercomputers generate are becoming excessive. More important is the machine's reliability as more power to the system means more heat to the components, significantly increasing failure rates. Developing hardware and software infrastructure to increase performance while ignoring the effects on power consumption and reliability will not be feasible in the future. Seven grants have been awarded under the ACI program to teams composed of members from academia, industry and the national laboratories.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. Multipath Exploitation and Knowledge-based Imaging Using Compressive Sensing
Professor Fauzia Ahmad, Villanova University, Single Investigator Award

The objective of this research is to create novel urban radar imaging using comprehensive sensing to provide a high resolution imaging capability and streamlined data acquisition with much fewer space-time samples for target localization and tracking under challenging urban environments. Detection, localization, and tracking of targets in urban canyons and inside enclosed structures using radio frequency sensors is critical to the Army's needs for meeting the challenges of asymmetric warfare in urban environments. There is increasing demand for radar systems to deliver high resolution images in both range and cross-range, which requires the use of wideband signals and large array apertures. Additionally, radar operation at all frequencies and all antennas can face logistic challenges, as some of the measurements can be difficult, or impossible, to attain. Furthermore, the presence of clutter and multipath can significantly contaminate the radar data and compromise the main intent of providing enhanced system capabilities for imaging of building interiors and tracking of targets in streets and behind walls.

In FY13, Professor Ahmad and her group at Villanova University established a new approach to radar imaging of building interior structures through compressive sensing. The new approach exploits prior knowledge of building construction practices to form an appropriate sparse representation of the building interior layout. A dictionary of possible wall locations, which is consistent with the fact that interior walls are typically parallel or perpendicular to the front wall, was created. Compressive sensing was applied to a reduced set of observations to recover the true positions of the interior and exterior walls. For interior imaging, ghost targets may appear in the scene due to specular reflections from interior walls and multiple reflections within the front wall. This approach leverages prior knowledge of interior geometry to eliminate ghost effects by explicitly including a multipath model in compressive sensing (see FIGURE 2). Effective methods were created for the reconstruction of stationary scenes through group sparsity. Target and wall contributions to the image are separated using a joint wall and target sparse reconstruction approach, which allows suppression of the ghosts and increases signal-to-clutter ratio at the target locations. Additional information about interior walls is obtained using a dictionary of possible corner reflectors. Results based on simulation and laboratory experiments have shown that the new sparsifying basis outperforms existing approaches for building interior layout detection.

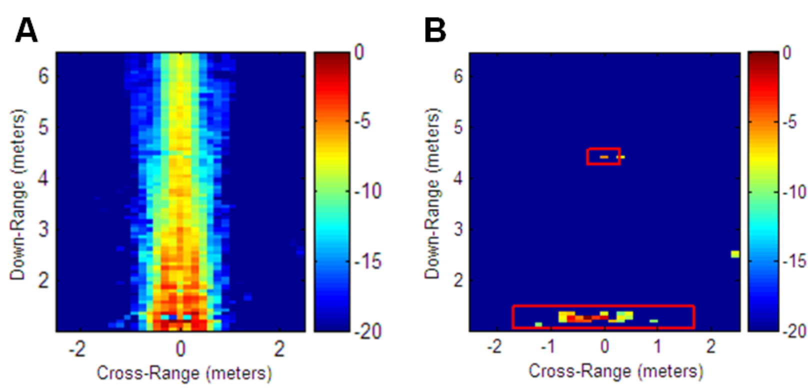


FIGURE 2

Compressive sensing based radar imaging. The target and wall are ambiguous in a traditional radar image (a) without wall mitigation using the full data set, but (b) visible in the new radar image with wall mitigation using 20% of the data.

B. Unobservable Re-authentication Techniques for Network Security

Professor Guoliang Xue, Arizona State University, Single Investigator Award

The objective of this research is to develop a novel authentication technique for handheld devices. More people are adapting to smartphones, which are lightweight and can provide extensive communication, computation, and sensing capabilities. These features make smartphones ideal for crowdsourcing, which is a new computing paradigm for human centric computing with collective intelligence. The widespread usage of smartphones gives rise to new security and privacy concerns, however. Smartphones are becoming a personal entrance to networks, and may store private information. Due to its small size, a smartphone could be easily taken away and used by an attacker. Using a victim's smartphone, the attacker can launch an impersonation attack, which threatens the security of current networks, especially online social networks. Therefore, it is necessary to design a mechanism for smartphones to re-authenticate the current user's identity and alert the owner when necessary. Such a mechanism can help to inhibit smartphone theft and safeguard the information stored in smartphones.

In FY13, Professor Xue designed a novel biometric-based system to achieve continuous and unobservable re-authentication for smartphones. The system uses a classifier to learn the owner's finger movement patterns (see FIGURE 3) and checks the current user's finger movement patterns against the owner's. The system continuously re-authenticates the current user without interrupting user-smartphone interactions. Experiments show that the system is efficient on smartphones and achieves high accuracy (see FIGURE 4).

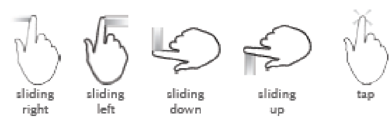


FIGURE 3

Five dominant gestures being monitored by the system for authentication.

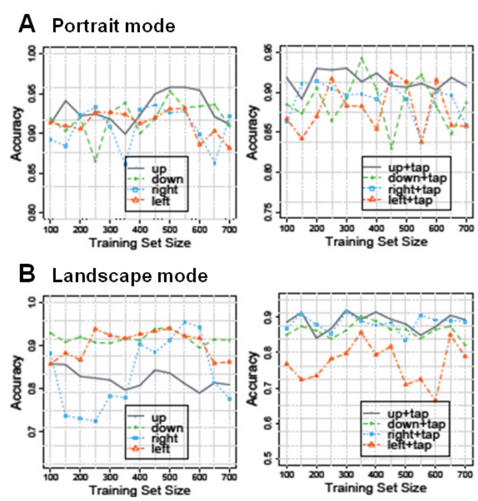


FIGURE 4

Training set size vs. classification accuracy. In general, as the training set size increases, the accuracy of a classification module first increases, approaches a maximum point, and then decreases.

C. Network Dependency Discovery

Professors Richard Kemmerer and Chris Kruger, University of California - Santa Barbara, MURI

The objective of this research is to create a new technique for modeling and tracking cyber dependency. Cyber-missions are sets of tasks that must be performed in a specified order and within a specified time frame to enable and support operational missions. High-level mission tasks that are composed of a series of more specific, low-level tasks could possibly be further broken down into even lower-level ones. To achieve cyber situation awareness, cyber analysts need to process a complete understanding of the mission hierarchical relationship and its dependency on information services.

In FY13, the research team created a new cyber dependency model and a prototype system to detect dependencies based on timing patterns. The system consists of both passive dependency detection and active dependency detection. The passive dependency detection system, which is application independent and network based, does not create any traffic and can be easily deployed in unknown environments. On the other hand, the active detection system injects small delays in the beginning of network connections to the under-study services, and these delays get propagated to the depending and dependent services. Statistical (hypothesis testing) analysis can detect these propagated delays to determine active dependency. The system can tune the system thresholds for gaining the desired false positive and false negative rates. The system has been deployed in a university lab for five months and correctly identified 54 network dependencies. When compared with previous approaches, which are generally passive-dependency detection systems such as NSDMiner, Orion, and Sherlock, the active dependency system provides a much better detection rate with a lower false error.

D. New Concepts in Semantic Organizing

Professor David Lazer, Northeastern University, Single Investigator Award

The objective of this research is to introduce a new concept of semantic organizing processes, mechanisms by which a set of authors come to produce observably similar discourse, as a means of inferring meaningful social and institutional networks from textual data. In FY13, the research team introduced three broad semantic organizing processes and showed that each leads to texts that tend to share phrases (n-grams) of different lengths (see FIGURE 5). To test these hypotheses, the researchers developed a novel n-gram extraction technique that captures textual overlaps in statements. The hypotheses of the three organizing processes and the extraction technique were tested on statements of the Members of the U.S. Congress. Ground truth against which the computed networks were compared were networks built from the Members' known party and group affiliation attributes. The computational results confirmed the hypothesis that the three organizing processes are reflected in three distinct kinds of textual similarity. These results are one step on the path toward the goal of this research to leverage social media to explore how groups of users reach consensus when no explicit external hierarchy or consensus mechanisms are present.

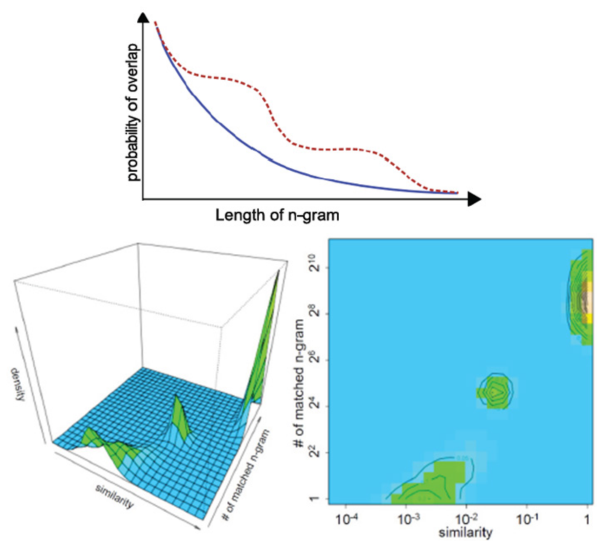


FIGURE 5

Phrases (n-grams) correspond to social groups. The top panel shows hypothesized similarity distributions over n-gram length. As n-gram length increases, the number of unique n-grams increases, and the probability of a match should decrease (blue solid line). Hypothesized semantic organizing processes can increase the likelihood of a n-gram overlap, producing "bumps" in the distribution (red dashed line). The bottom panel shows empirical evidence of these "bumps" in the distribution of observed n-gram similarity, based on a sample of 20% of documents in the corpus.

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. Spatial-temporal Correlation Analysis of Large-scale Sensor and Social Data

Investigator: Professor Alfred Hero, The University of Michigan, MURI Award
Recipient: ARL Computational and Information Sciences Directorate (ARL-CISD)

Spatial-temporal correlation analysis of data captures pairwise interactions between variables and is the basis for many machine learning and computer vision algorithms (e.g., algorithms for pattern classification and anomaly detection). For example, the analysis of patterns of spatial-temporal correlation between spatially distributed sensors can lead to better classification of intruders and improve situational awareness. To obtain reliable results, such correlation analysis requires collection of a larger number of data samples than standard mean analysis because a correlation matrix typically has many unknown parameters. Consequently, such correlation analysis tends to be computationally challenging and numerically unstable in practice.

Professor Hero and his research group at the University of Michigan have for the first time created a novel sparse Kronecker product representation of correlation matrix and established a ground breaking approach to correlation analysis of large scale spatially-temporal data. Numerical examples have shown that the new approach achieved five orders of magnitude improvements in computational speed and root mean square error reduction. This research will help address the large-scale data analysis challenges facing the defense community. The research has been conducted in close coordination with CERDEC Intelligence and Information Warfare Directorate (I2WD) and ARL-CISD, and the results transitioned to ARL-CISD for sensor network management.

B. An Experience-aided Reasoning Support System for Cyber Defense

Investigator: Professor John Yen, Penn State University, MURI Award
Recipients: ARL-CISD

Cyber analysts have been facing increasing challenges for detecting and responding to cyber attacks due to the huge amount of noise-abundant monitoring data and the increasing complexity of the attack strategies. Hence, supporting the analytic process of cyber analysts to better deal with these challenges is essential. While naturalistic decision making models recognize the important role of experiences in expert decision making, experiences have not been effectively leveraged in the existing reasoning support system due to the difficulty of elicitation and reuse.

Professor Yen and his research team have developed an experience-aided analytic reasoning support framework that automatically captures the experience of expert cyber analysts and subsequently recommends them to guide the reasoning process of novice analysts. The framework, realized through a support system, offers several important features. First, drawing on cognitive theory, experience is modeled as a reasoning process involving "actions," "observations," and "hypotheses," which are organized into a flexible tree structure that facilitates navigation by analysts and retrieval by the system. Second, the recommendation of experience enables the most relevant analytical sub-processes (within an experience) to be identified, ranked, and recommended based on its similarity to the current context. Third, in addition to successful experiences, failure experiences are also captured and recommended to assist the analyst to reduce the time spent on analyzing false positive alerts. Fourth, the system is non-intrusive in that it does not require any modification of existing data sources to be included in the system and can easily integrate new data sources. Computability and adaptability are key advantages of this framework because the hypotheses capture the analysts' internal mental reasoning using free text (understood by analysts, but currently viewed as a black box by the machine), while "actions" and "observations" are represented to capture the analysts' evidence exploration activities. A pilot study of the tool using a multi-step attack scenario indicated that the system can efficiently capture experts' experience without disrupting their analytical reasoning process. In FY13, the reasoning support system transitioned to ARL-CISD to develop a deeper understanding on how cyber analysts gain situation awareness.

C. Interactive Computational Algorithms for Acoustic Simulation in Complex Environments

Investigator: Professor Dinesh Manocha, UNC - Chapel Hill, Single Investigator Award
Recipient: U.S. Army Cold Regions Research and Engineering Laboratory (CRREL)

The objective of this research is to develop new interactive algorithms for acoustic simulation for analyzing wave propagation in complex environments. This research offers fundamental scientific capabilities for solving wave/sound propagation problems in highly complex, vast domains for seismology, geophysics, meteorology, geomagnetism, urban planning, immersive training, etc. The research includes development of accurate numerical methods for the wave equation, fast solutions based on sound field decomposition or geometric propagation, and development of hybrid numeric/geometric solutions. Parallel algorithms that can exploit the parallel capabilities of current multi-core CPUs and many-core GPUs for fast computations were also developed.

In FY13, software for non-linear ray tracing was developed and transferred to CRREL, one of the U.S. Army Corps of Engineers' Engineer Research and Development Center's laboratories. Accurately and efficiently modeling such propagation through large volumes has been a major challenge to CRREL acoustic scientists. The CRREL researchers are interested in developing new and fast algorithms for sound field computations for situations where neither prior low-frequency nor high-frequency methods are appropriate and when there is some randomness in the propagation but not enough that the problem can be modeled using a random scattering theory. The non-linear ray tracing formulation is used in simulations of large volume outdoor scenes to model high frequency propagation through inhomogeneous medium, including variations in temperature and pressure. Several large computational models have been developed at UNC-CH (see FIGURE 6) to validate the non-linear ray tracing method, along with other techniques, by making comparisons with measured acoustic data.

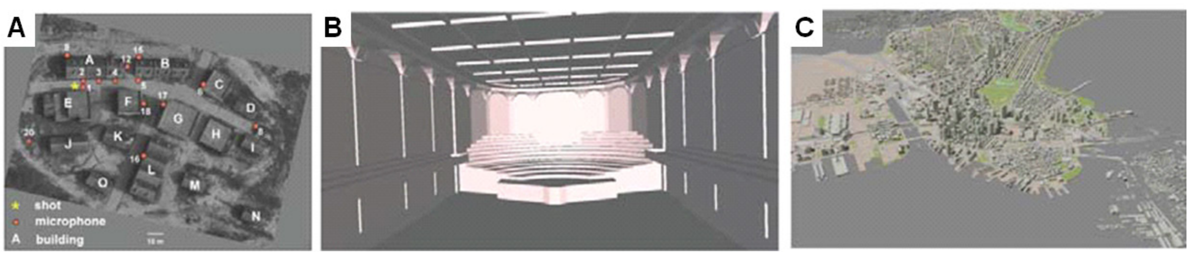


FIGURE 6

Large benchmark models to evaluate performance of ray-tracing and geometric acoustic simulation algorithms. From left to right: (**A**) An urban scene of dimensions 150m × 150m × 20m. Acoustic measurement data was provided from collaborators at CRREL for nearly 100 source-listener locations for frequencies up to 5 kHz. (**B**) Concert theater of dimensions 40m × 30m × 15m. The theater was designed by UNC's partner Arup (a major engineering design firm) and measurements were obtained for multiple locations for frequencies up to 20 kHz. (**C**) Boston city models of dimensions 3km × 3km × 100m. The data is made available by the Boston Redevelopment Authority. A UNC small business partner, Shotspotter, installed acoustic sensors in the city to gather the measurement data.

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. Value Driven Information Processing and Fusion

Professor Biao Chen, Syracuse University, Single Investigator Award

The objective of this research is to create a general framework for value driven decentralized information processing that is applicable to various information value metrics as determined by different inference tasks. This research builds on the two universal properties of various notions of information: data processing inequality (DPI) and additivity with independent observations. The DPI states that processing alone does not create information. It's desirable to establish a framework that guides data processing that optimizes information value, or minimizes information loss, while complying with various practical constraints. It is anticipated that in FY14, the research will examine a new class of DPI that characterizes information preservation and loss in information processing, which will have ramifications not only in optimal processing for inference, but also in many other design issues in information integration (*e.g.*, in the direction of communication and the selection of fusion center, among others). Each individual notion of information will be examined, including: Shannon's mutual information, Fisher information, Kullback-Leibler distance, Wyner's common information, and J-divergence. The research will also explore new approaches for data processing to maximally preserve the value of information. The paradoxical case exists only when data dependence is present such that globally sufficient statistics are no longer optimal when local processing is subject to stringent resource constraints such that those statistics cannot be conveyed to the fusion center in its entirety. Furthermore, a tandem fusion network where information exchange occurs in a lateral fashion will be carefully studied.

B. A Behavior-based Classification System for Bots

Professor Haining Wang, The College of William and Mary, Single Investigator Award

The objective of this research is to address the challenges of distinguishing bots from human users on Internet applications. Normally the behaviors of human users are irregular or unpredictable, but those of bots are regular or predictable. The proposed research will explore human observational behaviors that are inherently difficult for bots to mimic, but can be classified to distinguish between bots and human users. The research conducts a series of user behavior measurements through various online applications to characterize the observational behaviors of human users. The characterized observational behaviors include (i) user sending behaviors like inter-message delay and (ii) user biometric behaviors like mouse movement.

It is anticipated that in FY14 a classification system which consists of the entropy classifier and the neural network classifier will be built. The entropy classifier checks message interval as a measure of behavior complexity, while the neural network classifier checks for user-input actions such as keystrokes and mouse events to classify bots from human users. Each component assigns a score to the feature(s) it checks, which indicates the likelihood of automation, and makes a decision to categorize an unknown user as human or bot.

C. Disciplined Approximate Computing

Professors Luis Ceze and Mark Oskin, University of Washington, Single Investigator Award

The objective of this research is to investigate how to make approximation a useful feature of system design so that practical programmers can take advantage of it, especially with regard to energy efficiency. Through careful co-design of the hardware (approximate circuits and architecture), programming environment (exposing approximation through the type system), and runtime environment (dynamically monitoring and adjusting approximations to the application), approximation can become a useful core system building technique that will lead to orders of magnitude improvements in energy efficiency. The motivation is that as Denard scaling nears an end, traditional approaches to scaling energy efficiency are drawing to a close. At the same time, the scope and scale of problems to be addressed with computing continues to expand exponentially. Novel approaches that provide significant, not just incremental, gains in energy efficiency are required to meet this demand. One such approach is approximate computing.

Historically, approximation has been used only sparingly in computer systems and instead computer systems attempt to guarantee perfect correctness. However, many real world problems are naturally amenable to approximation. For example, when computing occurs on real-world data whose effective precision is limited by noise, computing with precision beyond the intrinsic accuracy of the data is wasted effort. Another class of applications is naturally tolerant of approximate approaches due to the algorithms employed: machine learning, optimization, Monte Carlo simulation, and other probabilistic computations.

It is anticipated that in FY14 language specifications for approximate extensions to C will be designed as well as a prototype LLVM compiler for approximate programs and approximate program evaluation tools.

D. Taming Twitter: Using Social Media Networks to Identify Deviant Behavior
Professor Tyler McCormick, University of Washington, Single Investigator Award

The objective of this research is to identify actors in social media networks who are likely to engage in non-normative or deviant behavior (e.g., drunk driving or use of marijuana) or have a non-normative attribute (e.g., obesity). It is anticipated that in FY14, the investigator will develop a calibrated case-control sampling framework to collect data on social media users and their social network. This design is similar to the case-control study, which is commonly used in epidemiology to learn about rare populations groups, but incorporates uncertainty about the reliability of reported (and unreported) information. Actors will be identified using theoretical paradigms to understand the factors associated with disclosure of deviant or stigmatizing behavior combined with statistical tools for data collected in open, unstructured environments. The investigator will develop a scalable data collection infrastructure data/strategy and identifying phrases and word combinations associated with deviant behaviors. Ground truth is difficult to obtain in social media. Professor McCormick's laboratory will attempt to create a surrogate for ground truth, namely, demographic and anthropometric information provided by Amazon Mechanical Turks. The research will evaluate multiple data collection platforms (e.g., Twitter Streaming and Search APIs) and various ways of asking Amazon Mechanical Turks about the characteristics of individuals presented in profile images. The research will also develop a way to randomly sample from the Twitter stream, a necessary component of case control methodology. This work in designing data collection and analysis mechanisms will set a foundation for further research using data collected in open environments.

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

B. Directorate Scientists

Dr. Randy Zachery
Director, Information Sciences Directorate

Dr. Bruce West
Senior Scientist, Information Sciences Directorate

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 2013* is to provide information on the programs and basic research supported by ARO in FY13, 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 FY13.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of research in the ARO Electronics Division is to gain new fundamental knowledge of phenomena that involve charged particles and their resulting wave phenomena. 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 and plasma mechanisms and concepts. The results of this research 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." Army-relevant research in electronics spans areas such as (i) solid-state and high-frequency electronics to provide components that require less power, operate in extreme conditions, and enhance the creation and processing of information, (ii) studies in electromagnetics, microwaves, and power to enable multimodal sensing for detection, identification, and discrimination of environmental elements critical to decision-makers in complex, dynamic areas, (iii) optoelectronics, which involves the use of electromagnetic (EM) radiation from radio frequency (RF) to X-ray, to interrogate, disrupt, and defeat hostile electronic and threat systems, and (iv) action-reaction relationships in electronic materials and structures that may lead to new devices and methods for sensing and communication over long ranges and variable terrain.

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 coordinates and leverages research 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 its research portfolio 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

The Electronics Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY13, the Division managed research 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 to pursue the program's long-term goal. Nanoelectronic Engineering Sciences' research involves 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 to 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 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 and plasmas, 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 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 seek 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 Photonic Detection 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 Thermal, Mechanical, and Magnetic Effects Thrust includes the modalities of acoustic, magnetic, infrasound, and “passive” environmental signals such as radio or TV broadcasts as well as thermal effects for infrared detection. Research in 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 FY13 were $27.5 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY13 ARO Core (BH57) program funding allotment for this Division was $6.8 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 $3.6 million to projects managed by the Division. The Division also managed $5.0 million of Defense Advanced Research Projects Agency (DARPA) programs, and $5.2 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $3.1 million for contracts. Finally, $3.8 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 creation, leadership, and management of 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 FY13 (*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 FY13 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 FY13, the Division awarded 10 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 microstructure of mercury based materials as a function of growth and annealing treatment, demonstrate enhancement of light emission from inherently low quantum efficiency emitters such as silicon nanocrystals, and demonstrate a new kind of bolometer material based on dispersed metal nanoparticles. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Ki Wook Kim, North Carolina State University; *Topological Insulators for Novel Device Applications*
- Professor Do-Hoon Kwon, University of Massachusetts - Amherst; *Fundamental Limitations of Phased Array Antenna Elements*
- Professor Martin Margala, University of Massachusetts - Lowell; *Ballistic Deflection Transistors for THz Amplification*
- Professor Vinod Menon, Queens College of the City University of New York (CUNY); *Enhanced Light Emitters based on Metamaterials*
- Professor Margaret Murnane, University of Colorado - Boulder; *Photon Energy Limits of Bright High Harmonic X-Ray Generation*
- Professor Roberto Myers, Ohio State University; *Dopantless Diodes For Efficient Mid/deep UV LEDs and Lasers*
- Professor Cun-Zheng Ning, Arizona State University; *Deep Subwavelength Scale Plasmonic Nanolasers under Electrical Injection*
- Professor David Smith, Arizona State University; *Advanced Microscopy and Analytical Studies for Hg-based Infrared Detector Materials and Substrates*
- Professor Zhi Yu, SRI International; *Dispersed Metal Nanoparticles for Low-Noise Bolometer Materials*
- Professor Yong-Hang Zhang, Arizona State University; *Increased Lifetime Beyond Radiative Limit Using Carrier Separation in Direct Bandgap Semiconductors For IR*

2. Short Term Innovative Research (STIR) Program. In FY13, the Division awarded three new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to determine the potential for optimization in order to reduce measurement errors from spurious reflection sources, to discover a novel approach to p-doping (hole doping) of ZnMgO semiconductors based on polarization doping and explore the improved efficiency and power handling capability of a new approach to coherent beam combination of laser diodes. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Ronald Pogorzelski, California State University; *Electromagnetics, Microwaves, and Power: Advanced Antenna Measurement Processing*
- Professor Winston Schoenfeld, University of Central Florida; *Polarization doping p-ZnMgO*
- Professor Lin Zhu, Clemson University; *Improve the Performance of Integrated Diode Laser Beam Combining Through Grating Regrowth*

3. Young Investigator Program (YIP).

No new starts were initiated in FY13.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conference was held in FY13 and was supported by the Division. As with other grants in this category, the support was provided via a competitive grant to academic researchers responsible for organizing or leading the conference.

- *Beyond Graphene: Advanced 2D Electronic and Optoelectronic Crystals and Devices for Next Generation Applications*; University Park, PA; 6-7 March 2013

5. Special Programs. In FY13, 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 Electronics Division; therefore, all of the Division's active MURIs are described in this section.

1. 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 to develop new sensing modalities for chem/bio sensing based on materials development in nanotechnology and nanoscience, and to interface nanoelectronic and nano-optical components to biologically relevant physical properties.

In order to tap the requisite contributions from different academic disciplines (DNA chemistry, electrophysiology, nanoelectronics, optics and THz spectroscopy), three sensing hardware testbeds are being developed for further testing, functionalization, and analysis: (i) bottom up carbon electronics (graphene, nanotubes); (ii) top down silicon nanoelectronics (top down Si nanowires); and (iii) nano-optics (CdSe and other nanowire emitter/detector architectures). Two functionalization schemes are being be applied to these testbeds to enable sensing: DNA origami aligned to nanowire arrays and ion channel functionalization for electrophysiology at the nanoscale. Unique aspects of this sensing research include multiplexing (massively parallel sensor arrays) via DNA self assembly. Using this approach, in principle, each nanowire in an array can have a different sensing functionality, at unprecedented pitch. In addition, direct integration of bio-electrical signals (ion channel currents) to nanoelectrodes (carbon, silicon, and nano-optics) are being explored. A key discovery in the recent year is that the ion channel current pulses can be used to charge the quantum capacitance of graphene, demonstrating a qualitatively new sensing modality for nanoscale electrophysiology. Lastly, single-molecule sensitivity and novel mechanisms for selectivity at THz frequencies are being pursued. Once the three test beds are functionalized, their THz spectra may provide non-trivial information about chemical composition. Advances in this MURI will enable a new class of sensors for applications in biomedical diagnostics for civilian and warfighter health care, chemical agent detection, nano-optical devices for sensing, and neural-electrical interface at unprecedented spatial resolution.

2. 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 of 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.

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

Research 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 FY13, the Division managed 11 new-start SBIR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of four Phase I contracts, two Phase I Chemical Biological Defense SBIR (CBD-SBIR) contracts, four Phase II contracts, and one Phase III contract. These new-start contracts aim to bridge fundamental discoveries with potential applications, including the development of an ultra-sensitive, room-temperature, long-wavelength detector that utilizes the mechanical-optical coupling of a toroid or sphere on a nano-pillar, the development of a plasmonic metamaterial with strong absorption within a narrow band that is dynamically tunable over the 8-10 micron range, and the development of methods that combine UV illumination and Raman spectroscopy into a rapid diagnostic tool for the detection and classification of bacteria in clinical samples.

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 FY13, the Division managed seven new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of four Phase I contracts and three Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications, including the development of high-performance MgZnO based photodetectors that operate in the solar blind region of the spectrum and the development of an economical thermopile array with sensitivity maximum in the long wavelength regime for detection and identification of chemical agents and simulants.

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 FY13, the Division managed one new ARO (Core) HBCU/MI project and seven 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 FY13.

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 FY13, the Division managed five new DURIP projects, totaling $0.8 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of flexoelectric materials, plasmonics, and crystal growth of metamorphic heterostructures.

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

ARO currently manages nine MRI programs for the High Energy Laser Joint Technology Office (HEL-JTO) 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. These three MRIs were reviewed in FY13 and decisions were made to continue their funding for the options (years 4 and 5). 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. The new MRIs are led by professors at Rutgers, University of Illinois, Texas Tech, University of California – Riverside, Clemson, and the University of Central Florida (Center for Research in Electro-Optics and Lasers). These MRIs are on the following topics: single crystal fiber lasers, reduced stimulated Brillouin scattering fiber materials, rare-earth doped GaN, polycrystalline AlN ceramic gain media, leaky wave and gas-filled hollow-core fiber lasers, and nonlinearity mitigation in fiber lasers. 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.

I. 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.

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

The objective of this program 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 in FY13, 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.

K. 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.

L. 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 and Crystal IS 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. ARO co-manages efforts within this program. 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.

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

The AWARE program focuses on technologies to enable wide FOV, higher resolution and multi-band imaging for increased target discrimination and search in all weather day/night conditions. The Electronics Division works with this program by suggesting and monitoring basic research projects with complementary goals. In FY13, the AWARE program provided funding for five new university projects that fit nicely into the Electronic Sensing program area. These included projects in theory of germanium based photodetectors, Ge and Si-Ge avalanche photodiodes (APDs), nanowire APDs, and 4 pi steradian imaging. The 4 pi steradian imaging proposal grew from a result in the Electronics Division's single investigator program. In addition, another ongoing single investigator project on band engineering for APDs received additional funding for continuation from AWARE.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. Type-I Quantum Well Cascade Diode Lasers Emitting Near Three Microns

Professor Gregory Belenky, State University of New York - Stony Brook , Single Investigator Award

The objective of this research is to advance the science of antimony based semiconductor epitaxy and lasers by developing lasers in the 3.0-4.2 μm (or greater) wavelength range. In FY13, the research team designed and fabricated cascade GaSb-based type-I quantum well diode lasers (see FIGURE 1). Cascade pumping was achieved utilizing efficient interband tunneling through "leaky" window in band alignment at GaSb/InAs heterointerface. The carrier recycling between stages was confirmed by twofold increase of the slope efficiency in two-stage devices as compared to reference single-stage lasers. Moderate internal optical loss increase was observed in cascade lasers with interband injector located near the optical mode peak. Cascade pumping scheme increased the continuous wave output power of room temperature operated 3 μm semiconductor lasers up to 590 mW and led to improved power conversion efficiency.

This interband cascading approach is novel and takes advantage of the high gain of type-I quantum wells while re-using the original electrons in more than one recombination event. Although this approach resulted in power outputs twice as high (roughly) as previous records also set by the same group (under ARO funding) with type-I diode lasers, the cascade approach has not been optimized or studied in detail. Thus, further significant improvements in power output are expected.

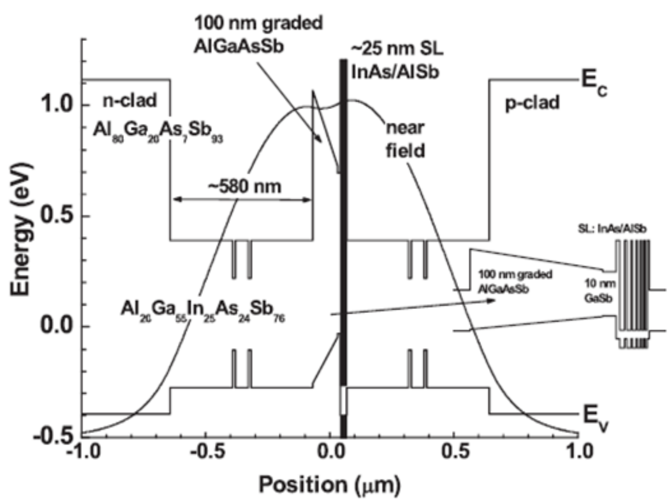


FIGURE 1

Schematic band diagram of the laser heterostructure under flat band condition. The calculated fundamental mode is shown. The inset shows the details of the electron/hole injector design.

B. Nonreciprocal Light Transmission in Parity-time-symmetric Whispering Gallery Mode Microcavities

Professor Lan Yang, Washington University at St. Louis, PECASE Award

The objective of this research is to exploit significantly enhanced light-matter interactions in ultra-high-Q Whispering Gallery Mode (WGM) optical resonators for the development of a new generation of synthetic optical systems for on-chip manipulation and control of light propagation. In FY13, the research team demonstrated (i) lasing in WGM resonators by free space pumping, (ii) nanoparticle detection and sizing, (iii) WGM biosensing, as well as (iv) non-reciprocal light transmission (see FIGURE 2). The key to the nonreciprocal behavior was time-reversal-symmetry breaking. As shown in the figure, they used coupled WGM resonators to implement a classical analogue of a non-Hermitian parity-time (PT-) symmetric Hamiltonian. The team observed a transition to strong nonreciprocity at the PT symmetry-breaking phase due to strong field localization, which significantly enhances nonlinearity. In the linear regime, light transmission is still reciprocal regardless of whether symmetry is broken or unbroken. The team's results provided a direct experimental proof of nonreciprocity in PT-symmetric optics. They anticipate PT-symmetric microcavities to be a starting point for unconventional optical systems utilizing resonance effects. For example, WGM resonators could be used for building CPA-lasers and photonic analogues of topological insulators and for studying exceptional points in lasers. These results represent a significant advance towards a new generation of optical systems enabling on-chip manipulation and control of light propagation.

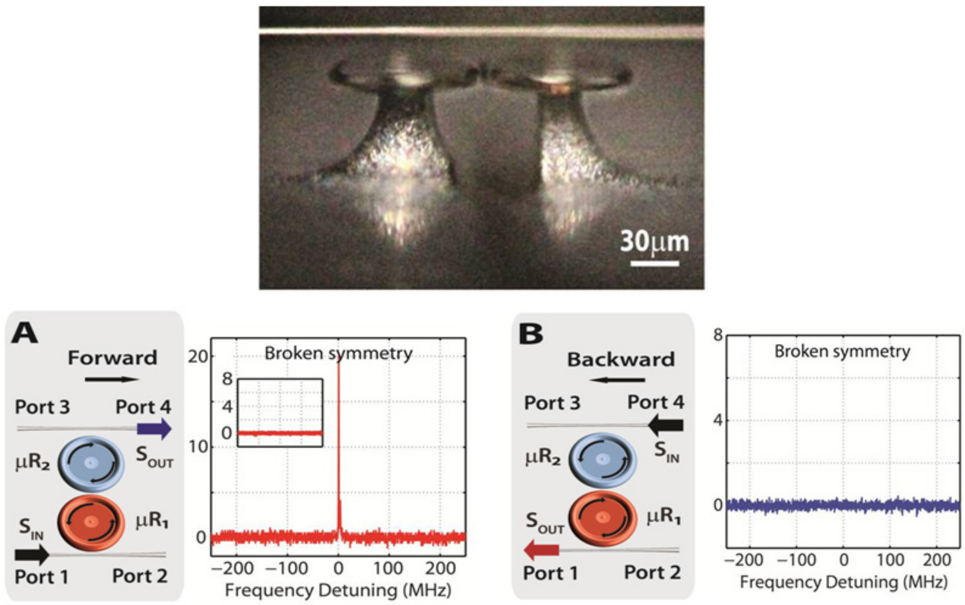


FIGURE 2

Nonreciprocal light transmission. (TOP) Two coupled WGM resonators with single coupling fiber (bright line). Distance between them can be adjusted to increase or decrease coupling. In the experiment, strong pump power which produces broken symmetry is input into Port 1 which couples into uR1. uR1 is designed to create a Raman shift to a signal that couples to uR2. The probe beam at the shifted frequency is coupled into (**A**) port 1 or (**B**) port 4. (**A, RIGHT**): probe beam transmission in forward direction from port 1 to port 4, insert is without probe beam showing pump is not transmitted. (**B, RIGHT**): No probe beam transmission from port 4 to port 1 with same pump power as A.

C. Self-assembled Nanomaterials for Hybrid Electronic and Photonic Systems

Professor Chris Dwyer, Duke University, PECASE

The objective of this research is to discover new ways to build integrated molecular-scale systems which can interface with traditional electronic systems. Building on prior work in DNA nanotechnology, this project is directed toward understanding three enabling phenomena: (i) the self-assembly of precise nanoscale networks of chromophores, (ii) exciton transport in RET devices, and (iii) self-organizing processes for integrating RET and biological components for future computer architectures. Through theoretical and experimental methods this project has begun to expose important properties of RET devices and the computational systems that they could one day enable.

In FY13, the research team successfully demonstrated an optical media system with a storage density of >1000X present-day media (*e.g.*, DVD/BluRay) with a technological scaling path toward a physical limit of ~ 5500X per layer (>100 layers) yielding an areal density of 19.3 petabits/in^2 (see FIGURE 3). The technology leverages components found in commodity optical drive hardware and uses precise molecular-scale assemblies of chromophores to achieve world record densities. Dwyer's group also discovered a new kind of optical switching device through a theoretical study of chromophore networks. The device operation, coined a diffuse exciton valve, has been proven experimentally and is currently being optimized. Exciton valves will enable more sophisticated systems to be built from molecular components since they exhibit high on-off ratios which can help compensate for circuit losses. Along theoretical fronts, Professor Dwyer's group published several design automation tool suites to aid in the design and engineering of RET-based devices and circuits. Without such tools it had never been possible to design complex RET circuits either for study or application.

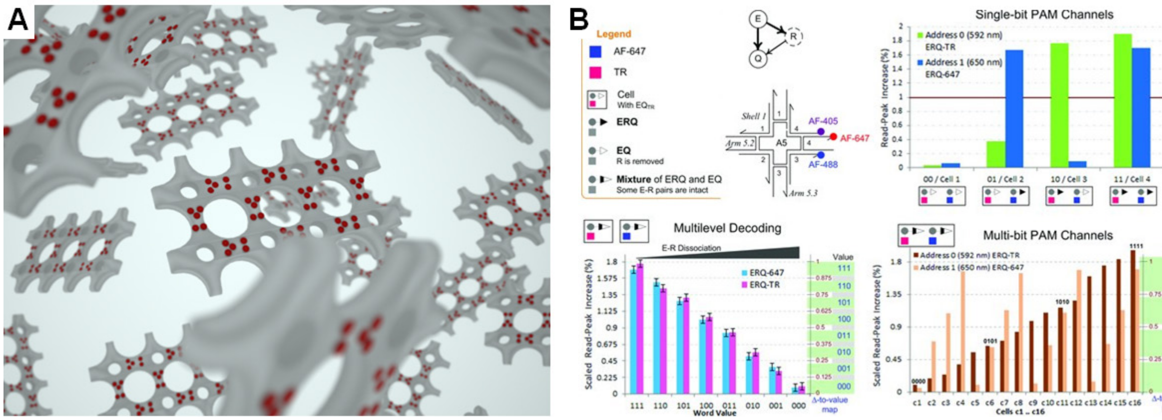


FIGURE 3

Poly-chromatic addressing enables >1000X storage density vs. conventional optical media. (A) Schematic of DNA nanostructures with RET circuits that implement the storage media, and (B) RET circuit structure and demonstration of multi-channel read-out with multi-valued data encoding.

D. Voltage-Activated Bulk Acoustic Wave (BAW) Devices and Filters

Professor Robert York, University of California - Santa Barbara, Single Investigator Award

The goal of this research is to understand voltage-induced piezoelectricity in thin-film strontium titanate (STO) and barium-strontium titanate (BST). This study may ultimately improve piezoelectric resonator technology for RF filter applications. In FY13, the research group achieved record-high Q-factors of 180 in thin film barium strontium titanate (BST) BAW solid mounted resonators at frequencies greater than 10 GHz, providing the opportunity for 5-element electrically switchable filters with 10% tuning range, 4 dB insertion loss, and 100 dB out of band rejection (20-30 dB for a single resonator). The BST was deposited by MBE, followed by a chemical mechanical polishing, which Professor York showed to be critical to the Q-factor improvement by smoothing down the surface roughness (see FIGURE 4). These piezoelectric resonator based electrically tunable filters offer competition to the higher Q but more lossy GaAs technology and the more costly, less reliable MEMS approach.

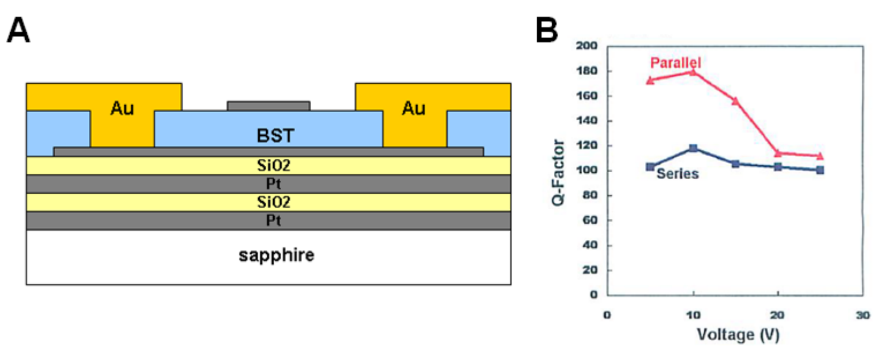


FIGURE 4

Thin film barium strontium titanate BAW resonators. The schematic (a) illustrates the MBE layered structure of the solid mounted BST BAW resonator, while the plot (b) shows the Q-factor for the series and parallel resonances of the polished surface BST BAW resonator as the bias voltage is varied.

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. Quantum Cascade Laser Improvements

Investigator: Dr. C. Patel, Pranalytica Inc., STTR Phase II Contract
Recipients: Northrop Grumman, ORNL, others

The goal of this STTR contract is to advance the frontiers of intersubband AlGaAs (Aluminum Gallium Arsenide) semiconductor lasers. Spectral emission in the mid-wave infrared (MWIR) and long-wave infrared (LWIR), collectively covering a wavelength range from three to twelve microns, are of very high importance for a number of critical military applications. Light with wavelength in either of these spectral regions propagates through atmosphere with very low losses. As a consequence, infrared laser sources are widely employed in situations when free space light propagation over long distances is required. Such applications include infrared beacons for search and rescue missions, target designators for covert operations and infrared countermeasures for protection of aircrafts from MANPADS. In addition, the LWIR spectral region covers spectral features of most chemical warfare agents and explosives, making LWIR lasers the cornerstone in IED sensors.

The large size, low efficiency, and low reliability of available infrared laser sources severely limit their use by the Army. Quantum cascade lasers (QCLs), a novel type of semiconductor lasers, are considered to be the most promising technology to address these pressing needs. QCLs are ultra-compact primary lasers that efficiently convert electrical energy into infrared laser radiation. This STTR program was dedicated to development of a new generation of QCLs with radically improved characteristics. Using its revolutionary laser design approach, Pranalytica has developed first multi-watt QCLs, dramatically improving state-of-the-art QCL performance. Reliability of over three thousand hours has been demonstrated for fully packaged lasers with a characteristic package dimension of less than one cubic inch. In a strategic alliance with Northrop Grumman Laser Systems division, Pranalytica has transitioned double-digit power level QCL systems with very high beam quality, needed for the next generation of infrared countermeasures systems. This collaboration resulted in a ten-watt QCL module with a footprint comparable to that of a smart phone (see FIGURE 5). Pranalytica has also transitioned these results to Oak Ridge National Laboratory (ORNL), and is collaborating to develop QCL-based stand-off sensors for IED detection. Pranalytica is seeking pursuing follow-on work to establish large throughput production capability to address the emerging applications and drive laser cost below $1,000.

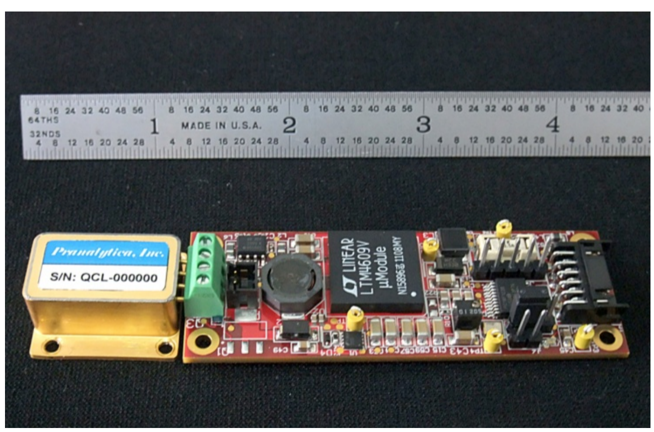


FIGURE 5
Quantum cascade laser module.

B. Strong Electron-Photon Coupling using Plasmonic Light Compressors
Investigator: Professor Hooman Mohseni, Northwestern University, Single Investigator Award
Recipients: DARPA

The objective of this research was to demonstrate the strong coupling of infrared photons and surface plasmona polaritons in metal-dielectic-metal (MDM) structures. Professor Mohseni has developed a hybrid antenna with a high directivity and very low loss to couple far-field optical modes to near-field modes with a dimensional scale approaching the electronic sizes (see FIGURE 6). The hybrid antenna uses a two stage approach and is composed of a dielectric antenna which couples optical power from the far-field to a metallo-dielectric antenna which in turn couples the power to the semiconductor absorbing volume. The dielectric antenna is a lossless dielectric microsphere which focuses the radiation into a "photonic jet" whose width and depth is narrower and deeper than a conventional microlens. This photonic jet lens transitioned to DARPA for continued study in DARPA's Advanced Wide FOV Architectures for Image Reconstruction and Exploitation program, entitled "4π-Steradian Curved and Lensless Imagers (4π-SCALE)." This project will develop a new passive three-dimensional imaging platform that allows the ultimate field of view of 4π Steradian, or a complete sphere, while maintaining extremely thin conformal and flexible geometry. Moreover, the proposed platform will be capable of producing high quality 3D images in short-wavelength infrared (SWIR).

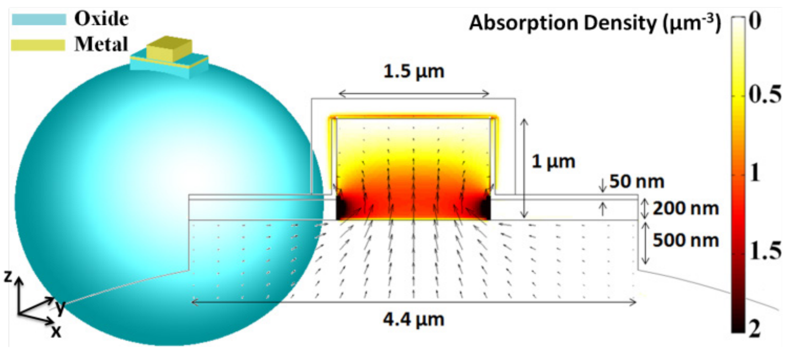


FIGURE 6

Schematic of the hybrid antenna (left) and cross sectional view of the microcavity (center). The cross section view is superimposed by the map of power flow (Poynting vectors scaled with relative strength) and normalized power consumption density throughout the cavity at the operating wavelength of 8 μm.

C. Extrinsic-GaAs Photomixers, Arrays and Spectrometers
Investigator: Professor Elliott Brown, Wright State University, Single Investigator Award
Recipient: TeraPico, LLC

The goal of this research is to demonstrate new types of THz photoconductive sources (PCSs) based on extrinsic photoconductivity rather than the usual intrinsic photoconductivity. In extrinsic photoconductivity, a photon creates a single type of photocarrier (electron or hole) by internal photoionization of energy states lying in the band gap of the host semiconductor (see FIGURE 7A). This is in contrast to intrinsic photoconductivity where a photon creates an electron-hole pair by ionizing valence-band states of the host semiconductor. The band-gap states can be created by impurities, nanoparticles, defect states, and possibly other mechanisms. The preferred approach is ErAs nanoparticles embedded in GaAs based on our discovery in 2012 of a very large and ultrafast photoconductive response in a ErAs:GaAs PCS switch (see FIGURE 7B) when pumped by 1550-nm laser radiation. Another reason is that GaAs has much higher resistivity and electrical breakdown than InGaAs and other possible THz PCS materials that operate at 1550 nm. A typical THz output from the 1550-nm driven, ErAs:GaAs photoconductive switch is displayed in FIGURE 7C, for which the average THz power was ≈100 μW. This marks an important development for the THz field because it enables the fabrication of PCS arrays with 1550-nm distributed, fiber-optic drive and control networks, a concept that has been discussed for a long time but never realized because of the lack of a suitable PCS device. This research team is pursuing basic research to better understand this exciting new device technology, but also developing the first PCS arrays to produce output power levels ~10x greater than available from single THz PCS devices today

In FY13, these results transitioned to the start-up company TeraPico, LLC, which was launched in concert with Wright State University and the Ohio Research Scholars Program. The new extrinsic-photoconductive THz sources is highly relevant as there is worldwide demand for useful 1550-nm-driven PCS devices.

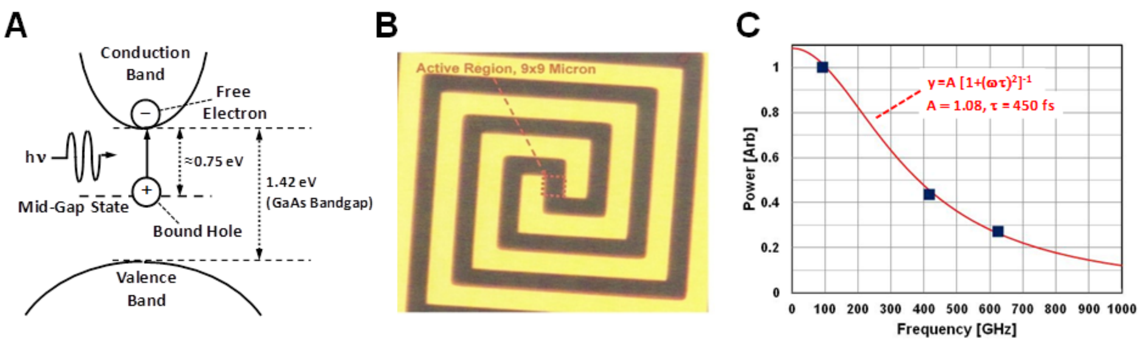


FIGURE 7

New types of THz PCS based on extrinsic photoconductivity. (**A**) Energy diagram for n-type extrinsic photoconductivity in ErAs:GaAs associated with a very dense mid-gap state created by the embedded nanoparticles. (**B**) Top-side view of new PCS switch showing square-spiral antenna and device active region at center. (**C**) Spot-frequency power spectrum of new 1550-nm-driven PCS switch.

E. Field/Circuit Computational Modeling and Simulation Software Tools

Investigators: Drs. C. Penney, S. Fast, G. Moss, Remcom, Inc, and Professor M. Steer, NC State University, STTR Phase II Contract
Recipients: CERDEC, ARL-SEDD, Remcom, Inc., others

Remcom, Inc. and NCSU have developed and are marketing a unique US commercial simulation code capability to model active and passive RF circuits directly within a transient electromagnetic environment. This research will allow configurations of large electromagnetic elements, such as antenna arrays, to be modeled simultaneously with RF circuits containing passive elements such as filters and active elements such as oscillators or amplifiers within an overall FDTD simulation or co-simulated with the FDTD computation (see FIGURE 8). The current released version of the code will handle passive RF elements within the electromagnetic environment, for example large portions of a cell phone circuit together with antenna and radiating elements. A version which will include a co-simulation of active circuits with an FDTD electromagnetic simulation has been validated. This capability rests on extensive previous research at NCSU supported by ARO single investigator and MURI programs. The code has a unique capacity for custom adaptation to DoD analysis and design problems. A massively parallel version of the code has been developed. These findings have transitioned to ARL-SEDD and CERDEC, as the simulation is particularly capable of simulating electromagnetic structures with embedded or integral active electronic circuitry of interest to ARL-SEDD and co-site interference problems of interest to CERDEC.

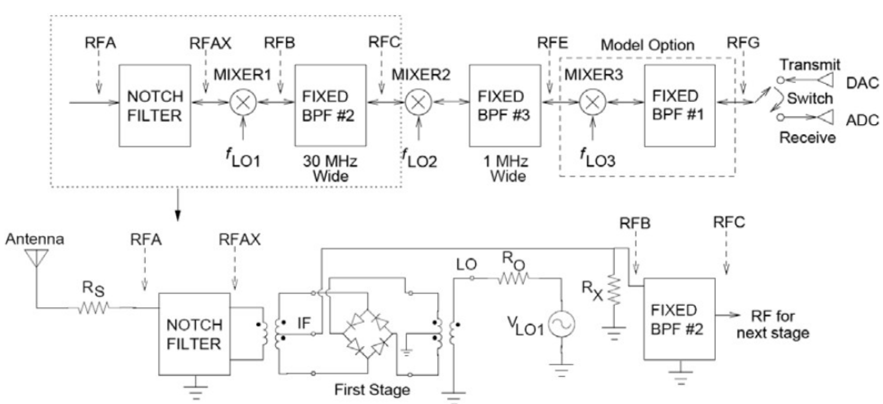


FIGURE 8

Singars-like radio circuit. The schematic illustrates a Singars-like radio circuit and antenna.

V. ANTICIPATED ACCOMPLISHMENTS

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

A. Optical Magnetism

Professor Kevin Webb, Purdue University, STIR Award

Every material has electric and magnetic properties that affect how a material responds to electromagnetic (EM) waves. The electric properties of a naturally-occurring material respond very rapidly to an EM wave and are key to the design and operation of modern-day electronic and optical devices. In contrast, the magnetic properties of a natural material remain relatively static and only respond to EM waves at low frequencies. However, scientists recognized that if these magnetic properties could be harnessed in the optical regime, it could theoretically allow for the control of visible light in new ways. This concept, called transformation optics, has been demonstrated in specific instances but it is still uncertain whether broad-band and multidirectional properties can be realized.

The objective of this research is to show that homogeneous magnetism is possible at optical frequencies. It is anticipated that in FY14, Professor Webb's research team will perform theoretical and numerical studies of metamaterials with coil-like unit cell elements (see FIGURE 9). The focus will be on carbon and related structures that can be chemically synthesized without recourse to lithography. The lattice boundary conditions will be designed to suppress chirality, by mixing an equal amount of left-handed and right-handed coils, and the resulting tensor dielectric constant and permeability will be determined. Numerical results will be viewed both in terms of spatial dispersion (due to the material's structure) and equivalent circuit concepts. These numerical results should point the way towards experimental follow-on work. Development of homogenized magnetic material properties at optical frequencies would present new domains for energy collection, filters, spectroscopy, sub-wavelength imaging, and camouflage, as well as homogeneous cloaking. In addition, spin-offs from this research will enable electronic and photonic equipment of the warfighter to be lighter and more rugged.

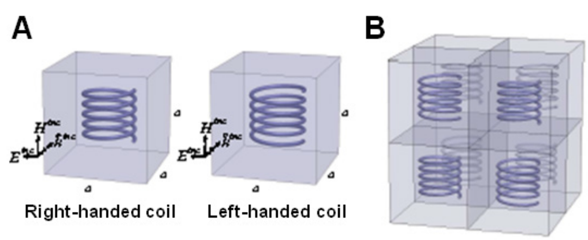


FIGURE 9

Metamaterial modeling structure. (A) Left-handed and right-handed carbon coils that are placed in a x a x a cells. The coil diameter and length is 0.5a, and the wire diameter is 0.02a. (B) Non-chiral unit-cell of periodic metamaterial that comprises four left-handed coils and four right-handed coils.

B. Terahertz Devices Based on Photo-excited Low-dimensional Electron System

Professor Ramesh Mani, Georgia State University, Single Investigator Award

The objective of this project is to broadly study the electrical properties of low dimensional electronic systems, with an emphasis on comparing the equilibrium properties, with the steady state non-equilibrium properties that is realized by photo-exciting the electronic system using electromagnetic waves in the microwave and THz parts of the radiation spectrum.

It is anticipated that in FY14, Professor Mani's team will characterize the dark- and photo-excited magneto-transport response of graphene grown by chemical vapor deposition (CVD) and compare with the results obtained in epitaxial graphene. In epitaxial graphene, Professor Mani's team reported an unexpectedly strong microwave-induced electrical response and dual microwave-induced resonances in the dc resistance. The observed resonances corresponded to the resistive detection of spin resonance. In CVD graphene, the measurements in the dark thus far show a logarithmic change in the resistance vs. temperature, as expected for weak localization. Microwave photo-excitation reveals a heating response, which is being followed as a function of power and microwave frequency. Professor Mani's team is attempting to quantitatively determine the carrier temperature as a function of the experimental variables. This research may help to provide further understanding of the electronic and spin properties of the carriers in CVD- and epitaxial- graphene.

C. Photon Energy Limits of Bright High Harmonic X-ray Generation

Professor Margaret Murnane, University of Colorado, Boulder, Single Investigator Award

Previous work by Professor Murnane and her group have demonstrated extreme high harmonic generation (HHG) of bright UV and soft X-ray radiation in the plasma created by femtosecond, ultra-high power laser pulses propagating through atomic gases at several atmospheres of pressure. In this extreme regime over 5000 photons from the source laser are converted to a single UV or X-ray photon. She has demonstrated that the energy (frequency) of the emitted radiation increases with increasing wavelength of the femtosecond laser source, with mid-IR laser sources producing X-ray radiation at 1 keV energies. This relation is due to the phase matching requirement for the source laser field, the motion of the electrons in the atomic gas, and the resulting X-ray radiation (see FIGURE 10). The phase matching condition becomes more favorable at longer source laser wavelengths, but the quantum mechanical dissipation of the electronic wave functions also become greater. In FY14, Professor Murnane will explore the unknown phenomena of generation using longer wavelength sources lasers (in the 8-12 micron wavelength range) and other approaches to achieving the phase matching condition, such as "quasi-phase matching." Ultimately this research has the promise of leading to table top plasma sources of attosecond X-ray radiation with potential applications in biological research, medical imaging and treatments, and directed energy military uses. It is anticipated that the research team will discover the long wavelength limitations to this process and the potential for quasi-phase matching approaches.

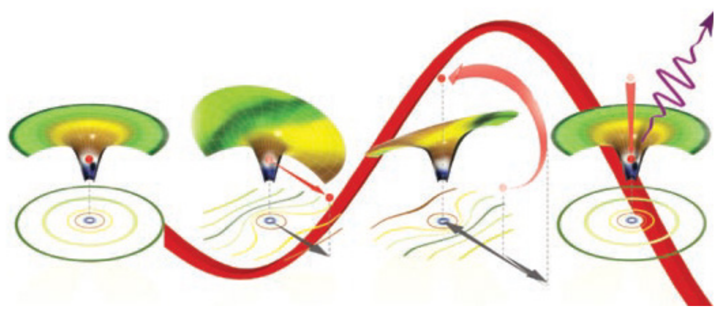


FIGURE 10

Classical picture of extreme HHG. In extreme HHG, the source laser field bends the atomic coulomb potential, allowing tightly bound electronics to tunnel out, where the source laser field accelerates them first in the outward direction, then back to the atomic ion, where they are re-captured, emitting UV or X-ray radiation.

D. New Plasmonic Materials: Highly-doped InAs

Professor Seth Bank, University of Texas - Austin, STIR Award

The objective of this research is to achieve high electron carrier concentrations in InAs semiconductors via enhanced doping. It is anticipated that in FY14, the research team will demonstrate doping levels in excess of $3x10^{20}$ donor atoms /cm^3 and possibly even as high as $7x10^{20}$ cm^{-3} needed for plasmonic applications. Incorporation of higher doping concentrations in InAs (currently $9x10^{19}$ cm^{-3}) will enable surface plasmon propagation along the surface with longer propagation lengths. Plasma frequency is inversely proportional to electron effective mass and since InAs has the smallest (lightest) electron effective mass known in standard semiconductors, it is being pursued to achieve plasma frequencies high enough for incorporation of InAs plasmonic materials along with useful laser diodes. Mid-infrared diode lasers can be incorporated with the highly doped semiconductors to enhance the properties of the optoelctronic devices or create plasmonic waveguides of small dimensions relative to the photonic wavelengths. Ultimately, semiconductor plasmonics could lead to extremely high bandwidth and small dimensioned photonic systems and devices.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

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Division Chief
Program Manager, Electronic Sensing

Dr. Michael Gerhold
Program Manager, Optoelectronics

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Program Manager, Electromagnetics, Microwaves, and Power

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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 2013* is to provide information on the programs and basic research supported by ARO in FY13, 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 FY13.

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 and the terrestrial domain of the natural environment. 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 managed by the Environmental Sciences Division provides 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 the environmental sciences 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 DoD agencies, including the Navy, Marine Corps, Air Force, the Defense Advanced Research Projects Agency (DARPA), the Environmental Security Technology Certification Program (ESTCP), the Environmental Protection Agency (EPA), the National Aeronautics and Space Administration (NASA), the National Oceanic and Atmospheric Administration (NOAA), the National Science Foundation (NSF), and the Department of Agriculture - Agricultural Research Service.

B. Program Areas

The Environmental Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified two sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY13, the Division managed research within these two Program Areas: (i) Atmospheric Science and (ii)

Terrestrial Sciences. 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.

C. Research Investment

The total funds managed by the ARO Environmental Sciences Division for FY13 were $4.0 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY13 ARO Core (BH57) program funding allotment for this Division was $2.4 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 $0.8 million to projects managed by the Division. The Division also managed $0.4 million provided by other DoD agencies. Finally, $0.4 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 creation, leadership, and management of 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 FY13 (*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.

The following subsections summarize projects awarded in FY13 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 FY13, the Division awarded four 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 surface fluxes in the atmospheric boundary layer over complex topography, determine controls of grain-grain interactions on sediment transport, and characterize single aerosol particles using optical trapping-cavity ringdown spectroscopy (OT-CRDS) in combination with conventional aerosol characterization methods/techniques to obtain new experimental data. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor William Anderson, Baylor University; *Numerical Simulation of Atmospheric Boundary Layer Flow: Surface Fluxes From Resolved and Subgrid Scales*
- Professor Douglas Jerolmack, University of Pennsylvania; *Granularity and Jamming: A New Approach to Understanding and Predicting Near-Threshold Sediment Transport*
- Professor Simon Mudd, University of Edinburgh; *Constraining the Topographic Signature of Erosion Rates and Processes Using High Resolution Topography*
- Professor Chuji Wang, Mississippi State University; *Physical And Chemical Study of Single Aerosol Particles Using Optical Trapping-Cavity Ringdown Spectroscopy*

2. Short Term Innovative Research (STIR) Program.

No new starts were initiated in FY13.

3. Young Investigator Program (YIP).

No new starts were initiated in FY13.

4. Conferences, Workshops, and Symposia Support Program. The following symposium was held in FY13 and was supported by the Division. As with other grants in this category, the support was provided via a competitive grant to academic researchers responsible for organizing or leading the symposium.

- *Bioaerosols: Characterization and Environmental Impact Symposium*; Portland, OR;
  30 September - 4 October 2013

5. Special Programs. In FY13, 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 one new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grant to support summer research efforts by promising high school or undergraduate students, to be completed at an academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

No projects were active in FY13.

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

No new starts were initiated in FY13.

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

No new starts were initiated in FY13.

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

No new starts were initiated in FY13.

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

No new starts were initiated in FY13.

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 FY13, the Division managed five new DURIP projects, totaling $0.8 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of Earth surface processes and aerosol characterization.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. Measurement of Raman Spectra from Single Airborne Aerosol Particles

Professor Yong-qing Li, East Carolina University, Single Investigator Award

The objective of this research is to demonstrate that Raman spectroscopy can be performed on single aerosolized particles in a flow. Raman spectroscopy is a noninvasive technique that can be used to analyze molecular composition. As such, it has been recognized and pursued as a means of characterizing atmospheric aerosols. Unfortunately, Raman signals are relatively weak, and it takes significant integrations, either over time or over particle numbers, to obtain a useful signal. Such a measurement of single aerosol particles in a point-sensing system is challenging. In FY13, the research team successfully demonstrated a new method using a single Gaussian laser beam to trap, manipulate the position, and acquire the Raman spectra from a single aerosol particle in a flow (see Figure 1).

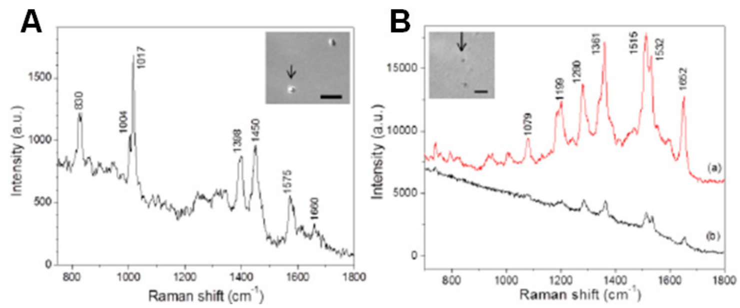

FIGURE 1

Raman spectra of optically trapped aerosol particles. (**A**) Spectrum of single trapped B. cereus spore. The insert shows images of the trapped spore with a scale bar of 5 µm; (**B**) Raman spectrum of a cluster of 80-nm gold particles.

B. Determining Planetary Boundary Layer Height Using Three-wavelength Lidar

Professor Patrick McCormick, Hampton University, PIRT Award

The objective of this research is to demonstrate novel capabilities of characterizing the atmosphere using lidar systems. Within this research, a new technique to obtain the height of the planetary boundary layer (PBL) has been developed. Lidar backscatter resulting from scattering in the atmosphere contains information about the optical and physical properties of aerosols and molecules. The lidar backscatter signal can provide information about the PBL stratification by using aerosol as a tracer for convective and mixing processes. A PBL height and structure detecting technique based on the fractal dimension (FD) of three-wavelength backscatter signals was explored. The FD was calculated using all three wavelengths of the lidar. The PBL heights obtained from the FD is compared with PBL heights obtained from the potential temperature profiles, which are provided by the NASA Langley Research Center (approximately 10 miles from the lidar located at Hampton University). Results of the two methods agree well. Moreover, the new method has several advantages. The FD method can reduce the influence of the geometrical form factor on the PBL. In addition, the FD method can provide information on the PBL dynamics and its evolution more clearly. The FD signal is compared with potential temperature and the range-corrected lidar signal at 1064 nm. As shown in FIGURE 2, the PBL heights obtained from the range-corrected lidar using Wavelet-covariance-transform (WCT) method and the FD-WCT method agreed with the PBL height retrieved from the potential temperature profile using a gradient method (PT-GM). The PBL heights are 2.5 km retrieved using RCS-WCT, 2.52 km retrieved using FD-WCT, and 2.6 km retrieved using PT-GM for this case. In FY13, the research team successfully demonstrated that the PBL height can be retrieved accurately using 3-wavelength lidar.

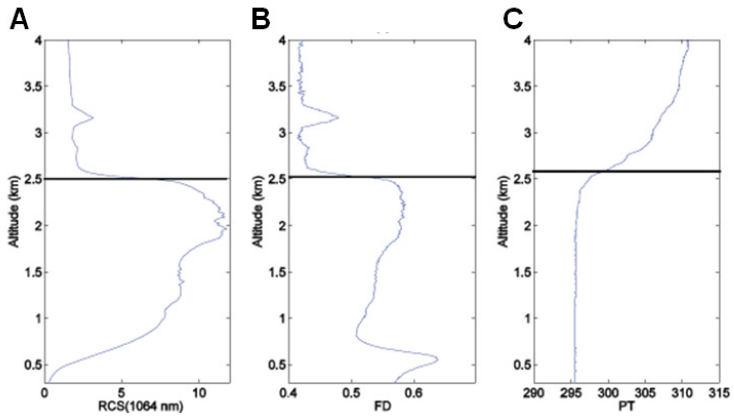

FIGURE 2

The planetary boundary layer height determined using three different methods: (**A**) RCS-WCT (at 1064nm), (**B**) FD-WCT, (**C**) PT-GM method on 05:08, 02 July2010 (ETS)

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-Resolution Atmospheric Studies Using DataHawk

Investigator: Professor Ben Balsley, University of Colorado, Single Investigator Award
Recipients: ARL-CISD; Dugway Proving Ground (DPG)

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 one second (temporally) and one meter (spatially) throughout the first few km of the atmosphere (see FIGURE 3). The DataHawk provided high-resolution data in support of the Materhorn field campaign that occurred at DPG in the fall of 2012. The goal of Materhorn is to increase weather-modeling capabilities in regions of complex terrain, such as in the vicinity of Granite Mountain at DPG. The DataHawk is a new technology that provided unique information of the fine-scale atmospheric dynamics during this project. The DataHawk identified several unique overturning features, whose origin is not known. These features have been identified and verified on data acquired using lidar instruments. Such data previously had been ignored as a blip, but the DataHawk's high-resolution capabilities using multiple instruments demonstrate that such blips are significant atmospheric structures. These results transitioned to ARL-CISD and DPG in FY13 and are being incorporated into efforts to increase modeling capabilities at those sites.

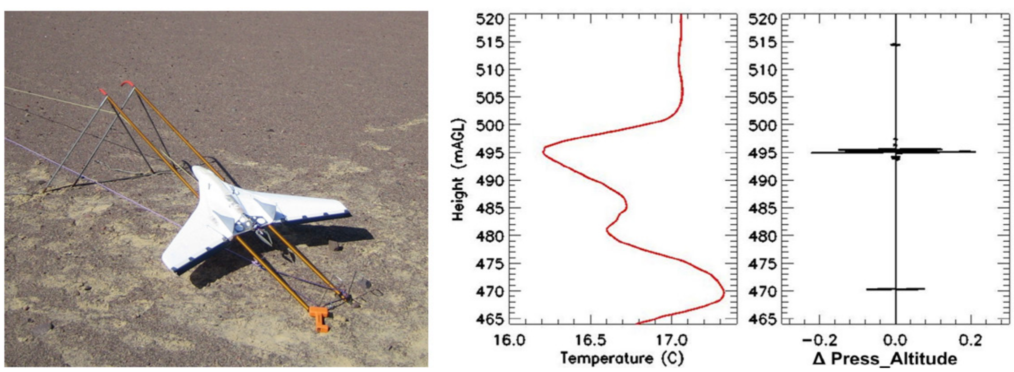

FIGURE 3

Micro-autonomous vehicle DataHawk. The DataHawk (left) is capable of providing real-time *in situ* measurements of the atmosphere. The DataHawk can be launched on the ground or by balloon for high-altitude measurements. An example of an overturn (right) was documented downwind of Granite Mountain.

B. Airborne Doppler Lidar measurements and verification of ADLAATS during Materhorn

Investigator: Dr. G. David Emmitt, Simpson Weather Associates, SBIR Phase II
Recipients: ARL-CIS; DPG

The objective of this SBIR contract was to measure and characterize the time and space variability of wind and wind hazards in the atmospheric boundary layers of complex terrain in real time. Using this information, the investigators developed an Airborne Doppler Lidar Analyses and Adaptive Targeting System (ADLAATS) that conducts continuous on-board measurement and processing of airborne Doppler wind lidar (DWL) data and transmits the data for further analysis. This system can be used to obtain directly measured wind profiles and aerosol plume concentrations to provide better information to the warfighter related to wind profiles in the action theater. ADLAATS also brings a numerical weather model and an airborne DWL together on the same platform. The DWL observations provide real-time high resolution measurements of Line of Sight (LOS) wind velocities, in addition to aerosol concentrations, that can be used by mission managers and flight planners independently or in concert with a numerical model, running on a laptop computer.

This system transitioned to ARL-CIS and DPG and was tested during ferry flights that took place between Monterey and DPG (see FIGURE 4). At DPG, airborne Doppler Lidar measurements were made in coordination with ground-based instruments, including additional Doppler Lidar systems operated byARL-CISD researchers. The data retrieved during these field experiments are being analyzed by researchers at DPG and ARL-CISD to increase weather-modeling capabilities in regions of complex terrain.

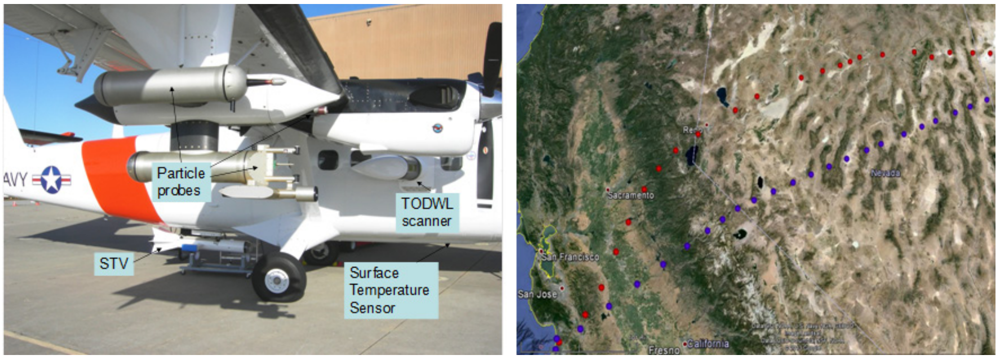

FIGURE 4

Airborn Doppler lidar measurements. Navy Twin Otter aircraft and Twin Otter Doppler Lidar system (left) are flown to DPG to take part in Materhorn. Data collection was made en route (right) to test the ADLAATS system.

C. Acoustic Tomography of the Atmospheric Surface Layer

Investigator: Professor Vladimir Ostashev, University of Colorado, Single Investigator Award
Recipients: ARL-CISD; CRREL

The primary goal of this research has been to perform detailed studies of the temperature and wind velocity fields in the atmospheric surface layer (ASL). The Boulder Atmospheric Observatory (BAO) acoustic tomography array allows robust and accurate reconstruction of temperature and wind velocity fields in acoustic tomography of the ASL. The specific objectives of the project are to process and analyze the data recorded during joint experiments; 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. This research has transitioned to NOAA/ESRL, CRREL, and ARL-CISD, which are closely collaborating to continue exploring potential applications of these data.

The acoustic array enables measurement of the travel times of sound signal propagation between different speakers and microphones, which constitute the tomography array. The results of temperature and wind velocity field reconstructions in the acoustic tomography experiment are shown in FIGURE 5. The BAO 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. In such experiments, the array provides information about both atmospheric turbulence and fluctuations in acoustic signals propagating through the turbulence. The data are now being used to test acoustic models being developed at CRREL and ARL-CISD.

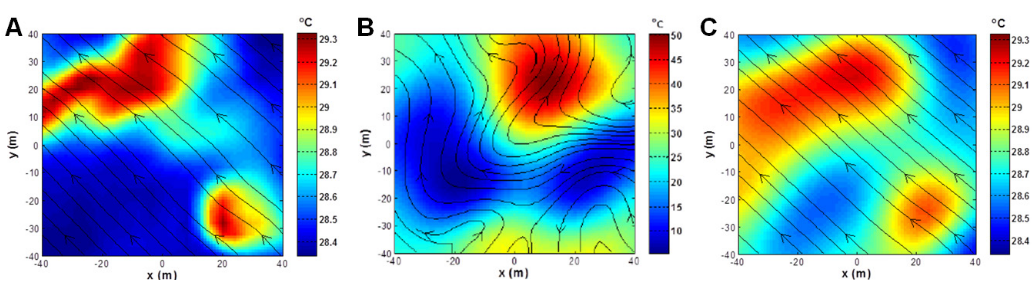

FIGURE 5

Reconstruction of the temperature field in numerical simulations. (**A**) LES temperature field. (**B**) Tomographic reconstruction without estimation of the systematic errors. (**C**) Tomographic reconstruction with an algorithm incorporating an assessment of the systematic errors.

V. ANTICIPATED ACCOMPLISHMENTS

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

A. A New Approach to Understanding and Predicting Near-threshold Sediment Transport

Professor Douglas Jerolmack, University of Pennsylvania, Single Investigator Award

The goal of this research is to determine the controls on grain-grain interactions on sediment transport, focusing on flow regimes close to the threshold of motion. This work will develop and test emerging ideas in soft-matter physics to extend their generality to fluid-driven granular movement using laboratory experiments that tomographically image an evolving sediment bed in turbulent and viscous flows along with field experiments in which the movement of pebbles in a natural stream are tracked. These complementary approaches will be employed to explore sediment transport in the context of jamming and may allow for a precise and mechanistic definition of the threshold of motion, which current does not exist, and the development of sediment transport models with higher accuracy than those that are currently available.

It is anticipated that in FY14, a new laboratory channel will be fabricated and preparations to perform experiments in which turbulent fluctuations in the fluid stress that act to obscure grain dynamics are suppressed will be completed. Preparations to perform a parallel set of experiment that explore the transition to inertia-dominated transport using a square acrylic tube filled with water and sediment to approximate a river channel will also be completed. Additionally, a two-week field campaign to measure particle and fluid motion during several floods in the Luquillo Critical Zone Observatory, Puerto Rico, will have been completed.

B. Probing the Effects of Topography on Bedrock Fracture in the Shallow Subsurface

Professor J. Taylor Perron, Massachusetts Institute of Technology, Single Investigator Award

The objective of this research is to test the hypothesis that topographic stresses significantly influence rock fracture patterns in the shallow subsurface, as the mechanical properties of rock are known to influence the erodibility of bedrock and the development of landforms, but the possibility that landforms in turn influence rock properties has not been thoroughly investigated. One way landform topography may influence bedrock is by perturbing the ambient stress field, and theoretical studies have concluded that net topographic stresses may be sufficiently large to fracture rock. This research will test these predictions through three tasks: (i) comparing modeled topographic stresses beneath real landscapes with rock fracture patterns observed in the field through the development of a numerical modeling approach for calculating the three-dimensional elastic stresses beneath an arbitrary topographic surface in the presence of an ambient tectonic stress field; (ii) a modeling study to investigate how topographic characteristics and ambient stresses influence the three-dimensional pattern of stress and fractures within a generic drainage basin, and (iii) surveys of fractures and rock damage in the shallow subsurface at three field sites (the Susquehanna-Shale Hills Observatory in Pennsylvania, the Southern Sierra Observatory in California, and the Boulder Creek Observatory in Colorado) with different geologic characteristics and tectonic contexts, which will be compared with the stress model predictions. It is anticipated that in FY14 the three-dimensional stress modeling procedure will be implemented and benchmarked, numerical experiments to investigate stress effects of drainage basin topography will have been performed, and field data will have been collected from a the Pennsylvania field site, including the logging of fractures from existing wells along with ground penetrating radar and seismic hammer surveys.

C. Real-time Aerosol Sampler Based on Negative Polarization of Backscattering

Professor Hui Cao, Yale University, Single Investigator Award

The objective of this research is to demonstrate experimentally that different aerosol classes of particles have a different polarization response in their backscatter. The strong elastic light scattering properties of airborne particles provide a natural means for rapid, noninvasive aerosol characterization. Recent theoretical predictions suggested that variations in the angle dependent scattering intensity of different polarization components could provide an efficient means of classifying different airborne particles. In order to experimentally validate this prediction, a high-throughput sampling system, capable of measuring the angle- and polarization-resolved scattering cross section of bio-aerosol particles and aggregates has been constructed. The system records the angle-resolved scattering light of both polarizations from individual particles or aggregates flowing through an aerosol jet stream excited by a single laser shot. The system has been calibrated by comparing the polarization-dependent scattering cross section of individual polystyrene spheres with the scattering cross sections predicted by Mie theory. The system currently is being used to study five different types of particle aggregates: Polystyrene aggregates composed of 1 µm and 500 nm spheres, BG (*Bacillus subtilis*) aggregates, Arizona road dust aggregates, and tryptophan molecules (~5 µm). The polarization aspect ratios as a function of scattering angle for all five particle types have been extracted for comparison (see FIGURE 6). It is anticipated that in FY14, the research team will demonstrate that the underlying nature of a cloud of aerosolized particles can be acquired from their backscattering polarization state.

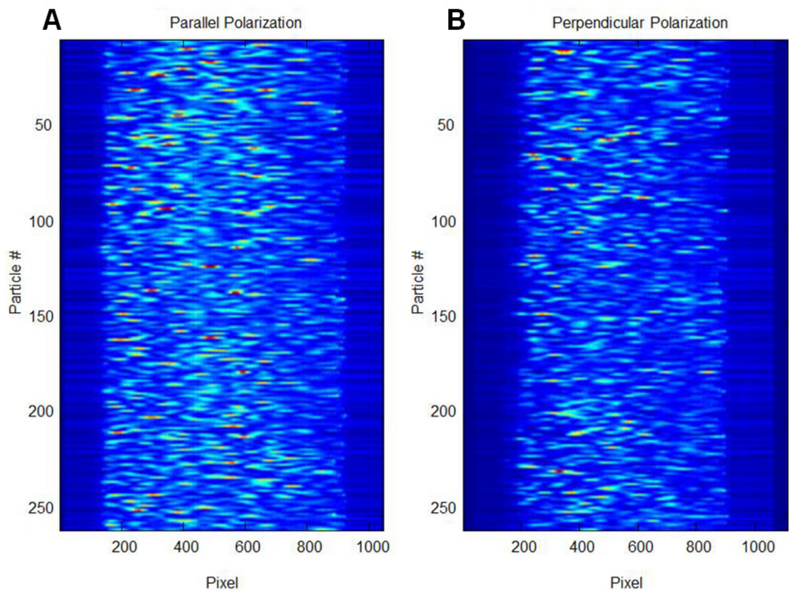

FIGURE 6

Scattering cross sections of aerosol clusters of polystyrene spheres. Light polarized (**A**) perpendicular and (**B**) parallel to the plane of incidence is detected separately. Each aggregate exhibits a different response depending on its orientation and packing configuration.

D. Real-time Holography of Aerosol Particles

Professor Matthew Berg, Mississippi State University, Single Investigator Award

The objective of this research is to demonstrate a new ability to use holography not only to image aerosol particles but to acquire information about their composition. 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 is under development. Particles flowing through the apparatus in a sample stream are illuminated by a pulsed UV laser. This illuminating light combines with light scattered by a particle across the face of a charged coupled device camera. The recorded pattern constitutes a digital hologram, from which an image of the particle can be reconstructed computationally. To gain composition information, the particle is illuminated by the UV laser twice in rapid succession while also being exposed continuously to light from an IR laser, forming two holograms on the camera. Performing the computational reconstruction operation on this double-exposed digital hologram yields an image of the particle superimposed by interference fringes. These fringes originate from any change in the physical form of the particle occurring between the two UV pulses. Absorption of the IR light by the particle should cause thermal expansion, which would thus register as fringes in the reconstructed image. Since the degree of expansion varies with composition, the fringes should contain information related to the particle material. It is anticipated that in FY14, the research team will demonstrate that double-exposed holography will be able to be used to retrieve additional particle information.

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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 2013* is to provide information on the programs and basic research supported by ARO in FY13, 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 FY13.

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 this research 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, for advances in synthetic biology for energy production, intelligence, and bioengineering, and for new capabilities for predicting group behavior and change.

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 research 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 its research portfolio 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

The Life Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY13, the Division managed research within these five Program Areas: (i) Genetics, (ii) Neurophysiology and Cognitive Neuroscience, (iii) Biochemistry, (iv) Microbiology, and (v) Social and Behavioral 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.

This Program Area 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. Neurophysiology and Cognitive Neuroscience. 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) Multisensory Synthesis, and (ii) Neuronal Computation. 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 Multisensory Synthesis Thrust aims to understand how the human brain functions in relation to the interaction of sensory, cognitive and motor processes during its performance of real-world tasks. Basic research focused on mapping, quantifying and modeling distributed neural processes that mediate these features are being used to develop better understanding of cognition for eventual application to Soldier performance enhancement. Research in the Neuronal Computation Thrust is focused on understanding how living neuronal circuits generate desirable computations, affect how information is represented, show robustness to damage, incorporate learning and facilitate evolutionary change. Cell culture, brain slice and in vivo models are being used to develop better understanding of living neural networks 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, identifying individual cognitive differences and new training paradigms for improved Soldier performance.

3. Biochemistry. The goal of this Program Area is to elucidate the mechanisms and forces underlying the function and structure of biological molecules. This research 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 Regulation, 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 and Regulation Thrust aim to identify the determinants of the specificity of molecular recognition and molecular activation/inactivation to modulate and control specificity and activity 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 the physiology, genetics, ecology, intercellular interactions, and adaptation of microbes, including viruses, prokaryotes, and single-celled eukaryotes. Microbes are distributed throughout nature and are essential for life; however, they can cause infections, spoil food, and degrade natural or artificial materials. Microbes also serve as a model system for exploring a variety of fundamental questions in biology that are too complex or costly to study effectively in more complex organisms.

This Program Area is divided into two research Thrusts: (i) Intercellular Dynamics and (ii) Microbial and Viral Adaptation. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goals. Efforts in the Intercellular Dynamics Thrust aim to discover and map the genetic, proteomic, and metabolic mechanisms involved bacterial and fungal intercellular communication. Research in this Thrust focuses on community aspects of bacteria and fungi and includes studies in areas such as quorum sensing, host-pathogen/symbiont interactions, programmed cell death, and interactions in mixed populations. The Microbial and Viral Adaptation Thrust focuses on understanding how bacteria, fungi, and viruses adapt at the individual level, including studies at the molecular level (*e.g.*, genetic and proteomic) and macroscale (*e.g.*, cell morphology). This Thrust includes studies of viral infection and replication mechanisms (*e.g.*, changes in production of virus-like particles), microbial stress resistance (*e.g.*, biodegradation, toxin sequestration and removal, microRNA production, growth in extreme environments).

While these research efforts focus on high-risk concepts, research supported by this program promotes a range of long-term applications for the Army, including strategies for detecting and classifying microbes, for controlling bacterial, viral, or fungal infections, for harnessing microbes to produce novel materials, to protect materiel, and/or to efficiently produce desirable commodities. In addition, understanding how microbes adapt is crucial for advancing studies in other fields, including genetics, environmental science, materials science, and medicine.

5. Social and Behavioral Science. The goal of this Program Area is to gain a better theoretical understanding of human behavior at all levels, from individuals to whole societies, for all temporal and spatial scales, through the development of mathematical, computational, simulation and other models that provide fundamental insights into factors contributing to human socio-cultural dynamics and societal outcomes (see FIGURE 1).

This Program Area is divided into two research Thrusts: (i) Predicting Human Behavior, and (ii) Complex Human Social Systems. The program supports research that focuses on the 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, movements for social justice), 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 systems, 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, comparative-historical analyses, 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. A component of supported research includes the collection of primary data for model development and testing. The program also supports research to develop methodologies (*e.g.*, measurement, data collection, statistical methods, and research designs) that may provide an improved scientific understanding of human behavior.

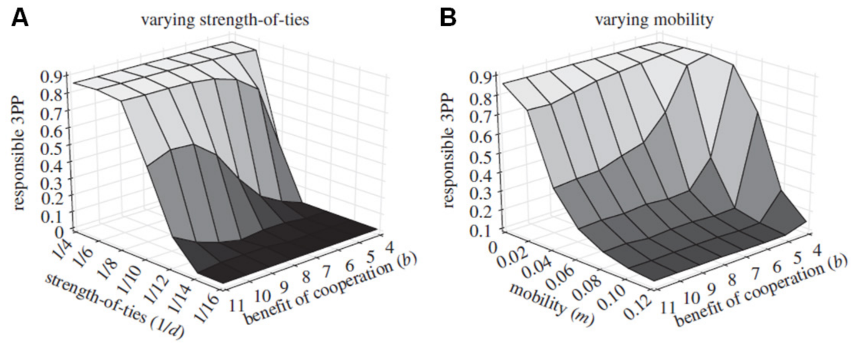

FIGURE 1

Results of research on third-party punishers (3PP) of injustice. These data demonstrate the key role of social dynamics in generating justice. The stronger the social ties within a community and the lower the socioeconomic mobility among community members, then the more likely the members are to punish social injustice, even if they did not directly experience the injustice. They also show the key role that support of others plays in punishing injustice (*i.e.*, benefit of cooperation). When social ties are weak and mobility is low, incentivizing others to cooperate in punishing injustice becomes more important.[1]

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 and allied intent, and produce integrated data and modeling in situ for rapid socio-cultural assessment in conflict zones and in humanitarian efforts.

C. Research Investment

The total funds managed by the ARO Life Sciences Division for FY13 were $62.7 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY13 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 $10.8 million to projects managed by the Division. The Division also managed $20.1 million of Defense Advanced Research Projects Agency (DARPA) programs and $6.3 million for active Minerva Research Initiative projects. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.7 million for contracts. The Institute for Collaborative Biotechnologies received $13.8 million. Finally, $4.5 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.8 million provided through the ARO Core (BH57) allotment, in addition to funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

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[1] Roos P, Gelfand M, Nau D,Carr R. (2014). High strength-of-ties and low mobility enable the evolution of third-party punishment. *Proc. R. Soc. B.* 281:20132661.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of 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 FY13 (*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. Research opportunities 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.

The following subsections summarize projects awarded in FY13 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 FY13, the Division awarded nine 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 the metabolic impact of mitochondrial biogenesis and bicarbonate pool expansion, to investigate a new method to control reversible payload sequestration and release in hydrogels, and to analyze single nanoparticles, viruses and bacteria using ultra-wide field imaging. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Berry Brosi, Emory University; *Identifying Pollen In Mixed Samples Based On Plastid DNA*
- Professor Michael Davis, Oklahoma State University; *Metabolic Impact Of Mitochondrial Biogenesis And Bicarbonate Pool Expansion*
- Professor Hanna Engelberg-Kulka, Hebrew University of Jerusalem; *Novel Stress-Induced Translation Machinery As a Unique Mechanism For Bacterial Cell Death And Survival*
- Professor Ralph Greenspan, University of California - San Diego; *Systems Biology Of the Actinomycete Rhodococcus*
- Professor Neel Joshi, Harvard University; *Reversible Payload Sequestration And Release In Hydrogels*
- Professor Aydogan Ozcan, University of California - Los Angeles; *Ultra-wide Field Imaging of Single Nano-Particles, Viruses and Bacteria*
- Professor Russell Stewart, University of Utah; *Connecting Molecular Structure to Silk Fiber Properties*
- Professor Benjamin tenOever, Mount Sinai School of Medicine; *The Antiviral Biology of Drosha*
- Professor Marvin Whiteley, University of Texas at Austin; *Polymicrobial Virulence Mechanisms*

2. Short Term Innovative Research (STIR) Program. In FY13, the Division awarded two new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to synthesize and structurally characterize peptide-based, self-assembled nanostructures and to explore novel peptides as a potential mechanism to improve protein stability and activity. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Shaoyi Jiang, University of Washington; *Peptides to Improve Protein Stability and Activity*
- Professor Kristi Kiick, University of Delaware; *Synthesize And Structurally Characterize Peptide-Based, Self-Assembled Nanostructures*

3. Young Investigator Program (YIP). No new starts were initiated in FY13.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY13 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *4th International Workshop on Advances in Electrocorticography*; New Orleans, LA; 11-12 October 2012
- *Future Directions of Basic Research in Chemical and Bioengineering Workshop*; Austin, TX; 16-18 January 2013
- *The Institute of Biological Engineering Annual Conference*; Cary, NC; 7-9 March 2013
- *19th International Meeting on DNA and Molecular Computing*; Tempe, AZ; 22-27 September 2013
- *Conference on Foundations of Nanoscience*; Snowbird, UT; 15-18 April 2013
- *Biological Mechanisms in Evolution: in Basic Biology, Cancer, Infectious Disease and Medicine Gordon Research Conference*; Easton, MA; 2-7 June 2013
- *Microbial Population Biology Gordon Research Conference*; Andover, NH; 21-26 July 2013
- *Workshop on Visual Search: A Comprehensive Treatment*; Washington, DC; 5-6 December 2013
- *Workshop on Cell-Based Sensing*; College Park, MD; 25 January 2014

5. Special Programs. In FY13, 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 Division; therefore, all of the Division's active MURIs are described in this section.

1. 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 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 2). 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.

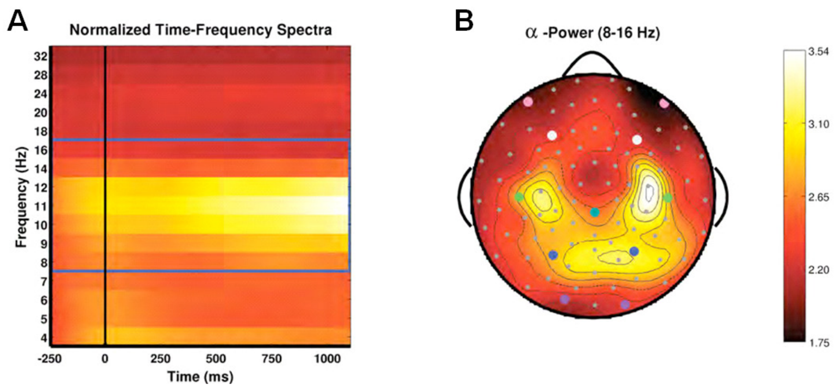

FIGURE 2

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.

2. 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 3).

FIGURE 3

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. This MURI includes research that spans multiple methodologies (qualitative, experimental, survey, archival, computational) within each of these objectives.

3. 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 4). 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 4

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.

4. 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.

5. 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.

6. 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. This research 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.

7. 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.

8. 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 research 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.

9. 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.

10. 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.

11. Artificial Cells for Novel Synthetic Biology Chassis. This MURI began in FY13 and was awarded to a team led by Professor Neal Devaraj at the University of California - San Diego. The goal of this MURI is to understand how biological and biomimetic synthetic cellular elements can be integrated to create novel artificial cells with unprecedented spatial and temporal control of genetic circuits and biological pathways. This research is co-managed by the Life Sciences and Chemical Sciences Divisions.

The field of synthetic biology aims to achieve design-based engineering of biological systems. Toward this goal, researchers in the field are identifying and characterizing standardized biological parts for use in specific biological organisms. These organisms serve as chassis for the engineered biological systems and devices. While single-celled organisms (e.g., bacteria, yeast) are typically used as synthetic biology chassis, the complexity of even these relatively simple organisms presents significant challenges for achieving robust and predictable engineered systems. A potential solution is the development of minimal cells which contain only those genes and biomolecular machinery necessary for basic life. Concurrent with recent advances toward minimal biological cells, advances have also been made in biomimetic chemical and material systems, including synthetic enzymes, artificial cytoplasm, and composite microparticles with stable internal compartments. These advances provide the scientific opportunity to explore the integration of biological and biomimetic elements to generate an artificial hybrid cell that for the first time combines the specificity and complexity of biology with the stability and control of synthetic chemistry.

The objective of this MURI is to integrate artificial bioorthogonal membranes with biological elements to create hybrid artificial cells capable of mimicking the form and function of natural cells but with improved control, stability, and simplicity. If successful, these artificial cells will provide a robust and predictable chassis for engineered biological systems, addressing a current challenge in the field of synthetic biology that may ultimately enable sense-and-respond systems, drug-delivery platforms, and the cost-effective production of high-value molecules that are toxic to living cells (e.g., alternative fuels, antimicrobial agents).

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

Research 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 FY13, the Division managed six new-start SBIR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of four Phase I contracts and two Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications, such as the development of label-free methods for chemical detection and a nano-pharmaceutical platform for creating artificial vaccines.

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 FY13, the Division managed nine new-start STTR contracts, in addition to active projects continuing from prior years. These contracts consisted of six 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 nanostructured carbon nanosheet electrode for enzymatic fuel cells, and DNA-origami systems for potential use in assay 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 FY13, the Division awarded six 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 FY13.

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 FY13, the Life 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 protein transport and adsorption, and cognitive/perception processing.

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 $13.8 million was allocated to the ICB in FY13, which was the fifth year of a $70 million contract that was renewed in FY09 for a five-year period. Of these FY13 funds, $10.4 million was allocated for 6.1 basic research and $3.4 million was allocated for six 6.2 projects, including two new projects.

In FY13, the ICB supported 64 faculty, 130 graduate students, and 74 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 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. ARO Life Sciences, ARL-SEDD, and DARPA 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.

J. DARPA Reliable Neural-Interface Technology (RE-NET) Program

The goal of this program is to develop high performance and clinically viable in-vivo neural interfaces to control dexterous functions made possible with advanced prosthetic limbs, enabling service members with amputations to return to active duty and improve their quality of life. ARO Life Sciences co-manages projects in the Reliable Peripheral Interfaces (RPI) focus area, which 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. One approach supported through this program involves the use of 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 example uses an implantable device to measure electromyogram activity from residual muscles to provide the control signal to the robotic limb. A third approach is exploring the design of a sensory feedback interface from the prosthetic fingers to the user's skin to enable intuitive touch feedback during use.

K. 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 research 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 this research 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.

L. DARPA Stochastic Computing Machines Enabled by DNA Self-Assembly Project

The Life Sciences Division currently co-manages a DARPA project focused on creating stochastic computing machines using self-assembled DNA nanostructures. This joint project aims to demonstrate the feasibility of a new class of computing machine that is physically implemented by DNA self-assembly and molecular-scale devices. The computing machine will be based on digital stochastic state machines, unlike traditional digital circuits, which are based around deterministic finite state machines. The planned computing machine has potential to deliver improved performance at vastly reduced power and size by using architectures that are implemented using nanoscale physical devices.

M. 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.

N. 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. Two projects initiated in the previous year continued in this second year of the program. 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.

O. 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 were two active projects pursuing research under this topic in FY13.

P. 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. 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 FY13.

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

The objective of this MRI topic is to examine the relationship between trans-national 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 FY13.

R. 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 FY13.

S. 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 FY13.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. 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. The goal of the MURI award led by Professor Hao Yan at Arizona State University is to develop 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.

In FY13, the multidisciplinary research team organized a two-enzyme reaction pathway on a planar DNA nanostructure to identify the inter-enzyme distances necessary for maximal pathway activity. The team also developed new conjugation methods to attach enzymes to DNA structures with reliable control at the three-dimensional level, which will be used to determine the impact of 3D spatial arrangement on pathway activity in coming years. In addition, the directed diffusion of reaction intermediates between enzymes was demonstrated using an engineered swing arm (see FIGURE 5). The swing arm dramatically increased the efficiency of the reaction, increasing the effective concentration of the intermediate by 200-fold. The swing arm also provides a mechanism to avoid competition from side reactions in a three-enzyme cascade, thereby improving the specificity of the reaction pathway. Single molecule fluorescence measurements of a model system were used to determine the optimal distance between the swing arm and the enzymes and to verify successful transfer of intermediates. These results will be used to construct more complex, bioelectroactive enzyme pathways that in the future may be interfaced with external conductive materials for new capabilities in photo-energy generation and energy storage.

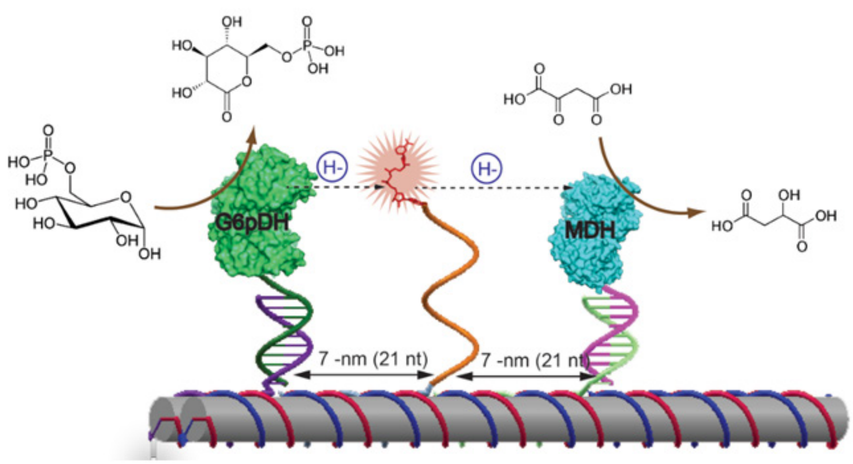

FIGURE 5

Organizing and controlling biochemical pathways outside of the cellular environment. The MURI team has designed a molecular swing-arm system which efficiently channels a reaction intermediate between two enzymes, Glucose-6-phosphate dehydrogenase (G6pDH; green) and Malate dehydrogenase (MDH; blue). The cofactor Nicotinamide adenine dinucleotide (NAD; red star) is attached to a short DNA arm (orange) that swings between the two enzymes. G6pDH will oxidize glucose-6-phosphate to glucolactone and reduce NAD+ to NADH. The swing arm will then specifically transfer NADH to the second enzyme, MDH, which uses the NADH to catalyze the formation of oxaloacetate from malate.

B. Ghrelin and Stress Resilience
Professor Ki Goosens, Massachusetts Institute of Technology, Single Investigator Award

The objective of this research is to identify molecular and neurophysiological pathways of stress and stress resilience. In FY13 the Goosens laboratory published a landmark paper identifying a new stress pathway. For over one hundred years neuroscientists have believed that the hypothalamic-pituitary-adrenal axis, which produces adrenaline, cortisol, and other hormones, is the critical and only command center for the human stress response. The Goosens laboratory demonstrated that not only is stress also mediated through the ghrelin pathway, but that the ghrelin pathway acts independently of the hypothalamic-pituitary-adrenal axis.

In addition to profoundly altering how neuroscientists understand stress, the recently published work from the Goosens laboratory also pointed the way to new avenues for preventing and treating stress induced disorders such as post traumatic stress syndrome, suicide, and depression. The investigators discovered that ghrelin, previously known as the "hunger hormone," is released during chronic stress and that this ghrelin release makes the brain more susceptible to long-term debilitation from stress. While some stress can improve performance, too much stress often results in short- or long-term declines in performance capabilities. How much stress is good and how much is bad varies from individual to individual. With the results from this research, scientists now understand that one factor affecting individual stress resilience is long-term ghrelin levels. This implies that regular meals can protect against stress induced illnesses, and that ghrelin-suppressors could potentially protect warfighters (and civilians) against the long-term impact of severe traumatic events. While developing new drugs can easily take a decade and cost millions, at least a dozen drugs that interfere with ghrelin have already been developed by various pharmaceutical companies. These ghrelin inhibitors were initially developed to reduce obesity, but were a failure for the indication of weight loss. However, their safety was demonstrated in earlier clinical trials and therefore may be able to be more quickly tested and if successful in trials, transitioned to vaccines to proactively protect warfighters against PTSD, and to alleviate dysfunction in soldiers suffering from stress induced psychiatric disorders.

C. Electroencephalography-based Translation of Neural Activity
Dr. Rajesh Rao, University of Washington, Single Investigator Award

The field of brain-machine interfacing has witnessed rapid progress in the last decade in developing technology to aid paralyzed and disabled individuals. An important question that could significantly expand the realm of applicability of brain-machine interfaces (BMIs) is whether they can be operated by able-bodied subjects while they engage in normal physical activity. The objective of this research is to use a non-invasive BMI based on electroencephalography (EEG) to detect and translate neural activity from both imagined and overt movement and quantify the degree to which they are coupled via advanced pattern recognition and machine learning methods.

In FY13, the research team leveraged previous findings on the coupling between imagined and overt EEG patterns and used this information to develop and demonstrate the first-ever direct transfer of signals between the brains of two human subjects, a brain-to-brain interface (BBI). The researchers created a BBI by detecting EEG patterns from one subject who imagined moving his hand. The control signal detected by the brain activity of intended movement was immediately sent over the internet to a transcranial magnetic stimulation helmet worn by the second subject, who then involuntarily (subconsciously) moved his hand (see FIGURE 6). Although this experiment demonstrated that a brain impulse from one human can be used to control specific muscles in a different subject, it represents the unidirectional control of a pre-selected movement. Researchers are now attempting longer-term studies to determine if this approach can be expanded to detect a subject's conscious intent and then transmit that information remotely to a device or another person. This research may ultimately be useful for developing new training paradigms based on BMI and brain-brain interfaces.

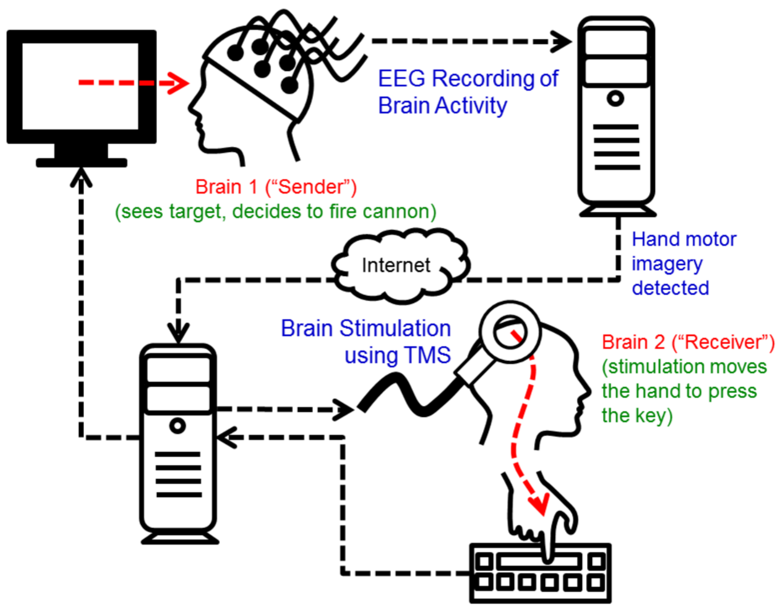

FIGURE 6

Brain-to-brain signal transfer. Brain signals from Subject 1 (the "Sender") were recorded using EEG. When imagined hand movements were detected by the computer, a "fire" command was transmitted over the internet to the TMS machine, which caused an upward movement of the right hand of Subject 2 (the "Receiver").

D. Anisotropic Nanostructured Materials

Professors Bradley Chmelka and Songi Han, University of California - Santa Barbara, Institute for Collaborative Biotechnologies (UARC)

The goal of this research, led by Professors Bradley Chmelka and Songi Han, is to create and explore the properties of inorganic-organic hybrid materials. In FY13, the research team developed and characterized a novel inorganic-organic hybrid materials platform that allows for (i) the controlled synthesis of ordered synthetic membrane materials with tunable nanochannel dimensions over macroscopic length scales with (ii) the capability to incorporate diverse active biological guest species including membrane proteins. One such membrane protein is the light responsive bacterial proteorhodopsin (PR) which actively pumps H^+ ions across cell membranes creating an H^+ gradient that is used to generate chemical energy that powers cellular functions.

This group proposes to achieve a proton motif force (PMF) by creating an H^+ gradient across the synthetic membrane material upon light activation in the presence of PR and converting the PMF into a voltage potential. Toward this end, Chmelka and Han have developed robust synthesis and evaluation protocols for incorporating PR into these nanocomposite membranes. This research has included the development of solution-processing conditions and inclusion of appropriate surfactants for maintaining correct folding and activity of high levels of PR within the nanochannels and the demonstration that light-induced conformational changes are sustained within the synthetic membranes. More recently, the team demonstrated that (i) PR molecules within the nanostructured hybrid thin films exhibit higher thermal stabilities than within native *E. coli* membranes or membrane-mimetic surfactant micelles, (ii) the photocycle kinetics and other functional properties of PR are tunable by water content and pH, and (iii) high degrees of alignment of PR molecules in the hybrid membranes are achievable over macroscopic (cm) length scales by applying strong electric fields during film syntheses.

With further refinement, this synthetic membrane constructed with well-ordered and tuned nanochannels capable of hosting active PR has the potential to serve as a platform for the development of lightweight photovoltaic and electrochemical energy conversion and storage devices. The same fundamental knowledge that has gone into the engineering of these synthetic membranes has contributed to a successful ICB 6.2 project led by Teledyne Scientific and Imaging and ARL-SEDD. This research is integrating acid-functionalized nanostructured proton conducting membranes from Prof. Chmelka's group into low-power-density microbial fuel cells that are under development at ARL for unattended ground sensors in desert environments.

E. A Molecular Subtyping Scheme for Understanding the Epidemiology of *Salmonella Enterica*

Professor Edward Dudley, Pennsylvania State University, Single Investigator Award

The objective of this research is to determine whether a unique genetic feature in bacteria, known as a clustered regularly interspersed short palindromic repeat (CRISPR), in addition to molecular subtyping methods such as pulsed field gel electrophoresis (PFGE) and multilocus sequence typing could be used in concert to discriminate between strains of *Salmonella Enterica*, to better understand the population structure of Salmonella, to understand bacterial-bacteriophage interactions in an environmental system, and to estimate the rate at which Salmonella CRISPR spacer arrays evolve in gram negative bacteria such as Salmonella.

CRISPRs 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. Professor Dudley and colleagues previously devised a sequencing approach that incorporates sequencing of CRISPR regions with known virulence genes, designated CRISPR-multi-virulence-locus sequence typing (CRISPR-MVLST).[2] The researchers sought to determine whether this method could discriminate between common *Salmonella* strains and may be useful for identifying isolates that associate with specific environmental niches and those that have increased capacity to cause human disease.

In FY13, Professor Dudley and colleagues demonstrated that their CRISPR-MVLST method could distinguish between particular *Salmonella* strains that were not possible to positively identify using other methods alone.[3-4] The team assayed isolates from ten previous *Salmonella* outbreaks using CRISPR-MVLST. In repeated studies, they found that analyzing various *Salmonella* strains (serovars) using conventional methods alone, such as pulsed-field gel electrophoresis (PFGE), could not distinguish among many of the key isolates. However, the combination method of CRISPR-MVLST was more effective in accurately distinguishing various isolates and at a faster turnaround than PFGE (see FIGURE 7).

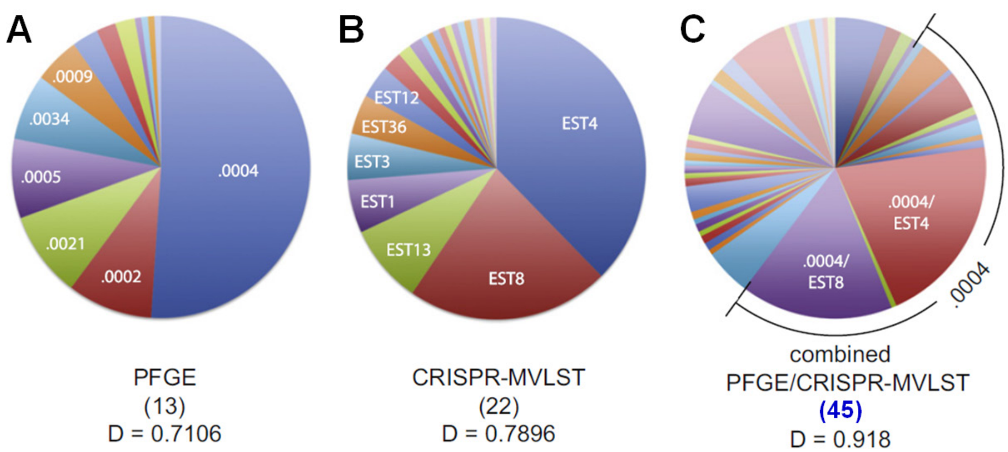

FIGURE 7

Combined PFGE and CRISPR-MVLST provides increased discriminatory power. The pie charts showing the number of distinct subtypes of *Salmonella* that could be distinguished using (A) PFGE, (B) CRISPR-MVLST and (C) a combination of both PFGE and CRIPSR-MVLST. The number of distinct groups defined by each method is listed in parenthesis and discriminatory power (D) is listed at the bottom.[3]

The rapid and accurate identification of isolates can have a profound impact on the speed and effectiveness of isolating the source of an outbreak. This research will likely lead to long-term applications such as more effective methods for monitoring food safety, the rapid detection of outbreaks from gram-negative bacteria, and also a more accurate determination of the optimal treatment regimen for affected patients.

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[2] Liu F, Kariyawasam S, Jayarao BM, et al. (2011). Subtyping Salmonella enterica serovar enteritidis isolates from different sources by using sequence typing based on virulence genes and CRISPRs. *Appl Environ Microbiol*. 77:4520-6.

[3] Shariat N, Kirchner MK, Sandt CH, et al. (2013). Subtyping of Salmonella enterica serovar Newport outbreak isolates by CRISPR-MVLST and determination of the relationship between CRISPR-MVLST and PFGE results. *J Clin Microbiol*. 51:2328-36.

[4] Shariat N, DiMarzio MJ, Yin S, et al. (2013). The combination of CRISPR-MVLST and PFGE provides increased discriminatory power for differentiating human clinical isolates of Salmonella enterica subsp. enterica serovar Enteritidis. *Food Microbiol*. 34:164-73.

F. Dynamic Models of the Effect of Culture on Collaboration and Negotiation
Professor Michele J. Gelfand, University of Maryland - College Park, MURI Award

The goal of this resaerch is to systematically examine the effects of culture on negotiation, with particular attention to developing models that account for Western and Non-Western cultures. It is widely believed that social norms – expected repertoires for behavior – vary across cultures and affect negotiations. Existing theory and research, however, has failed to systematically represent and test how cultural differences affect negotiation processes and outcomes.

In 2013, the Gelfand team demonstrated that negotiation involves both tangible outcomes (e.g., policy settlements, delivery of resources) and intangible outcomes (e.g., honor, trust). The team also showed that intangible outcomes are linked to cultural values. Moreover, parties at the negotiating table may place different weights on these tangible and intangible outcomes. For example, building trust may be more important to one party than the other in the negotiating context. If valued intangibles are not realized in the outcome of a negotiation (e.g., an actor valuing trust emerges distrustful), the Gelfand model demonstrates that subsequent negotiations between different actors representing the same cultures will suffer from a "contagion of conflict" that generates difficulty in even bringing the actors representing the different cultures to the table for subsequent negotiations. This is because the negative after-effects of the failure to secure desired intangible outcomes reverberates across the culture through different institutions. For example, distrust experienced by an actor in a political negotiation, can generate suspicion by another actor from the same culture entering into economic negotiations, according the model. The Gelfand team has not only mathematically modeled the role of cultural values in negotiating styles and interactions, they have also validated the model through a series of experiments and case studies published in 2012 and 2013. Their attention to cultural differences demonstrates that the outcomes of negotiation have a lasting and profound impact beyond the negotiation table primarily through the less-visible, intangible outcomes negotiators experience. This has important implications for developing effective negotiation and bargaining strategies and points to the importance of understanding the cultural values of all parties at the negotiation table.

G. Game Theory, Culture and Institutional Path Dependence
Professor Scott Page, University of Michigan, Single Investigator Award

The goal of this research is to generate computational models to represent how one institution influences behavior in other institutions through the diffusion of normative information. In FY13, the research team experimentally demonstrated that (i) strategies for negotiation are learned from negotiating partners; (ii) those strategies are carried over and exercised in subsequent negotiations with different partners; and (iii) when strategies are carried over, they are revised to extreme levels. For example, if a negotiating partner moderately violates the trust of a focal actor, the focal actor becomes highly distrustful in future interactions with unrelated others and behaves accordingly. Their research also demonstrated that governance structures in society can incentivize desired negotiating strategies through rewarding negotiators for deploying them or punishing them for failing to deploy them. Rewards, however, are more effective at eliciting desirable behavior in negotiations than punishments. Using a combination of mathematical modeling and network analytic strategies, the research team has developed a breakthrough generalizable representation of this path dependence in sequential negotiation that parameterizes the dynamics of path dependence and path revision in negotiation. This is important because it allows understanding of these dynamics to move beyond sets of examples for describing the dynamics to being able to simulate and predict negotiation dynamics and outcomes across a broader range of negotiation contexts. Furthermore, the Page team's model provides a framework for drawing on genetics and ecological sciences to further explore the interplay between stability and change in negotiating strategies and their diffusion across time and institutions. The breakthroughs made in 2013 by this team offer new insights on not only the persistent and influential role that initial negotiation norms play beyond a single negotiation setting, but also the most efficient ways that governing agents can reinforce desired negotiation strategies.

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. Protein Nanoparticles from Ivy Adhesive for Advanced Sunscreen Formulations

Investigator: Professor Mingjun Zhang, University of Tennessee - Knoxville, Single Investigator Award
Recipient: Advanced Skin Technology, Inc.

Professor Zhang's laboratory made the initial discovery that ivy adhesive is composed of nanoparticles suspended in a polymer matrix, which was the first time that naturally secreted plant nanoparticles had been observed. The goal of this research was to elucidate the biochemical and mechanical properties of these nanoparticles which lead to the impressive strength of the ivy adhesive. Results from this research demonstrated that the ivy nanoparticles were primarily composed of protein, and further characterization of these protein-based nanoparticles led to the discovery that ivy nanoparticles protect against UV radiation 4-fold better than metal-based nanoparticles currently used in sunscreens. These naturally produced plant nanoparticles were also found to be non-toxic when administered to cell cultures, identifying an additional benefit relative to the traditional sunscreen nanoparticles. These results transitioned to Advanced Skin Technology, which is testing ivy nanoparticle samples for potential use in advanced sunscreens with reduced toxicity.

B. Actionable Variation in Human Genes

Investigator: Professor Jasper Rine, University of California - Berkeley, Single Investigator Award
Recipient: VitaPath Genetics

The human genome contains approximately six hundred genes that encode proteins dependent on vitamin or mineral cofactors for proper function. The sequence of each individual human's genome is quite variable, due to both inherited and de novo polymorphisms. As a result a typical human is deficient in one or more of these six hundred proteins, with resulting suboptimal function of one or more of these critical enzymes. Although these six hundred enzymes are nutritionally responsive – and the deficiency is easily remedied if one knew which supplement any particular individual needed – the vast majority of the human population remains unsequenced and the individual variations remain unknown. While the state of the art is a one size fits all approach to supplements (i.e. multivitamins); excessive amounts of minerals and vitamins are well known to cause increased susceptibility to cancer, bacterial and viral infections, and reduced longevity. A further complication is that even in sequenced genes it remains extremely difficult to accurately predict the effect of a change in amino acid sequence on protein structure and function.

The long term objective of this research is to develop accurate assays for rapidly determining the effect of polymorphisms in these six hundred cofactor dependent enzymes. Professor Rine's laboratory aims to interrogate all identified nonsynonymous single nucleotide polymorphisms in five protypical B6, niacin, riboflavin, and thiamine-dependent enzymes for both functional impact and cofactor responsiveness.

The initial results from the Rine lab transitioned in FY13 to a partnership between VitaPath Genetics and Alere to create a molecular assay for spina bifida vulnerability in women of childbearing age. Spina bifida is caused by the incomplete closure of the embryonic neural tube. Spina bifida is one of the most common birth defects, with a world-wide incidence of about one in a thousand live births. Affected children often have learning and social disabilities as well as muscle, orthopedic, urinary, skin, and ocular problems.

The incidence of spina bifida can be reduced by 70% by folic acid supplementation in the three months prior to becoming pregnant. However the recommended dose for at risk women is 4-5 mg/day, whereas the recommended dose for not at risk women is 0.4mg/day. The intent of the Vita-Path-Alere partnership is to identify at risk women before they become pregnant, so that the risk of spina bifida can easily and safely be dramatically reduced with pe-pregnancy supplementation with appropriate levels of folic acid.

The long term goal of the Rine lab is to extend this approach to the other 599 cofactor dependent enzymes, so that each warfighter's genome can be known and so that each individual's daily mineral and vitamin uptake can be tailored to maximize that person's cognitive and mental performance capabilities.

C. Modeling Cultural Factors in Collaboration and Negotiation

Investigator: Professor Katia Sycara, Carnegie Mellon University, MURI Award
Recipient: Air Force Culture and Language Center, Maxwell Air Base

The objective of this research is predict the effects of cultural factors on cooperation and negotiation through the development of validated theories; construction of flexible and scalable computational models that incorporate cultural and social parameters and generate new theoretical insights; and investigation of the role of sacred values in conflict resolution. Sacred values are fundamental beliefs that reflect moral norms – beliefs about what is right from a moral standpoint, independent of material and instrumental values and outcomes (such as acquisition or access to important resources). Sacred values provide a framework not only for action, but also for rationalizing one's actions and interpreting the actions of others, and as such, they play a central role in negotiation.

In 2010, the researchers began collecting dictionaries of sacred values for different cultures, focusing on the Middle East. The investigators recognized that not only do types of sacred values vary cross-culturally, individuals within cultures may be more or less competent in identifying and enacting values and may respond to violations of sacred values more or less radically. The researchers have incorporated these insights into their models, providing them with a tool to simulate negotiation and conflict resolution in cross-cultural scenarios and demonstrate how individual differences with respect to cultural competence and radicalization of response effect outcomes. In FY13, this model transitioned to the Air Force Culture and Language Center at Maxwell Air Base for use in the General Officer Pre-Deployment Acculturation Course.

D. MicroRNA-mediated Control of Viral Gene Expression

Investigator: Professor Benjamin tenOever, Mt. Sinai School of Medicine, PECASE Award
Recipient: DARPA

The objective of this research is to understand how small RNA molecules in the cells of many organisms interact with invading viruses and to explore methods that could potentially harness these natural mechanisms to control viral growth in mammalian cells. Although there are variations across organisms, small RNA molecules bind to messenger RNA molecules with complementary or near-complementary sequences, causing the degradation of those pairs by the cell and suppressing translation in a process generally referred to as RNA interference (RNAi). In effect, these small RNA molecules provide another mechanism for controlling gene expression.

The cells of some organisms, including bacteria, arthropods, nematodes, and plants, release a class of small RNA molecules called virus-derived interfering RNA (viRNA). In these organisms, viRNA sequences are coded to bind directly to the gene products of viruses commonly encountered by the organism, thereby preventing viral replication. Interestingly, eukaryotes (e.g., humans and other vertebrates) do not use this mechanism, instead relying on a protein-based defense strategy in which cells shut down various functions that are essential to viral replication. Despite these differences, eukaryotes utilize a class of small RNA molecules called microRNAs as a mechanism for rapidly controlling the levels of proteins native to the cell.

Professor tenOever and colleagues have made many notable discoveries in the past ten years regarding the molecular-level responses of cells to viral invasion. In 2003, he was one of the first scientists who discovered a unique series of signaling cascades through which cells detect and respond to invading viruses.[5] With support from ARO and others, Professor tenOever began examining (i) the mechanism and locations of viral microRNA production in a host cell, (ii) whether microRNAs can be used to control virus tropism, and (iii) whether viruses can be attenuated by modifying the viral genome to be an exact complement to a native microRNA expressed in the host tissue of interest.

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[5] Sharma S, tenOever BR, Grandvaux N, et al. (2003). Triggering the interferon antiviral response through an IKK-related pathway. *Science*. 300:1148-51.

Professor tenOever's laboratory has made significant progress in each of these areas. His research team discovered a small RNA produced by influenza A virus that, while not a microRNA, accumulates to >10000 copies per cell and has a significant impact on the virus' replicative cycle.[6] His laboratory also developed a molecular and genetic method for tracking the types of cells targeted by a given virus, which was then validated by delivering small RNAs of pre-designed sequences, providing a level of resistance for the cells against specific infections (see FIGURE 8).[7] He also found that viruses could be engineered to produce functional microRNAs regardless of whether the viruses replicated in the nucleus or cytoplasm.[8-9] Given that certain microRNAs are cell-specific and/or species-specific, he also demonstrated that a similar approach can be used to control virus tropism.[10-11] These discoveries mark a potential revolution in the tools available to study viral replication mechanisms and to combat infection.

In FY13 these results transitioned to DARPA, which is funding research to determine whether these discoveries are compatible for use in other organisms and adaptable for different types of viruses. The safety and effectiveness of these methods must also be demonstrated through rigorous laboratory and clinical studies. These follow-on studies are building on the fundamental discoveries made possible through ARO basic research funding.

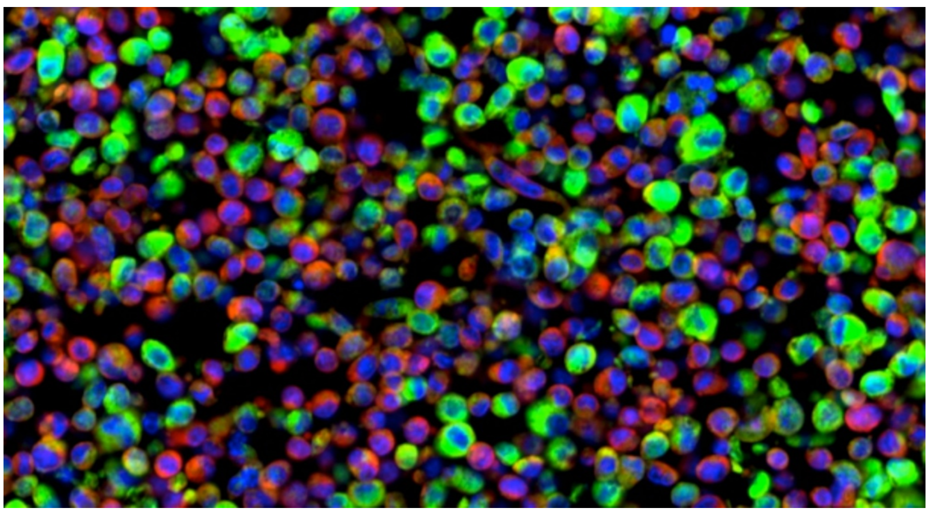

FIGURE 8

Abundant small RNA in virus-infected cells. Virus infected cells labeled with RNA to depict the nucleus (blue), the cytoplasm (red) and viral production of small RNA (green). *[Courtesy tenOever laboratory]*

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[6] Chua MA, Schmid S, Perez JT, et al. (2013). Influenza A virus utilizes suboptimal splicing to coordinate the timing of infection. *Cell Rep*. 31:23-9.

[7] Pham AM, Langlios RA, tenOever BR. (2012). Replication in cells of hematopoietic origin is necessary for dengue virus dissemination. *PLoS Pathog*. e1002465.2.

[8] Shapiro JS, Varble A, Pham AM, Tenoever BR. (2010). Noncanonical cytoplasmic processing of viral microRNAs. *RNA*. 16:2068-74.

[9] Langlois RA, Shapiro JS, Pham AM, tenOever BR. (2012). In vivo delivery of cytoplasmic RNA virus-derived miRNAs. *Mol Ther*. 20:367-75.

[10] Langlois RA, Varble A, Chua MA, et al. (2012). Hematopoietic-specific targeting of influenza A virus reveals replication requirements for induction of antiviral immune responses. *Proc Natl Acad Sci U S A*. 109:12117-22.

[11] Langlois RA, Albrecht RA, Kimble B, et al. (2013). MicroRNA-based strategy to mitigate the risk of gain-of-function influenza studies. *Nat Biotechnol*. 31:844-7.

V. ANTICIPATED ACCOMPLISHMENTS

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

A. Forensic Palynology

Professor Berry Brosi, Emory University, Single Investigator and DURIP Awards

Identifying the origin and recent history of people and materiel is a major technological challenge and critical to the success of current and future operations. One often needs to quickly know whether the person wanting to enter a sensitive area is who they say they are, or not. In addition, it would be useful to be able to verify their recent activities, such as travel to certain regions of the world. The rapid identification of pollen is an underutilized avenue for extracting information about a person's recent location and activities.

The objective of this research is to identify and characterize pollen obtained from mixed samples. There are four major characteristics of pollen that make it particularly informative. (i) Pollen is microscopic, generally ranging from 10-70 um in diameter. (ii) Pollen is abundant, being produced in vast abundance by male plants in order to fertilize female plants of the same species. As most pollen is generally dispersed by either wind or insects, the male plants must produce pollen in vast amounts (up to 100,000 grains of pollen per anther) to ensure that some of it will reach a female of the same species. (iii) Pollen is very stable and has been identified in some cases after millions of years. (iv) Pollen is exceedingly complex and varies widely from species to species. (v) Pollen types are specific to time and place. A particular combination of pollen may enable the accurate identification where a human, body, computer, or other item has been, based on the variability in where plants can grow, when they produce pollen, how far a particular species of pollen can travel, and how stable a particular pollen is under specific conditions (see FIGURE 9).

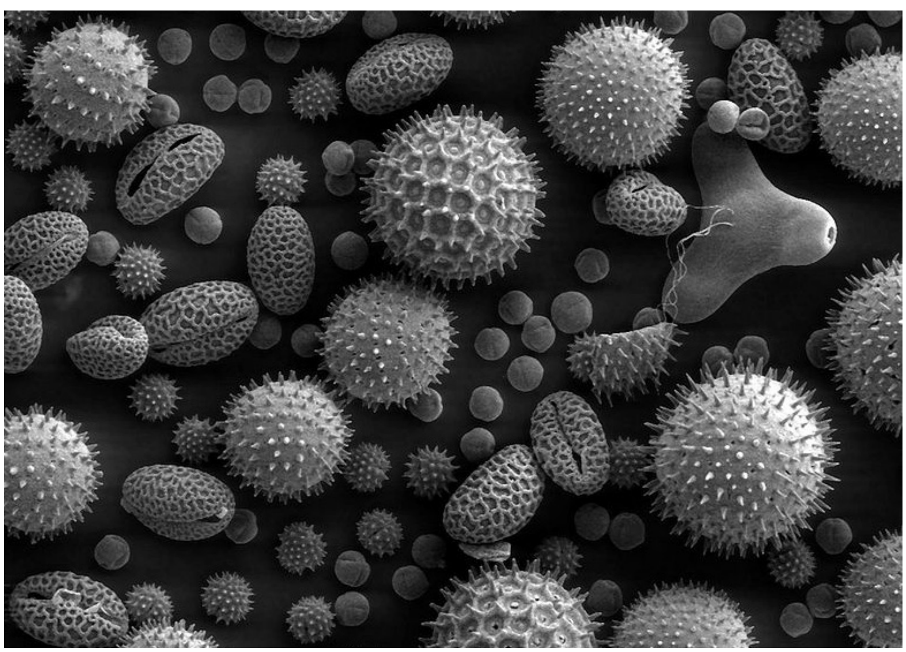

FIGURE 9

Pollen diversity. Scanning electron microscope image of pollen grains from a variety of common plants including sunflower, morning glory, prairie hollyhock, oriental lily, evening primrose, and castor bean reveals some of the diversity of pollen types and characteristics. The identification and relative ratios of different types of pollen pinpoints the origin of the pollen both temporally and spatially.

In close collaboration with FBI and Army forensic scientists, Professor Brosi at Emory University is determining whether pollen identification can be automated using DNA analysis. The challenge has been that pollen identification is currently done by humans, training takes years, very few humans are trained palynologists, and even the most highly trained palynologist is still very slow. While pollen is already used in DoD and non-DoD forensics, current technological challenges prevent use of the information encoded in pollen in real time for DoD intelligence, security, and forensic applications. It is anticipated that in FY14, Professor Brosi's laboratory will evaluate plastid DNA presence and copy number across a nested, detailed swath of the Spermatophyte lineage. Forty of the seventy families, sixty families within the forty focal orders, and five genera within the focal families will be examined. He is also working to improve the efficiency and reliability of DNA extraction from pollen samples, including elimination of non-pollen DNA. If successful this work is anticipated to lead to rapid, automated palynology, so that pollen can be analyzed in real time. Real time capabilities would greatly increase the ability of DoD to use the information embedded in pollen composition to rapidly track down terrorists and other nefarious objects and personnel.

B. Organic Matrix Templating and Function in an Ultrahard Biological Composite
Professor David Kisailus, University of California - Riverside, Single Investigator Award

Nature has evolved efficient strategies, exemplified in the mineralized tissues of numerous species, to synthesize materials that often exhibit exceptional mechanical properties. These biological systems demonstrate the ability to control nano- and micro-structural features using organic templates that not only precisely guide the formation and phase development of minerals, but also significantly improve the mechanical performance of otherwise brittle materials. One such example is found in the heavily mineralized radular teeth of the chitons, a group of elongated mollusks that graze on hard substrates for algae. The radula, toothed ribbon-like structures which are used for this feeding (see FIGURE 10), are well known for their ability to efficiently erode the rocky surfaces on which the chitons feed. Professor David Kisailus at the University of California - Riverside is exploring synthesis-structure-property relationships in unique biomaterials that exhibit remarkable damage tolerance and abrasion resistance.

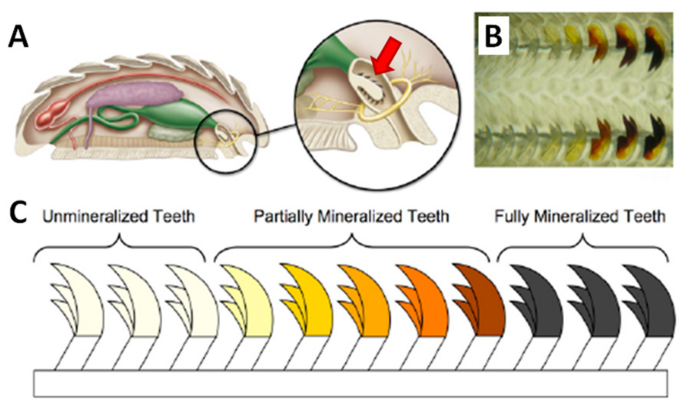

FIGURE 10

The Damage Tolerant and Abrasion Resistant Radular Teeth of Chitons. Professor Kisailus will explore the chemical and structural features of the mineralized radular teeth of chitons to elucidate structure-property relationships in these unique damage tolerant and abrasion resistant biological composite materials. (**A**) The internal anatomy of a chiton identifying the location of the radula (red arrow), a toothed conveyor belt-like structure used for feeding. (**B**) A photographic image of the mineralized teeth of the radula. New teeth are continually formed and are mineralized as they migrate toward the functional feeding position. Thus this system provides Professor Kisailus with unmineralized teeth, partially mineralized teeth and fully mineralized teeth for analysis (**C**).

The ultimate goal of this research is to investigate the chemical and structural features of both the fully mineralized radular teeth of the chiton *Cryptochiton stelleri* and the underlying organic framework which provides a template for mineral growth and a scaffold for the teeth. The results of this analysis will be used to design a biomimetic in vitro mineralization process to understand the organic-inorganic interactions and mineral growth mechanisms that lead to the architectural features of the radula that enhance abrasion resistance and damage tolerance. In the first year of this research, the fully mineralized teeth were comprehensively characterized using a variety of microscopy and spectroscopy methods to identify chemical and structural features and analyze mechanical properties. It is anticipated that in FY14, proteins that compose the underlying organic framework will be isolated and identified by protein sequencing, and partially mineralized teeth will be chemically, structurally and mechanically characterized using the same approaches employed for the fully mineralized teeth. This will provide an intermediate view of the mineralization process and aid in identifying the chemical and structural features that impact the final material properties.

This research will provide fundamental understanding of synthesis-structure-property relationships in unique abrasion resistant and damage tolerant biological composite materials that may enable the future development of the necessary tools for the design and fabrication of cost-effective and environmentally friendly engineered materials that mimic key design elements and performance properties present in biological systems.

C. Imaging How Neurons Compute

Professor Rafael Yuste, Columbia University, MURI Award

For decades, researchers have debated how information is integrated at the synaptic connections of neurons. There has been no conclusive answer, because the synaptic information content is dependent on the exact location of the synaptic contact on dendrites and on the cell types of the presynaptic and postsynaptic neurons and the spatio-temporal pattern of neuronal activity. This type of structural information was impossible to gather before, and must be combined with functional studies to truly understand neural computationwhich is among the most central questions in neuroscience.

The goal of this multidisciplinary research is to employ several novel and advanced optical imaging and stimulation techniques to visualize, for the first time, the relation between a neuron's firing output and the pattern of its synaptic inputs. Measurements will be performed in a variety of biological samples, from primary neuronal cell cultures, to brain slices, to in vivo mouse preparations.

It is anticipated that in FY14 structural and functional connectivity will be mapped with a combination of ultrastructural, super-resolution and two-photon imaging techniques to permit the resolution of synaptic inputs from interneurons and pyramidal cells that are activated with multielectrode arrays or two-photon photostimulation of presynaptic neurons, yielding, for the first time, the table of synaptic strengths of a neuron. A quantitative understanding of synaptic integration may offer the capability to generate computational models of pyramidal cells and of neocortical interneurons that may enable the prediction of their response to any arbitrary pattern of inputs. The successful completion of this research will result in a comprehensive understanding of dendritic integration. This technology has the potential to pioneer a novel approach to functional connectomics based on light microscopy, as opposed to static structural-only reconstructions from fixed tissue with electron microscopy.

D. Online Laboratory to Assess Problem-solving Dynamics

Professor David Lazer, Northeastern University, Single Investigator Award

In the modern military, large teams must collectively search for, process, and integrate information that leads to a problem resolution. Existing research suggests that actors use two different strategies to locate information to bring to bear in problem-solving: exploration and exploitation. Exploration involves the search for novel information, while exploitation involves searching for known information. Exploration comes at the cost of taking advantage of current best practices and slower gathering of information. Exploitation, however, may miss the identification of information that can lead to better solutions to problems. Additionally, more efficient communication networks (*i.e.*, ones in which information is quickly passed along to all members of a group) impede exploration, which requires more cognitive effort by actors. Such trade-offs have been studied extensively in small groups to identify optima in the balance between exploitation and exploration for a range of collective problems. These results have helped practitioners design networks that facilitate achieving that balance in small groups.

Scientists, however, have not yet successfully modeled and tested the hypothesized trade-offs between different problem-solving strategies within large networks, which more realistically represent many decision-making situations. This has hobbled the design and implementation of effective networks to facilitate problem-solving in real-world, real-time situations. One of the challenges for researchers has been the logistical difficulty of large-group experiments (*e.g.*, space limitations, enrolling large groups of participants) and capturing the network dynamics of a large group in the context of problem-solving.

The Lazer team is addressing this by developing an on-line platform for large group experiments and coupling it with a subject enrollment strategy built around Amazon Turk to populate massive on-line experiments. The researchers will then host games on the platform to test established hypotheses from small-group research regarding group problem-solving dynamics and network structures in large groups. This will allow the investigators to determine the scalability of validated small-group dynamics and network structures and the impact those dynamics and network structures have on problem-solving effectiveness in large groups. The team has developed nine game templates corresponding to established small-group experiments (see FIGURE 11).

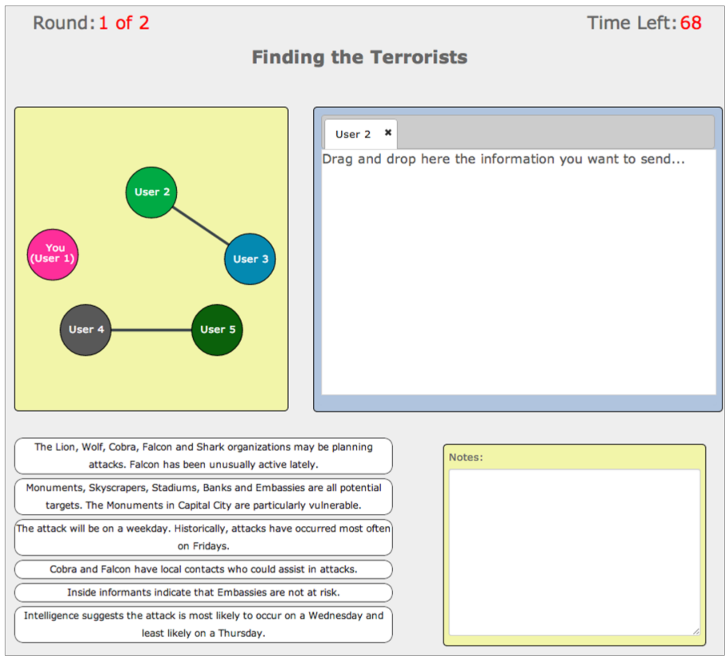

FIGURE 11

Small-group, hidden profile game experiment. In this problem-solving experiment, players work to replicate the hidden profile of a terrorist by culling through information and deciding what information should be communicated to which others in their network. The panel on the upper left displays the communication network in the case of a small group of five actors as typically studied. The Lazer team is scaling this approach to capture large group dynamics and assess how the structure of large-group networks affects the balance between exploitation and exploration strategies and problem-solving effectiveness.

The platform has been created and nine game templates have been developed and scaled for large-group experiments. Experiments in the game environments are now underway, with results anticipated in FY14. This research will be the first to shed light on whether network structures that facilitate small-group problem-solving also facilitate large-group problem-solving to the same extent and what modifications to large-group networks will improve efficiency and solution quality.

E. The Stress-Induced Translation Machinery of Bacterial Cell Death and its Role in Adaptation

Professor Hanna Engelberg-Kulka, Hebrew University of Jerusalem, Single Investigator Award

The objective of this research is to decipher the regulatory machinery and corresponding mechanisms that control programmed cell death in bacteria and enable the survival bacterial populations when exposed to severe stresses. The process of programmed cell death (PCD) in multi-cellular organisms, called apoptosis, is recognized as an essential mechanism ensuring the survival of the organism. For example, the cells that make up the webbing between the fingers during human embryogenesis must die to free the individual digits.

Until the mid-1990s, it was expected that this phenomenon was limited to multi-cellular organisms. Professor Engelberg-Kulka was one of the first researchers to demonstrate a mechanism for PCD in single-celled organisms.[12] More recently, her laboratory identified a toxin-antitoxin system (*maz*EF) that is involved in mediating PCD, and that this system was controlled due in part by a novel peptide called extracellular death factor (EDF).[13-14] Her laboratory showed that the protein toxin encoded by the MazF portion of the module is an endoribonuclease that cleaves a subset of messenger RNAs (mRNAs) at specific sites just upstream of the translation start sites, resulting in the generation of a population of leaderless mRNAs (see FIGURE 12). Further, they showed that MazF toxin also truncates the 16S rRNA, producing a subpopulation of ribosomes that selectively translate the leaderless mRNAs. Thus, the team has discovered a modified translational machinery that appears to be a mechanism used by bacteria for stress adaptation. These initial results were pioneering advances toward the larger goal of understanding the mechanisms of bacterial adaptation and survival, but the downstream proteins controlled by this system and the exact conditions that activate the process remain elusive.

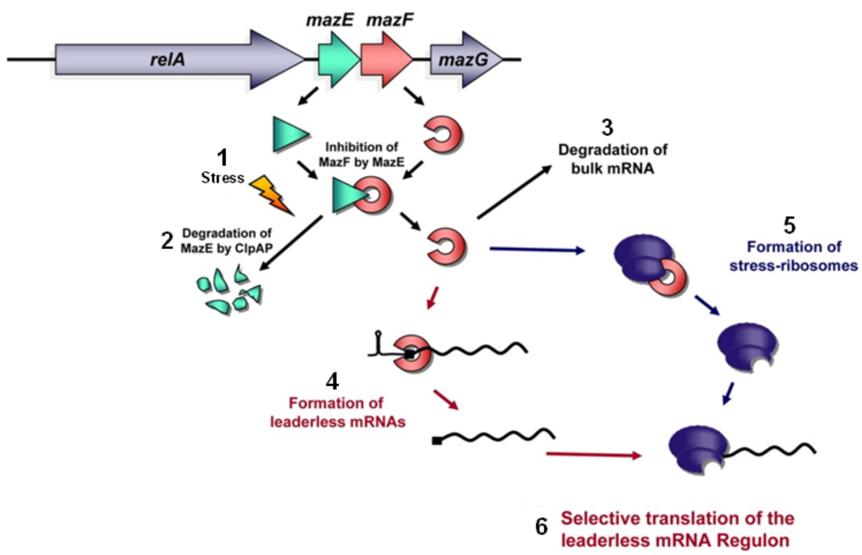

FIGURE 12

Model of mazEF-mediated leaderless mRNA and stress ribosome formation. The mazEF module can be triggered by stressful conditions (1), which results in (2) degradation of the antidote MazE. The activity of released MazF leads to degradation of the majority of transcripts (3) and removes the 50UTR of specific mRNAs, thus rendering them leaderless (4), and specifically removes terminal nucleotides of 16S rRNA (5), which is essential for the formation of a translation initiation complex on canonical ribosome-binding sites. As a result, (6) MazF activity leads to selective translation of a "leaderless mRNA regulon."

It is anticipated that in FY14 Professor Engelberg-Kulka's laboratory will identify the *E. coli* translation machinery that is mediated by *MazEF*, to determine the stress conditions that elicit changes in the systems, and to characterize the downstream proteins that are synthesized as a result of induction. If successful, these results will be an important step in understanding the growth conditions and molecular mechanisms that allow bacterial survival under various stressors, ranging from natural environmental changes to the presence of an antibiotic.

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[12] Aizenman E, Engelberg-Kulka H, Glaser G. (1996). An Escherichia coli chromosomal "addiction module" regulated by guanosine 3',5'-bispyrophosphate: a model for programmed bacterial cell death. *Proc Natl Acad Sci U S A*. 93:6059-63.

[13] Kolodkin-Gal I, Hazan R, Gaathon A, et al. (2007). A linear pentapeptide is a quorum-sensing factor required for mazEF-mediated cell death in Escherichia coli. *Science*. 318:652-5.

[14] Belitsky M, Avshalom H, Erental A, et al. (2011). The Escherichia coli extracellular death factor EDF induces the endoribonucleolytic activities of the toxins MazF and ChpBK. Mol Cell. 41:625-35.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

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C. Administrative Staff

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Ms. Jennifer Eaton
Contract Support

Ms. Valerie Johnson
Contract Support

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 2013* is to provide information on the programs and basic research supported by ARO in FY13, 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 FY13.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Materials Science Division seeks to realize slightly improved material 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 areas of interest include new approaches for materials processing, composite formulations, and surface treatments that minimize environmental impact. Finally, there is general interest by the Division in research to identify and fund basic research in 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 collaborating with 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

The Materials Science Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY13, the Division managed research 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, this research 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 this research 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 behind the observed physical properties (electronic, magnetic, optical, and thermal) in materials/composites through support of basic research that ultimately leads to development of future Army devices. General areas of research include modeling, innovative processing of materials with unprecedented physical properties, and novel physical property characterization techniques. The main Thrusts of this program are: (i) Defect Science and Engineering of Advanced Materials, and (ii) Novel 2D Free-standing Crystalline Materials (beyond graphene).

The Defect Science and Engineering of Advanced Materials Thrust involves studies related to various defects (such as point, line, area, volume, strain etc. in materials) and their origin, control, impact on physical properties in different materials (*e.g.*, oxides, nitrides, carbon-based materials etc) in bulk, thin-film, as well as at the interfaces. The Novel 2D Free-standing Crystalline Materials Thrust includes fundamental research with the goal of investigating the physical properties of novel free-standing graphene like crystalline 2D materials (*e.g.*, oxides, nitrides, chalcogenides etc.), and their composite/heterostructures and characterization of these structures for unique properties/phenomenon.

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) Stability of Nanomaterials and (ii) Manufacturing Process Science. The Stability of Nanomaterials Thrust focuses on the creation of thermally stable, high-strength nanocrystalline materials via interfacial grain boundary engineering, pinning nano-precipitates or internal coherent boundaries. The Manufacturing Process Science Thrust supports research with the goals of discovery of fundamental physical laws and phenomena of materials processes, and exploitation of unique phenomena that occur under extreme processing conditions for the creation of advanced materials.

These research areas 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 FY13 were $39.5 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY13 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 $8.4 million to projects managed by the Division. The Division also managed $19.0 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 $1.8 million for contracts. Finally, $3.1 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 creation, leadership, and management of 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 FY13 (*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.

The following subsections summarize projects awarded in FY13 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 FY13, 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 characterize fundamental device properties of 2D free-standing silicene and silicene/graphene heterostructures, to develop anisotropic, multiscale, statistical property assessments from flow-generated nano-rod or nano-platelet material dispersions, and to determine how segregation at grain boundaries can be used to manipulate boundary character in relation to the intrinsic stress states that evolve in nanocrystalline thin films. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Deji Akinwande, University of Texas at Austin; *Hexagonal Atomic Sheets of Silicon (Silicene); Towards Heterogeneous Layered Solids*
- Professor M. Gregory Forest, University of North Carolina - Chapel Hill; *Statistical Multiscale Property Metrics for Nanorod and Nanoplatelet Composite Membranes and Films*
- Professor Theodore Goodson III, University of Michigan - Ann Arbor; *Utilizing Quantum Size Effects with Novel Small Metal Cluster Systems*
- Professor Patrick Hopkins, University of Virginia; *Defect Engineering of Thermal Vibrations in Nanosystems*
- Professor Masaru Kuno, University of Notre Dame; *Colloidal Syntheses of Two Dimensional Titanium Disulfide and CdSe Nanosheets and Their Single Sheet Absorption Spectroscopy*
- Professor Peter Liaw, University of Tennessee - Knoxville; *Developing Advanced Light-Weight High-Entropy Alloys: Modeling and Experiments*
- Professor Konstantin Novoselov, University of Manchester; *Superstructures Based on 2D crystals*
- Professor Pramod Reddy, University of Michigan - Ann Arbor; *Engineering Near-Field Transport of Energy using Nanostructured Materials*
- Professor Suryanarayan Sankar, Advanced Materials Corporation; *Consolidation of Exchange Coupled Magnets Using Equal Channel Angular Extrusion at Low Temperatures*
- Professor Vivek Shenoy, University of Pennsylvania; *Multi-scale Modeling, Design Strategies and Physical Properties of 2D Composite Sheets*

- Professor Gregory Thompson, University of Alabama - Tuscaloosa; *Influence of Grain Boundary Structure on Nanocrystalline Thin Film Stress States*
- Professor Rodney Trice, Purdue University; *Fabrication of Complex-Shaped Ceramic Components by Room-Temperature Injection Molding of Ceramic Suspension Gels*
- Professor Christian Van de Walle, University of California - Santa Barbara; *First-Principles Investigations of Ga2O3 and Related Materials as Novel 2D Conductors*

2. Short Term Innovative Research (STIR) Program. In FY13, the Division awarded three new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to determine the effects of alloying and resultant microstructures on the size, density, and stability of nanotwins in stainless steels, to discover the influence of strain on catalytic properties, to demonstrate the feasibility of using innovative manufacturing technologies, namely spark plasma sintering (SPS) and high pressure torsion (HPT) to produce bulk amorphous alloys. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Raymundo Arroyave, Texas Engineering Experiment Station; *Stabilization of Nanotwinned Microstructures in Stainless Steels through Alloying and Microstructural Design*
- Professor Jason Nicholas, Michigan State University; *Strain Engineering Defect Concentrations in Reduced Ceria for Improved Electro-Catalytic Performance*
- Professor Julie Schoenung, University of California - Davis; *Materials Science: Novel Synthesis and Processing of Amorphous Mg Alloys*

3. Young Investigator Program (YIP). In FY13, the Division awarded two new YIP projects. These grants are driving fundamental research, such as studies to elucidate electron- phonon coupling (EPC) in metal chalcogenide nanosheets, and investigate novel heterostructures prepared by combining two dimensional (2-D) semiconductors and ultrathin, single crystalline complex oxides materials. The following PIs and corresponding organizations were recipients of the new-start YIP awards.

- Professor Linyou Cao, North Carolina State University; *Electron-Phonon Coupling in Atomic-Scale Two-Dimensional Chalcogenide Nanosheets*
- Professor Sayeef Salahuddin, University of California - Berkeley; *Novel Electronic Applications with 2D Semiconductors*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY13 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *2012 Materials Research Society Fall Meeting*; Boston, MA; 26-30 November 2012
- *Armor Ceramics Symposium 2013 - ACerS 37th International Conference on Advanced Ceramics and Composites*; Daytona Beach, FL; 27 January - 1 February 2013
- *2013 Materials Research Society Spring Meeting*; San Francisco, CA; 1-5 April 2013
- *Nanoscience and Nanotechnology with a Special Symposium/Workshop on Complex Oxides*; Corfu, Greece; 16-20 June 2013
- *50th Annual Technical Meeting of the Society of Engineering Science (SES)*; Providence, RI; 28-31 July 2013
- *9th International Conference on Composite Materials (ICCM-19)*; Montreal, Canada; 28 July - 2 August 2013
- *2013 Physical Metallurgy Gordon Research Conference on Materials at Extremes*; Biddeford, ME; 28 July - 2 August 2013
- *2013 Soft Condensed Matter Physics Gordon Research Conference & Seminar*; New London, NH; 18-23 August 2013

5. Special Programs. In FY13, 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 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 Materials Science Division; therefore, all of the Division's active MURIs are described in this section.

1. 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 project, which ended in FY13, was co-managed by the Chemical Sciences and Materials Science Divisions. This MURI explored 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 investigated 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 designed, synthesized, and characterized a revolutionary new class of mechano-responsive molecules, called mechanophores, which respond to mechanical stress with pre-designed chemical reactions. Based on 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.

2. 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 by the Materials Science and Chemical Sciences Divisions.

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.

3. 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.

4. Electrical Control of Magnetic Dynamics in Hybrid Metal-Semiconductor Systems. This MURI began in FY08 and was granted to a research team led by Professor Daniel Ralph at Cornell University. The objective of this research is to investigate fundamental phenomena that will enable the all-electrical manipulation of magnetic behavior (both static and dynamic properties) in hybrid structures incorporating magnetic metals, multiferroic oxides and semiconductors.

This research involves fundamental studies on spin injection and transport studies in hybrid metal-semiconductor systems and establish the materials growth and nanofabrication techniques needed to develop a new class of hybrid spin-based electronics. Five studies are being pursued: (i) to study spin injection across metal-semiconductor interfaces, (ii) to develop spin-transfer-torque oscillators and switches, (iii) to pursue the integration of multiferroic materials for electric-field control of exchange coupling bias, (iv) to investigate general approaches to electrical manipulation of spins (electron and nuclear spins), and finally (v) to identify electrical approaches to manipulation of coupled spins in diamond. One key goal is to obtain three orders of increase in the current density of injected spin polarized currents across metal-semiconductor interfaces.

5. 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 objective of this research is to investigate fundamental spin-based properties of novel hybrid structures incorporating magnetic metals, multiferroic oxides and organic semiconductors.

This research seeks to develop a new class of hybrid magneto-electronics that can move towards the seamless integration of memory and logic functions under a single device format. The research will conduct some very fundamental studies on spin injection and transport studies in hybrid metal-organic systems. In addition, this work will also look at aspects of nuclear spin imprinting in organics, spin-wave guiding, GHz spin precession and phase locking of sources, OLED modulation, electric-field tuning of spin injection from multiferroic contacts, and electrical switching of ferromagnetism in quasi 2DEG oxide heterostructures. Pioneering studies on magnetoresistance (OMAR) and nuclear spin polarization in organic systems and on conductor-insulator induced transitions in the magnetism of 2DEG oxide heterostructures ($SrTiO_3$ and $LaTiO_3$) are being conducted. It also proposes a very interesting task to use organic overlayers to image the evolution of spin waves from metallic spin torque devices. The program includes a significant theory and modeling task to help guide the experimental effort. As the material capabilities become better defined the program will seek to identify and prototype new device structures relevant to applications in sensors, magnetic storage, dynamic memory and logic, and spin-wave mediated data transfer.

6. 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.

7. 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.

8. 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 in 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

9. Stress-controlled Catalysis via Engineering Nanostructures. This MURI began in FY11 and was granted to a team led 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.

10. Atomic Layers of Nitrides, Oxides, and Sulfides (ALNOS). This MURI began in FY11 and was granted to a team led 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.

11. Materials with Extraordinary Spin/Heat Coupling. This new FY13 MURI was granted to a team led by Professor Roberto Myers of the Ohio State University. The objectives of this project include understanding the structure-property relationships for coupling heat and spin current in various materials and synthesize magnetic materials with extraordinary and tunable thermal conductivity due to spins, understanding non-equilibrium phonon-magnon transport and the mechanisms behind Spin Seebeck Effect, and finally measuring and understanding phonon-magnon drag and phonon-electron drag in materials.

If successful, this project may lead to long-term applications such as temperature sensors, thermal spintronic devices, solid-state Spin Seebect Effect -based power generators, thermal management in electronic and vehicular applications, and tunable thermal conductivity in materials via magnetic field, microwaves, and light.

12. Theory and Experiment of Cocrystals: Principles, Synthesis and Properties. This MURI began in FY13 and was awarded to a team led by Professor Adam Matzger of the University of Michigan at Ann Arbor. This MURI team is investigating molecular co-crystal formation and the implications for controlling solid-state behavior. This research is co-managed by the Chemical Sciences and Materials Science Divisions.

The largely untapped potential for creating new molecular crystals with optimal properties is just beginning to be realized in the form of molecular co-crystallization. Co-crystallization has the potential to impact the macro-scale performance of many materials, ranging from energetic materials, to pharmaceuticals, to non-linear optics. Unfortunately, the dynamics of molecular co-crystal formation is poorly understood. Molecular co-crystals contain two or more neutral molecular components that rely on non-covalent interactions to form a regular arrangement in the solid state. Co-crystals are a unique form of matter, and are not simply the result of mixing two solid phases. Organic binary co-crystals are the simplest type and often display dramatically different physical properties when compared with the pure ‘parent’ crystals. A significant amount of research on co-crystal design has been carried out by the pharmaceutical industry for the synthesis of pharmaceutical ingredients. However, co-crystal design has not been exploited in broader chemistry and materials science research areas. A recent breakthrough discovery demonstrates that co-crystallization can be used to generate novel solid forms of energetic materials.

The objective of this MURI is to develop a fundamental understanding of intermolecular interactions in the context of crystal packing, and to use the knowledge gained for the design of new co-crystalline molecular materials with targeted, optimized physical and chemical properties. In the long term, a better understanding and control of molecular co-crystallization has the potential to improve the properties of a variety of materials, including: energetic materials, pharmaceuticals, organic semiconductors, ferroelectrics, and non-linear optical materials.

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

Research 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 FY13, the Division managed three new-start SBIR 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 contracts aim to bridge fundamental discoveries with potential applications, including the development of Equal Channel Angular Extrusion prototype tooling and processing technology for large scale (250-350 kg) billets of ultrafine/nano grained light alloys, and lightweight nanostructured metallic alloy systems with high strength and ductility.

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 FY13, the Division managed four new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of two Phase I contracts and two Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications, including the development of a bulk acoustic wave (BAW) filter, a tunable microwave device based on multiferroic heterostructures, and a suitable method to grow epitaxial AlGaN films with reduced dislocation density.

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 FY13, the Division managed six 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. Engineering Ferroic and Multiferroic Materials for Active Cooling Applications. The objective of this PECASE, led by Professor Lane Martin at the University of Illinois at Urbana-Champaign, is to investigate the physical mechanisms and thermodynamic principles that underlie thermo-electrical responses, primarily pyroelectric and electrocaloric responses, in complex oxide materials and heterostructures.

This research program is exploring key materials properties that might permit one to manipulate and control temperature- and field-dependent entropic changes that occur in multiferroic/magnetoelectric systems and in frustrated ferroelectric systems, and probe the feasibility of using these for solid state cooling. The mechanisms that lead to strong magnetoelectric coupling in these systems will be studied to establish whether large entropy changes can be achieved in these systems. Finally, Ginzburg-Landau-Devonshire thermodynamic models will be developed to characterize the dominant pyroelectric and electrocaloric responses. First generation cooling devices will be fabricated and characterized for potential operation down to ~70K.

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 FY13, the Division managed five new DURIP projects, totaling $0.8 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of materials flow and deformation, dynamic behavior of granular materials, and friction stir processing.

H. 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.

I. DARPA LoCo Program

The goal of the Local Control of Materials Synthesis (LoCo) program is to develop a low-temperature process for the deposition of thin films whose current minimum processing temperature exceeds the maximum temperature substrates of interest can withstand (e.g., chemical vapor deposited diamond on polymers). The Division currently co-manages projects within this program seeking to realize chemical and physical processes to meet the energetic/chemical requirements of thin film deposition (e.g., reactant flux, surface mobility, reaction energy, etc.), without reliance on broadband temperature input used in state-of-the-art chemical vapor deposition.

J. 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.

K. 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.

L. 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.

M. 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.

N. 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.

O. 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.

P. 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.

Q. 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 funded and/or monitored by the Materials Science Division.

A. Germanium Graphane Analogues

Professor Joshua Goldberger, Ohio State University, Single Investigator Award

The objective of this research is to create and characterize the properties of novel hydrogen- and organic-passivated single atom thick 2D sheets of germanium as semiconductor building blocks for next generation DoD applications. In FY13, the research team successfully created germanane (GeH), an air-stable hydrogen-terminated germanium graphane derivative from the deintercalation of $CaGe_2$ in acidic media and started characterization of these materials (see FIGURE 1). GeH has a direct band gap in the near IR at 1.6 eV, and can be mechanically exfoliated into single layers of GeH onto SiO_2 / Si substrates. Theory predicts that 2D GeH has a room temperature electron mobility of 18,000 cm^2/Vs, which is five times of larger than 3D crystalline germanium. Additionally, the surface terminating hydrogen can be substituted with other organic moieties such as methyl groups, to yield methyl germanane ($GeCH_3$), thereby manipulating/tuning the properties. For example, methyl termination can increase the band gap to 1.7 eV and enhances the fluorescence quantum yield to 0.2%. This notion of creating a single atom thick electronically conductive direct band gap derivative of germanium is of potential interest to a wide variety of applications to DoD ranging from sensing, to optoelectronic communication to energy harvesting.

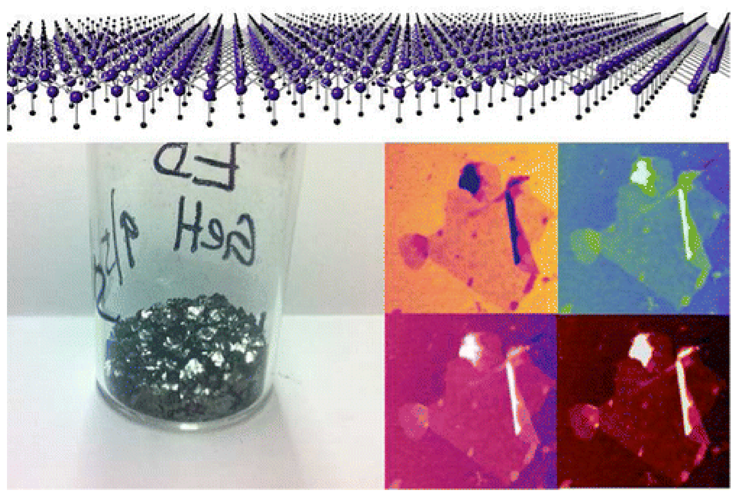

FIGURE 1

Germanane (GeH), an air-stable hydrogen terminated germanium graphane derivative. The panels include a schematic illustration of single-layer Germanane (GeH), gram-scale synthesis of bulk GeH crystals, and an atomic force microscope image of single-layer GeH.

B. Colloidal Syntheses and Characterization of 2D Titanium Disulfide and CdSe Nanosheets

Professor Masaru Kuno, University of Notre Dame, Single Investigator Award

The objective of this research is to develop basic understanding to obtain spatially-resolved *absorption* images of two-dimensional (2D) nanomaterials. This goal extends beyond conventional emission-based single molecule imaging, to allow one to study entire classes of *non-emissive* materials. In FY13 the research team initially focused on direct absorption measurements of single layer graphene oxide (GO) since this system possesses low absorption coefficients, is chemically heterogeneous and is reactive – being reduced to chemical graphene on prolonged exposure to light. These single layer GO studies have led to the first measurements of GO absorption coefficients as well as evidence of intrasheet absorption heterogeneities (see FIGURE 2A-B). More interestingly, it has enabled the first direct observation of GO during reduction, as followed in real time through correlated absorption/emission imaging. In turn, the PI has obtained detailed kinetic information about GO's photoreduction (see FIGURE 2C). To demonstrate the flexibility of the absorption imaging method, the PI has applied the technique towards the large-area absorption imaging of CVD-grown single layer graphene. In addition, the PI discovered what appeared to be grain boundaries as well as a bilayer islands, evident over single layer graphene (see FIGURE 2D).

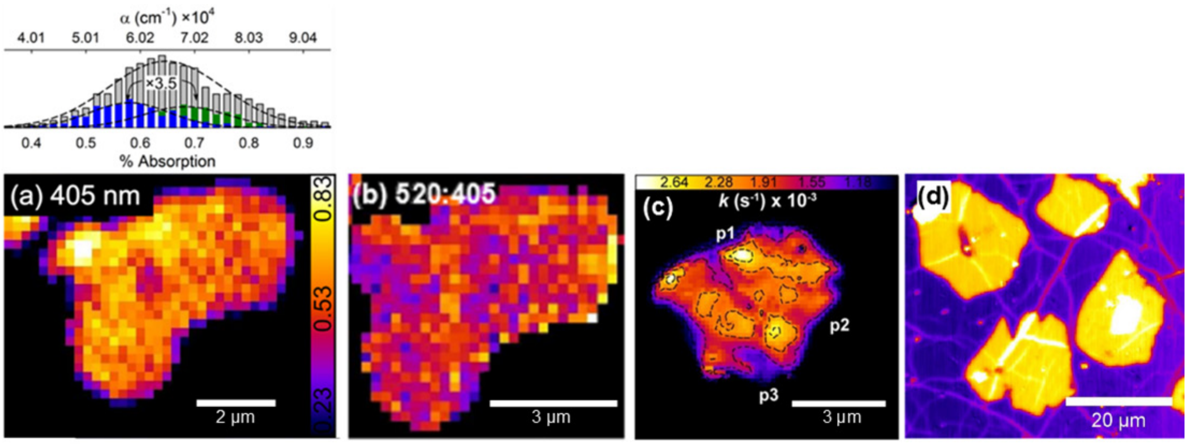

FIGURE 2

Spatially-resolved absorption images of non-emissive 2D nanomaterials. The figure illustrates (**A-B**) The research team's single-layer GO studies led to the first measurements of GO absorption coefficients and evidence of intrasheet absorption heterogeneities, (**C**) Kinetic data of GO's photoreduction, and (**D**) discovery of potential grain boundaries and bilayer islands evident over single layer graphene).

In FY13 the research team also successfully demonstrated the first synthesis of large free standing crystalline nanosheets composed of dinuclear sulfur bridged molybdenum complexes (see FIGURE 3). This material can potentially be used for the bottom-up synthesis of MoS_2 nanosheets. On a broader level, use of analogous bridged metal complexes may yield general routes to the chemical synthesis of 2D materials. These finding are highly relevant to DoD needs as (i) the developed absorption technique now enables virtually all 2D nanomaterials to be studied optically, and (ii) the synthetic approaches have begun to establish chemical routes to new 2D materials that have future applications such as sensing, electronics, power and energy.

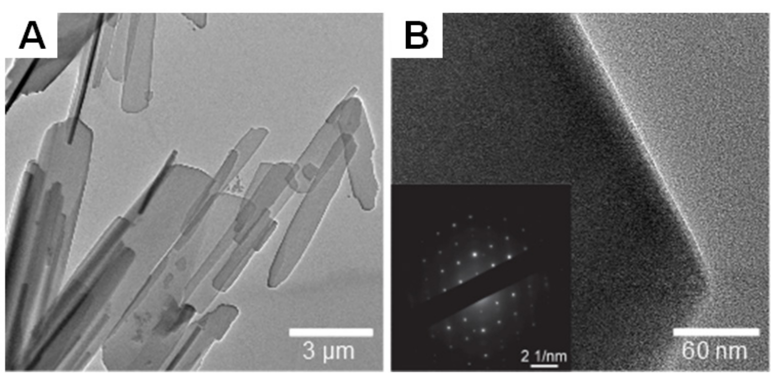

FIGURE 3

Nanosheets composed of dinuclear sulfur bridged molybdenum complexes. Transmission electron microscopy images of sulfur bridged molybdenum complex nanosheets with a representative selected area electron diffraction patterns.

C. Atomistic Calculation of Residual Stress in Nanocrystalline Polycrystalline Materials

Professor Mo Li, Georgia Institute of Technology, STIR Award

Residual stress plays in important role in mechanical properties of polycrystalline materials, including deformation, fracture, corrosion and fatigue; however, little is known about the residual stress in nanocrystalline due to size limitations in existing characterization methods. The objective of this STIR is to use molecular dynamic computational methods to quantitatively determine the internal stress and link the internal stress to microstructural components such as grain boundaries, triple junctions, and grains to residual stresses, and subsequently, establish quantitative relations between the microstructures and mechanical properties and residual stress.

The research team recently found that the celebrated Laplace relation still holds in nanocrystalline materials, that is, $p=2\gamma/R$, where p is the internal pressure, R is the mean grain radius, and γ is the so-called 'interface stress", however, the direct calculation of the "interface stress" from our their new method shows that the interface stress γ does not equal to the two-dimensional grain boundary (residual) stress, which is in direct contradiction to all existing theories, including Gibbs' (see FIGURE 4). This discovery represents a major finding that impacts all materials dominated by interfaces and surfaces (such as porous, granular, and also other nanocrystalline materials, and will be important for effective engineering design of new nanostructured materials.

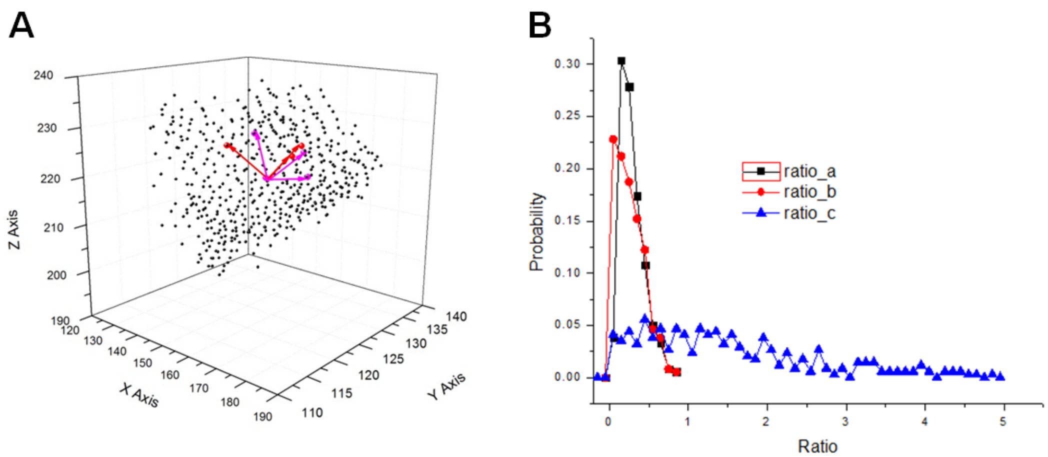

FIGURE 4

Non-two dimensional interface stress in nanocrystalline alloys. (**A**) The atomic configuration of a grain boundary (dots are shown as atoms) and the eigen directions of the interface stresses. This plot shows that the eigen stress is not two dimensional as expected with the non-vanishing third component; (**B**) The distribution of the ratios of the eigen stresses along directions perpendicular to and along the interface (blue triangles). The large spread of the ratio indicates that interface stress is not two dimensional.

D. Smart Core-Shell Nanowire Architectures for Multifunctional Nanoscale Devices

Professor Jonathan Spanier, Drexel University, PECASE Award

The objective of this research is to design, synthesize, and characterize a novel visible light-absorbing ferroelectric and photovoltaic perovskite oxide materials. Ferroelectric oxides possess characteristic features such as switchable polarity, and domain and domain wall variant structures that are enabling for novel modes of light-matter interaction, electronic carrier separation, and other functionalities well beyond those of ordinary non-centrosymmetric materials. However, ferroelectric oxide perovskites typically possess inherently large band gap E_g, typically >3 eV due to large electronegativity difference between oxygen and transition metal atoms. Because ferroelectric stability is typically driven by a select family of d^0 *B*-site transition metal cations, the synthesis of a robust system where the ferroelectric response is combined with a band gap in the visible range has remained elusive. Recently, a strategy for bandgap reduction without loss of ferroelectricity has focused on cation substitution chemistries that promote O vacancies and cation-vacancy clusters.

In FY13, the research team's efforts led to the discovery, synthesis and property characterization and analysis of a completely new family of visible light-absorbing ferroelectric and photovoltaic perovskite solid-solutions

$[KNbO_3]_{1-x}BaNi_{1/2}Nb_{1/2}O_{3-\delta}]_x$ (KBNNO).[1] KBNNO materials have large ferroelectric polarization and possess a wide variation of direct band gaps in the 1.1-3.8 eV range, 150% greater than that previously achieved by doping of a ferroelectric perovskite or a non-ferroelectric perovskite (see FIGURE 5). For example, the x = 0.1 composition has a band gap of 1.39 eV, switchable short-circuit current and an experimentally observed open-circuit voltage (V_{oc} = 3.5V), seven times larger than other narrow-gap semiconductor materials ($V_{oc} < 0.5E_g$). KBNNO is composed of non-toxic, earth-abundant, inexpensive elements. Advances in understanding of the bulk ferroelectric photovoltaic effect and in optical manipulation of ferroelectric polarization are required for future DoD applications in encoding, manipulating and storing information, optical detection, and sensing as well as photovoltaic energy conversion etc.

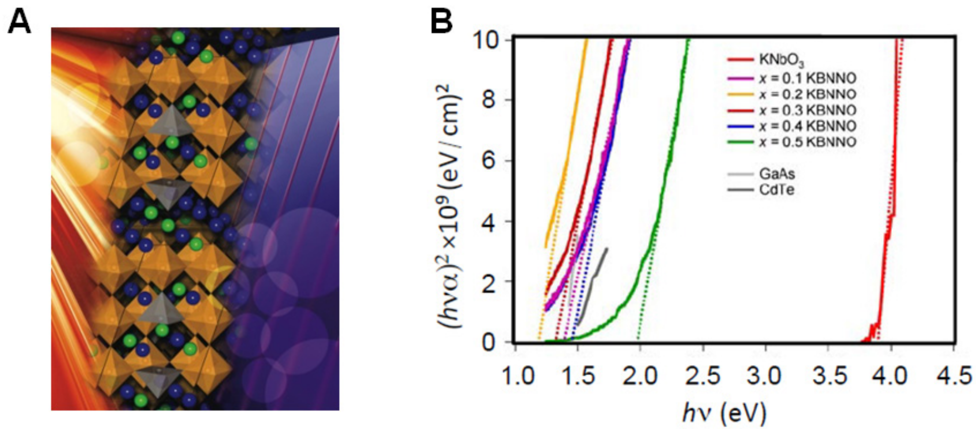

FIGURE 5

Structure and characterization of KBNNO. The panels illustrate (**A**) the structure of cation-oxygen vacancy cluster-driven ferroelectric semiconductor KBNNO and (**B**) ellipsometry measurements for KBNNO oxides with x=0.0-0.5, showing band gaps from 1.18 eV to 3.6 eV, making KBNNO promising for solar absorption.

E. In-Situ Observation of Densification in a Electric Field

Professors Klaus van Benthem and Troy Holland, University of California - Davis, Single Investigator Award

Currently, there are no less than five unique proposed mechanisms by which enhanced consolidation may occur in the presence of an electrical field. The objective of this research is to combine macroscopic sintering experiments using a modified thermo-mechanical analysis system with in-situ electron microscopy techniques to evaluate microstructure evolution and obtain a fundamental atomistic understanding of bonding phenomena during electric field-assisted sintering (EFAS).

In FY13, the investigators provided, for the first time, direct experimental evidence for dynamic surface cleaning during EFAS of metallic nanoparticles that are initially covered with ultrathin native oxide layers. The cleaning of nanoparticles from surface oxides or contaminants is critical during the initial stages of EFAS; however, until this study, only indirect evidence has suggested the occurrence of this phenomena. The investigators found that the "cleaning" of ultrathin NiO layers from the surfaces of nickel nanoparticles occurs through electric field-induced dielectric breakdown (see FIGURE 6). Furthermore, they propose a mechanistic description of the process wherein surface cleaning of metallic nanometric powder is initiated by defect formation and electron trapping of defects, as described by percolation models. Once the critical level of trapping is reached, local field enhancement drives the electrothermal depletion of surface oxides, with oxygen migrating away from the inter-particle contact, thereby inducing neck formation. These results provide a significant scientific advancement in the understanding of the local microstructural response during EFAS, and the elucidation of the true mechanisms for consolidation of new, advanced materials.

[1] Grinberg I, West DV, Torres M, et al. (2013). Perovskite oxides for visible-light-absorbing ferroelectric and photovoltaic materials. *Nature*. 503:509-512.

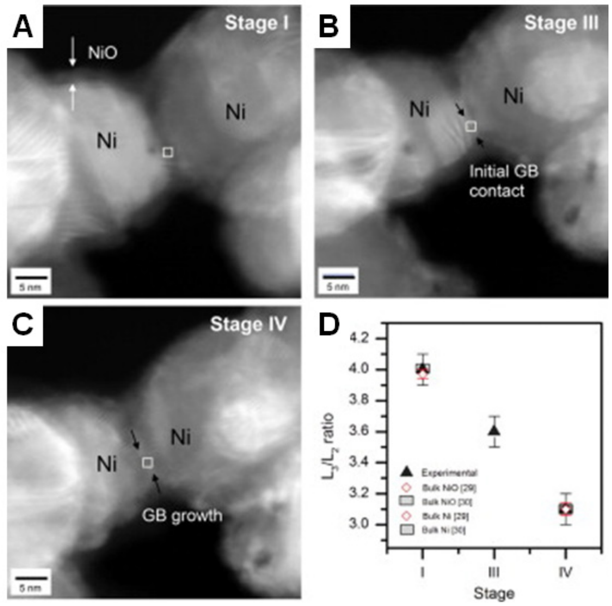

FIGURE 6

Dielectric breakdown of surface oxides in an electrical field. HAADF STEM images of two contacting particles before (**A**) the application of an electrical bias (stage I). The particles are covered with continuous NiO layers. (**B**) and (**C**) show the progression of surface oxide removal and the subsequent neck formation. EELS spectra of the Ni L2,3 absorption edges were recorded while the electron beam across the inter-particle contact area (box in A-C) was scanned. The L3/L2 EELS intensity ratio were calculated from experimental EELS data of the Ni L2,3 edges and plotted in (**D**). Reference spectra for bulk NiO and Ni are plotted for comparison.

F. Entangled Two-Photon Fluorescence Imaging

Professor Theodore Goodson, University of Michigan, Single Investigator Award

The objective of this research is to investigate the synthesis and self assembly of metal nanoparticles into clusters and larger assemblies. In FY13, the research team determined that the use of entangled photons can permit nonlinear optical spectroscopy measurements on organic molecules at greatly reduced laser intensities. They found that when using entangled photons it was possible to carry out two-photon excited fluorescence with a surprisingly small input flux 10^{10} photons/cm^{2}s compared to 10^{18} photons/cm^{2}s using conventional two-photon techniques. Because the photons are correlated, the absorption rate has linear intensity dependence instead of the normal quadratic dependence observed for classical two-photon absorption. The investigators also found that entangled photons are sensitive to the absorption mechanism of the molecule being probed and that new intermediate states and excitation pathways can be excited by the entangled photons that greatly enhance the absorption process, raising the possibility that strong fluorescence responses will be observed for materials that have very small classical two-photon cross-sections. The research represents a major breakthrough for future biological imaging, where laser damage to the sample limits current practice. In addition, it presents new possibilities and directions in the areas of quantum imaging, lithography, microscopy, and remote sensing.

G. Particle Shape Effects on the Stress Response of Granular Materials

Professor Heinrich Jaeger, University of Chicago, Single Investigator Award

The objectives of this research are 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. Researchers at the University of Chicago have recently measured the stress response of packings formed from a wide range of particle shapes. These measurements included spheres, convex shapes such as the Platonic solids, truncated tetrahedra, and triangular bipyramids, as well as more complex, non-convex geometries such as hexapods with various arm lengths, dolos, and tetrahedral frames. All particles were 3D-printed in hard resin. Initial packing states were established through preconditioning by cyclic loading under given confinement pressure. Stress–strain relationships for axial compression were then obtained at four different confining pressures for each particle type. For each of the shapes, the dependence of the aggregate stiffness on confining pressure was found to obey a power law of the form $E \propto (\sigma_{con})^n$, where n encapsulates the shape dependence (see FIGURE 7). Furthermore, when this shape dependence is parameterized by the particle sphericity, two branches emerge. One includes the faceted, polyhedral geometries that produce packing configurations where particles interact via several different types of contacts, in particular including those with large, rapidly varying contact area under compression. The other contains particles with arms (hexapods, dolos) and, as limiting case of vanishing arm length, the spheres, which can each interact only via point-like contacts.

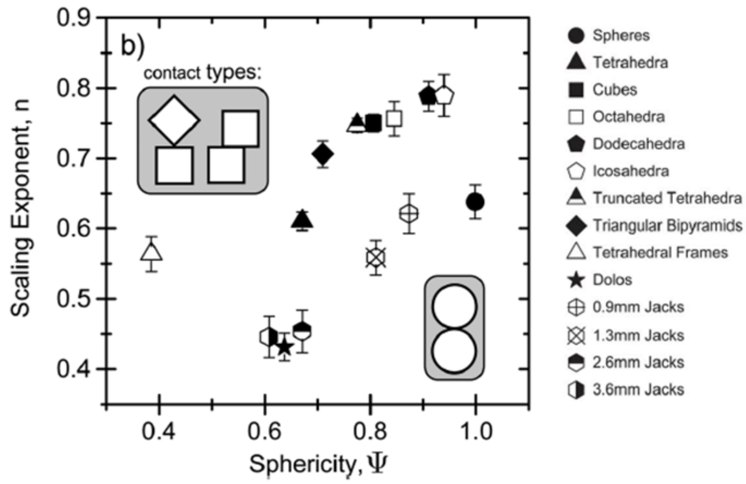

FIGURE 7

Scaling exponent n versus particle sphericity Ψ. The scaling exponents can be separated into two groups which each follow the same trend of increasing n with Ψ. The upper group includes all polyhedral shapes, which can interact via several types of contacts, depending on relative orientation (see inset). The lower group contains shapes with arms, all of which interact via one type of point-like contact, and includes the spheres as limiting, zero arm-length case.

H. Ultra-precise Size Sorting of Microspheres Using Resonant Optical Techniques

Professor Vasily Astratov, University of North Carolina - Charlotte, Single Investigator Award

Researchers at UNC - Charlotte have been investigating the resonant coupling of laser light to the whispering gallery modes of micron-sized polystyrene microspheres immersed in water, with the goal of developing techniques for sorting these spheres into size-matched groups with uniformities on the order of 0.01%. In FY13, experiments utilizing a tunable 50mW semiconductor laser (1100 to 1300 nm wavelength) revealed that laser light propagating down a tapered waveguide can couple strongly with nearby microspheres and exert large forces on select microspheres, propelling them at velocities in excess of 200 um/s. The propelling velocity was found to increase linearly with sphere diameter and appears to be much too high to be explained by the conventional nonresonant scattering forces. It is concluded that these high optical forces are a result of resonant coupling effects, and that they therefore represent a working principle for size sorting of super-monodisperse microspheres to an unprecedented small standard deviation of ~ 1/Q. This is important for the development of novel resonance-based photonic devices for such applications as spectral filters, sensors, micro-spectrometers and laser resonator arrays.

I. Novel Deformation-Induced Nanoscale Mixing Reactions

Professor John Perepezko, University of Wisconsin-Madison, Single Investigator Award

The objective of this research is to identify the governing process and control variable relationships during deformation-induced reactions in structural alloys. Researchers at the University of Wisconsin-Madison recently demonstrated unique intermixing behavior during deformation induced reactions. During the repeated cold rolling of Cu/Ni and Ag/Pd multilayers, a solid solution forms at the interfaces as nanoscale layer structure with a composition that replicates the overall multilayer composition. The interfacial mixing behavior was investigated by means of X-ray diffraction and scanning transmission electron microscopy, and the intermixing behavior of the Cu/Ni and Ag/Pd multilayers was found to be distinct from thermal diffusion processes (see FIGURE 8). More specifically, under cold rolling, there existed a plateau in the composition profile for the solid solution zone. The macroscopic average composition of the plateau was found to be approximately equivalent to the overall multilayer composition. Observations and analysis using scanning transmission electron microscopy established that the local alloying with composition variations occurs in a zone between the pure components, which means that the mechanism for the athermal alloying reaction induced by cold rolling is fundamentally different from the usual thermally activated diffusion processes.

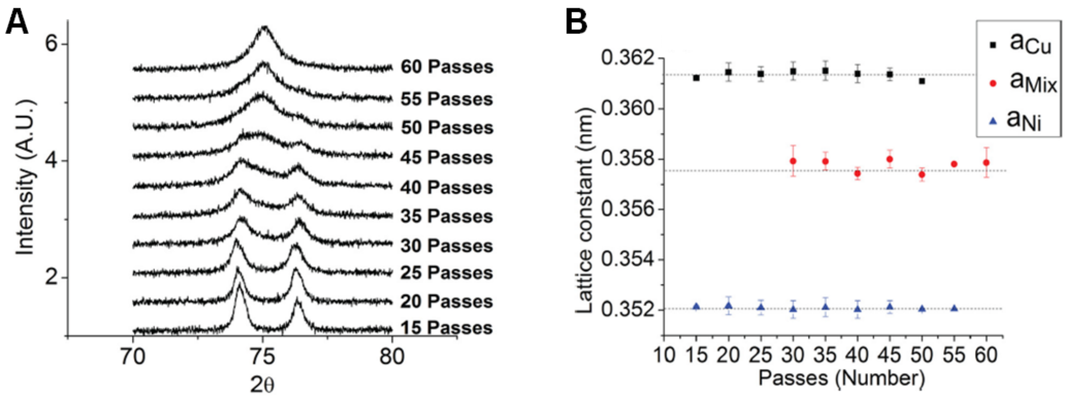

FIGURE 8

Interfacial mixing behavior between Ci/Ni and Ag/Pd multilayers. (A) Evolution of X-Ray diffraction between 70º and 80º 2θ with increasing deformation for the $Cu_{60}Ni_{40}$ multilayer sample. The peaks are the (220) peaks of the Cu, solid solution, and Ni from left to right, respectively. The pattern intensity for each pass number is normalized. (B) Summary of lattice constant behavior with increasing deformation for Cu/Ni multilayer. The reference lines from top to bottom are Cu, solid solution $Cu_{60}Ni_{40}$, and Ni, respectively.

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. Large Strain Extrusion Machining of Metal Foils and Sheet

Investigators: Professors Kevin Trumble and Srinivasan Chandrasekar, Purdue University, Single Investigator Award
Recipient: General Motors Research and Development Center

The objective of the ongoing research, which led to a recent technology transfer, is to advance the deformation processing science of hexagonal close packed (HCP) metals, such as Ti- and Mg-alloys, by employing the 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 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 9). This process can be 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.

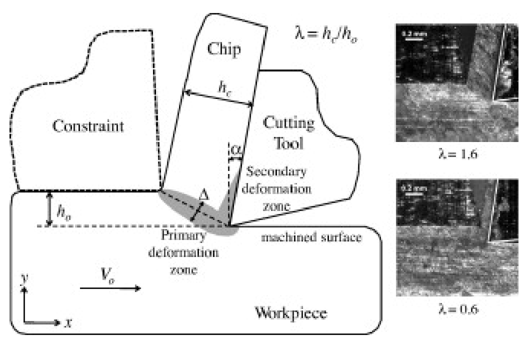

FIGURE 9
Plane-strain LSEM showing parameters. Inset shows images of process for two constraint levels.

In FY13, these results transitioned to General Motors in FY13, and will be used in studies to make and use lighter materials to meet with government Corporate Average Fuel Economy (CAFÉ) standards. The single-step LSEM process offers the possibility of making Mg-alloy sheet product quickly and economically, and GM is investing in research and development to expand and scale-up the results from Purdue.

B. Point Defect Reduction in Long Wavelength Infrared Materials via Surface Engineering

Investigator: Professor Joanna Millunchick, University of Michigan, Single Investigator Award
Recipient: ARL Sensors and Electron Devices Directorate (ARL-SEDD)

The objective of this research is to study the role of surface structure on the injection of defects in very low band gap materials, namely InAsSb that can be used in long wavelength (8-12 μm) infrared imaging. One important aspect to the successful implementation of InAsSb is the control of the composition and microstructure of this material. To accomplish this, the PI adopted an approach that closely couples experimental observation with ab initio computation and modeling. The PI currently is examining the role of a Bi surfactant on the composition and microstructural quality of InAsSb. These results transitioned to ARL-SEDD, which is collaborating with Professor Millunchick's. Characterization and analysis (shown in Figure 10) of these samples was conducted both at UM and ARL. FIGURE 10A shows a series of (004) triple axis x-ray diffraction (XRD) patterns that indicate the out of plane lattice parameter of the InAsSb film decreases as a function of Bi overpressure. Rutherford Backscattering (RBS) proves that no Bi was incorporated into the films, thus it is the Sb concentration that decreased with increasing Bi (see FIGURE 10B). Clearly, the presence of Bi on the surface frustrated Sb incorporation. There are indications in the RBS data that the compositional homogeneity varies in these samples. Prof. Millunchick's team is collaborating with the ARL to explore further details in this area.

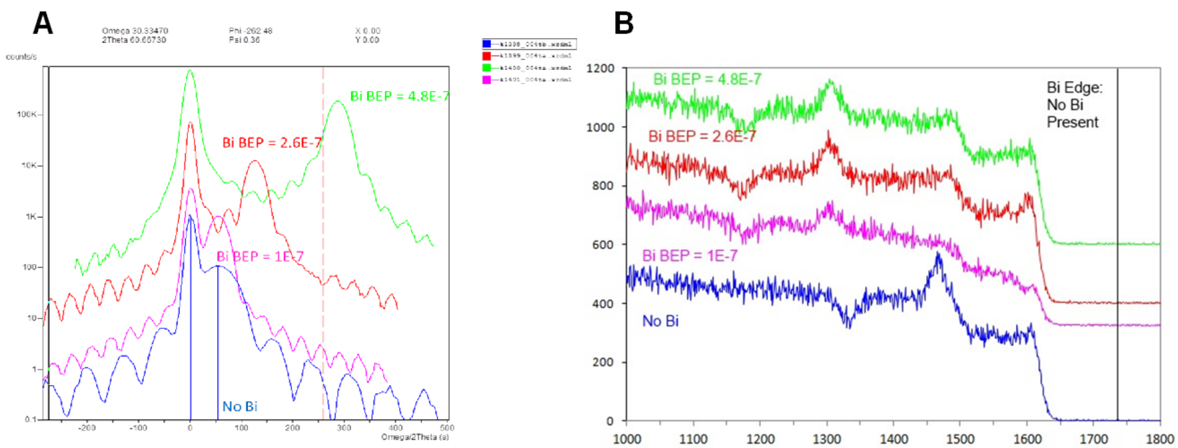

FIGURE 10

XRD and RBS characterization and anaylsis of InAsSb films. (**A**) A series of XRD scans for InAsSb films grown under different Bi overpressures. (**B**) A series of RBS spectra of the same samples.

C. Applications of SMM-THz Spectroscopy for Chemical Sensing

Investigator: Professor Frank De Lucia, Ohio State University, Single Investigator Award
Recipients: Applied Materials

The goal of this research at Ohio State University is to extend sub-mm THz spectroscopy techniques to the sensing of large molecules. Under a 'Long Horizons" grant from the Semiconductor Research Corporation (on behalf of its member industries IBM, Texas Instruments and Applied Materials), Prof. De Lucia's team is being supported to implement sub-mm THz chemical sensors in a low cost CMOS format. In addition, these results have transitioned to Applied Materials which is collaborating with the academic researchers to ascertain the feasibility of utilizing THz techniques for diagnostic and process control in semiconductor plasma reactors.

V. ANTICIPATED ACCOMPLISHMENTS

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

A. Epitaxial Semiconducting Heusler Alloy Heterostructures

Professor Chris Palmstrøm, University of California, Santa Barbara, Single Investigator Award

The objective of this research is to explore composition -processing- defects- structure- physical property relationships (electronic/optical) in multifunctional epitaxial semiconducting half Heusler alloy thin films and heterostructures. It is anticipated that in FY14, the research team will demonstrate the integration of lattice matched single crystal epitaxial CoTiSb with $In_{0.52}Al_{0.48}As$/InP(001) heterostructures and NiTiSn with MgO(001), among others. Materials such as CoTiSb, NiTiSn are expected to be semiconducting despite being composed entirely of metallic constituents. Theoretical calculations predict an indirect Γ-X bandgap of ~1 eV for CoTiSb. The investigator will employ atomic level growth control methods such as molecular beam epitaxy to grow these films/heterostructures for the first time. Temperature dependent transport measurements, photoluminescence and optical absorption etc. will be carried out to determine the semiconducting behavior (*e.g.*, mobility, carrier density) in these Half Heusler alloy films. If successful, this research could lead to develop future DoD applications such as spintronic devices for sensors, encryption, quantum computing, as well as novel thermoelectric devices.

B. Time-Dependent Dielectric Breakdown of Surface Oxide During Field Assisted Sintering

Professors Klaus van Benthem and Troy Holland, University of California - Davis, Single Investigator Award

The objective of this research is to evaluate the five proposed mechanisms by which electrical fields can enable the accelerated consolidation of materials during field assisted sintering: (i) local Joule heating at grain boundaries; (ii) generation of interfacial stress through applied electrical fields; (iii) nucleation of point defects; (iv) dielectric breakdown; and (v) interaction of the electrical field with space charge layers. It is anticipated that in FY14, the researcher's findings on real-time dielectric oxide breakdown (via in situ TEM observations) will be expanded to quantify the time-dependency and further elucidation important underlying mechanistic densification phenomena, such as the formation of local conductive pathways between individual particles.

C. Spin Manipulation in 2D Semiconductors

Professor Roland Kawakami, University of California - Riverside, REP Award

Because of their high surface sensitivity, 2D semiconductors present unique opportunities for controlling spin-dependent phenomena and exploiting magnetic proximity effects. The goal of this research is to characterize germanane (*e.g.*, 2D germanium with hydrogen termination) and monolayer MoS_2 systems. Both are direct gap semiconductors with optical selection rules that permit the optical injection and detection of conduction electron spin polarization, which similar to GaAs makes probing of the spin transport and dynamics relatively straightforward. Monolayer MoS_2 is of particular interest because it can produce large spin-orbit fields that can be used to manipulate and control the spin current. Together they provide some interesting device prospects. It is anticipated that in FY14, the research team will demonstrate spin injection into these 2D systems and identify unique spin properties and effects that can be exploited in the development of new spin-based electronic devices.

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 2013* is to provide information on the programs and basic research supported by ARO in FY13, 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 FY13.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mathematical Sciences Division supports research 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. This research 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 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, leverages, and transitions research within its Program Areas with Army scientists and engineers, such as the ARL Weapons and Materials Research Directorate (ARL-WMRD) and ARL Sensors and Electron Devices Directorate (ARL-SEDD), and also other DoD agencies such as 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 also coordinates its research portfolio with the 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 also complements 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 its research portfolio with the Physics Division to pursue fundamental research in quantum control. The Division 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

The Mathematical Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY13, the Division managed research 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 FY13, 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) Multiscale Modeling/Inverse Problems, (ii) Fundamental Laws of Biology, and (iii) Modeling Intermediate Timescales. Within these thrusts, basic, high-risk, high pay-off research efforts are identified and supported to achieve the program's long-term goals. Research in the Multiscale Modeling/Inverse Problems Thrust 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 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. Efforts in the Modeling at Intermediate Timescales Thrust attempt to develop new methods of modeling of biological systems, as well as their control, at intermediate timescales.

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 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 Sciences Division for FY13 were $28.4 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY13 ARO Core (BH57) program funding allotment for this Division was $4.5 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 $8.7 million to projects managed by the Division. The Division also managed $11.7 million of Defense Advanced Research Projects Agency (DARPA) programs, $0.6 million of Minerva Research Initiative programs, and $1.2 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, $1.0 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 creation, leadership, and management of 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 FY13 (*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 FY13 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 FY13, the Division awarded 15 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 approaches for quantum stochastic differential equation approximation, create new high-order accurate front-tracking methods, develop a framework for consensus approximation for multi-agent vehicle networks as a distribution-free learning problem, and to develop new mathematical techniques and models that allow for an understanding of ecological processes on relevant timescales with transient dynamics. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Rosalind Allen, University of Edinburgh; *Nutrient-cycling Microbial Ecosystems: Assembly, Function and Targeted Design*
- Professor Clinton Dawson, University of Texas - Austin; *Numerical Upscaling of Flow and Transport Through Obstructed Regions Over a Broad Range of Reynolds Numbers*
- Professor Lisa Fauci, Tulane University; *Locomotor Stability in a Model Swimmer: Coupling Fluid Dynamics, Neurophysiology and Muscle Mechanics*
- Professor James Glimm, SUNY at Stony Brook University; *Mathematical Models and Advanced Numerical Methods for Complex Flows and Structures*
- Professor Alan Hastings, University of California - Davis; *Dynamics at Intermediate Time Scales and Management of Ecological Populations*
- Professor Andrew Kurdila, Virginia Polytechnic Institute & State University; *Distributed Consensus Learning and Approximation for Geometric and Abstract Surfaces*
- Professor Xiaolin Li, SUNY at Stony Brook University; *Verification and Validation of the Spring Model Parachute Air Delivery System in Subsonic Flow*
- Professor Hideo Mabuchi, Stanford University; *Approximation of Quantum Stochastic Differential Equations for Input-Output Model Reduction*
- Professor David Nualart, University of Kansas; *Stochastic Evolution Equations Driven by Fractional Noises*
- Professor Joshua Plotkin, University of Pennsylvania; *Inferring Microbial Fitness Landscapes*
- Professor Julio Rossi, University of Alicante-Ministerio De Universidades E Investi; *Nonlocal Operators for Free Boundary Optimization*

- Professor Boris Rozovsky, Brown University; *Nonlinear Stochastic PDEs: Analysis and Approximations*
- Professor Guillermo Sapiro, Duke University; *Structured and Collaborative Geometric Signal Models for Big Data Analysis*
- Professor Alexander Tartakovsky, University of Southern California; *General Multidecision Theory: Hypothesis Testing and Changepoint Detection*
- Professor Byron Wallace, Brown University; *Sociolinguistically Informed Natural Language Processing: Automating Irony Detection*

2. Short Term Innovative Research (STIR) Program. In FY13, the Division awarded two new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to create a mathematical theory to determine the structure of an unknown gene network, and to develop a robust and reliable circadian phase estimation scheme for model generation and control design. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Desmond Lun, Rutgers, The State University of New Jersey - Camden; *Identification of Gene Networks: An Approach Based on Mathematical Modeling*
- Professor John Wen, Rensselaer Polytechnic Institute; *Light-based Modeling and Control of Circadian Rhythm*

3. Young Investigator Program (YIP).

No new starts were initiated in FY13.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY13 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *21st International Meshing Roundtable Conference*; San Jose, CA; 7-10 October 2012
- *18th U. S. Army Conference on Applied Statistics;* Monterey, CA; 24-26 October 2012
- *Dynamics Days 2013;* Denver, CO; 2-6 January 2013
- *International Conference on Difference Schemes and Applications;* Moscow, Russia; 27-31 May 2013
- *International Symposium on Fractional PDEs: Theory, Numerics and Applications;* Newport, RI; 3-5 June 2013
- *36th Conference on Stochastic Processes and their Applications*; Boulder, CO; 29 July - 2 August 2013
- *International Conference on Computational Cell Biology: From the Past to the Future*; 14-16 August 2013

5. Special Programs. In FY13, 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 Mathematical Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Model Classes, Approximation, and Metrics for Dynamic Processing of Urban Terrain Data. This MURI was active from FY07-FY13 and was led by Professor Andrew Kurdila of the University of South Carolina. The goal of this research was to develop theory, algorithms, software, and experiments for the highly compressed synthesis of urban terrain maps from dynamic point cloud sensor data. The specific technical goals were (i) to capture high-order topology through implicit representation of surfaces, (ii) to develop multiscale and adaptive algorithms that enable various resolutions of the rendered surface governed by the local density of the point clouds, (iii) to derive algorithms for fast computation of signed distances to the terrain surface thereby giving field of view from specified observation points, (iv) to derive fast and efficient methodologies for the use of dynamic point cloud measurements for the navigation and control of autonomous vehicles in three dimensions, and (v) to develop change detection theory and methods that employ point cloud observations taken at different times.

By the end of this project in January 2013, the MURI team had successfully developed a compression engine for terrain point cloud data. This engine uses the novel approach ("Hausdorff Tree Method") of measuring distortion and determining bit allocation by the Hausdorff metric (see FIGURE 1). The encoding generates an occupancy tree for dyadic cubes in Euclidean space for the point cloud data and then assigns a planar or quadratic fit on each cube. The performance of the local fit is measured locally in the Hausdorff metric. The occupancy tree is then pruned to balance the local performance on each cube. This gives a nonlinear partitioning of Euclidean space into dyadic cubes, each of which has an associated linear or quadratic polynomial. The encoder then assigns bits to determine the occupancy tree and bits to determine each of the polynomials on the terminal leaves. The result is a compression of the original point cloud into a succinct progressive bitstream. At the beginning of the project in FY07, the compression ratio of 100:1 was considered quite difficult to attain but was accepted as a goal. At the end of the project in 2013, compression ratios ranging from 100:1 to 500:1 were achieved in computational experiments for a variety of types of urban terrain. At these compression rates, the essential geometry and topology of the underlying terrain surface are preserved and high quality reconstruction can be achieved by decompressing the compressed file.

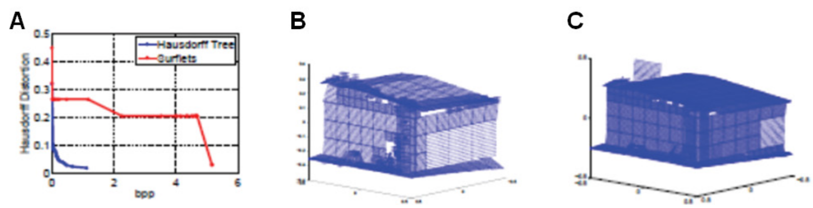

FIGURE 1

Hausdorff Tree method for encoding point cloud observations. (A) Comparison of the Hausdorff Tree Method with the Surflets Method of Chandrasekaran, et al.; the Hausdorff Tree Method achieves superior Hausdorff error with far fewer bits in the final encoding. (B) Hausdorff tree reconstruction with 1 bit/point. (C) The Surflets Method with 1 bit/point fails to capture the window of the house and does not adequately prune the roof.

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 effort 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 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.

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 Rakesh Nagi 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 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.

During the fourth year, the MURI team made several notable accomplishments. The team developed and refined an overall system concept for human-centered information fusion and information processing architecture. They developed a test and evaluation approach involving an evolutionary approach that proceeds from "truthed" synthetic hard and soft data to human in the loop campus based experiments. The team successfully developed object classification algorithms that use fused 2D and 3D video and 3D flash lidar data. Human-computer interaction for improved sense-making was a major research component in the fourth year and included scenario development, meta-data generation and analysis of requisite cognitive tasks and associated workload for sense-making, visualization for distributed sense-making study, and prototype implementation of human-computer interaction to support situation analysis of hard/soft data. A supporting infrastructure for integration of emerging algorithms was developed. A taxonomy for characterizing the human as a sensor and uncertainty characterization under environmental and observer characteristics—both of which are needed for source characterization of soft (human-based) data— were developed. Finally, the team extended a previously developed infrastructure for 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. Hard sensor processing techniques and a system for processing text messages are in the process of transitioning to ARL-CISD and ARL-SEDD.

6. 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.

7. Measuring, Understanding, and Responding to Covert Social Networks: Passive and Active Tomography. This MURI began in FY10 and was awarded to a team led by Professor Joseph Blitzstein at 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.

In its first two years, the MURI team 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. This theory enables one to make trade-offs between algorithmic performance and computational requirements.

In the third year of this effort, the MURI team used the previously developed signal detection theory for embedded insurgent sub-networks as a basis to (i) develop domain-specific models that characterize both background and foreground networks, taking prior information into account and (ii) develop scalable algorithmic frameworks for implementing optimal sub-network detection procedures with respect to these and other models. The team introduced a foreground model for sub-networks in which the total number of such sub-networks can grow with the overall size of the network. This was the first result showing that maximum likelihood estimation of group membership is consistent in this setting, meaning that true group memberships can be estimated with vanishingly small error as the size of the network becomes large.

8. 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.

9. 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.

10. 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.

11. 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 FY13.

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 FY13, the Division managed five new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of two Phase I contract, and three Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications, including the development of numerical methods and algorithms for predictably-accurate treatment of boundary conditions in electromagnetic and other wave-dominated phenomena that can be distributed within standard high performance computing libraries, highly scalable random number generators for use on multiple parallel computing architectures, and new methods for near-real time estimation of model parameter values from measured data for improved model performance and prediction.

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 FY13, the Division managed 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. Complex Phenomena in Stochastic Filtering. The objective of this PECASE, led by Professor Ramon van Handel of Princeton University, is to investigate conditional phenomena in probability theory and complexity of stochastic filtering. A number of complex phenomena in stochastic filtering theory will be investigated, where fundamental advances in mathematical understanding could potentially enable significant progress in the applicability of stochastic filtering to complex systems.

The research focuses on four areas where complexity is manifested in different ways: (i) complexity of mathematical filtering in spatially extended systems; (ii) mixing times and quantitative analysis of stochastic filters with emphasis on exploiting reversibility, functional inequalities, and the investigation of prototypical model systems; (iii) necessary and sufficient conditions for ergodicity and stability of quantum filters for applications in quantum information science; and (iv) stochastic analysis of optimal decision processes with partial observations in complex environments. Professor van Handel will develop new mathematical theory for conditional distributions as functions of time and spatial variables that involve the large-scale structure and ergodicity of filtering problems in order to understand the challenge of complex phenomena and high dimensionality in stochastic filtering. Stochastic models that are conditioned on observed data will be viewed as inhomogeneous Markov processes in random environments. The major approaches include: (a) developing ergodic structures for "random" systems; and (b) showing that these ergodic structures are inherited from their unconditional counterparts. Particular approaches of interest include Dobrushin-Shlosman mixing coefficients (as developed for the investigation of decay of correlations in random fields), dimension-free functional inequalities (of Poincaré or log-Sobolev type), and non-Markov ergodic theory for projections.

Advances in this area will motivate new mathematical problems at the foundation of stochastic filtering theory, and could hold the key to the next generation of filtering technology for complex and uncertain systems that play important roles in quantum information processing, quantum control, and decision sciences that will provide the scientific foundation for developing revolutionary capabilities for DoD and the Army.

2. The Computational and Neural Basis of Reinforcement Learning in Multidimensional Environments. The objective of this PECASE, led by Professor Yael Niv at Princeton University, is to explain how selective attention processes are neurally harnessed and computationally processed to enable efficient learning in complex environments.

Current models of reinforcement learning do not scale well to realistic scenarios involving many multidimensional stimuli. In most naturalistic tasks, however, only a few stimuli dimensions are relevant for obtaining reward and the majority can be safely ignored with no performance costs. Focusing attention on only the relevant dimensions can thus allow efficient reinforcement learning. The first goal of this project is to use functional neuroimaging to investigate whether neural reinforcement learning processes operate on a filtered representation of the environment that focuses on some dimensions and ignores others or whether they are pre-attentive. The next goal seeks to discover how the brain learns what stimulus dimensions are relevant to a particular task by developing and testing computational models of the process of learning what to attend to from trial-and-error feedback. The last goal involves developing a novel technique to enhance (or hinder) learning in multidimensional scenarios, by using a model's trial-by-trial predictions about the learner's focus of attention to select the next training example. The knowledge gained from this research likely will provide transformational new understanding of how humans achieve efficient learning in complex everyday tasks. This may ultimately provide the foundation for a practical means by which training examples can be tailored to individual learning strategies to accelerate learning in complex, multidimensional environments.

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 FY13, the Division managed two new DURIP projects, totaling $0.3 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of evolution of associative memory in bacterial populations, and innovative processing of Big Data.

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 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 2). 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.

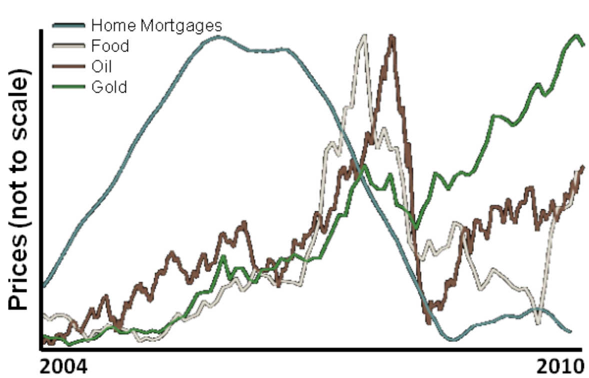

FIGURE 2

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 that 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 applied 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 funded and/or monitored by the Mathematical Sciences Division.

A. Inferring Microbial Fitness Landscapes

Professor Josh Plotkin, University of Pennsylvania, Single Investigator Award

The objective of this research is to develop mathematical models of the "fitness landscape" and analyze how it influences evolutionary dynamics. In FY13, the investigators made significant discoveries in a number of areas related to the fitness landscapes of microbes and proteins. In one sub-project, they studied the role of epistasis in protein evolution (epistatis refers to non-additive interactions among loci that collectively determine the fitness of an organism). By relaxing the normal unrealistic assumption that all amino acids observed at a given position in a protein alignment have equal fitness, they found that the observed patterns of amino-acid diversity at each site are jointly consistent with a non-epistatic model of protein evolution. In another project, the team used the NK mathematical model of fitness landscapes to examine how natural selection biases the mutations that substitute during evolution, based on their epistatic interactions. The team found that, even when beneficial mutations are rare, natural selection strongly biases the types of mutations that will become established; more importantly, the form of these biases changes substantially throughout the course of adaptation. In particular, epistasis is less prevalent than the neutral expectation early in adaptation and much more prevalent later, with a concomitant shift from predominantly antagonistic interactions early in adaptation to synergistic and sign epistasis later in adaptation; these same patterns were confirmed when reanalyzing data from a recent microbial evolution experiment (see FIGURE 3). A third project highlights the role of deleterious mutations during adaptation. Surprisingly, for many populations undergoing adaptation, fitness is expected to decrease in the short term, even though the expected fitness must eventually increase to its equilibrium value in the long term.

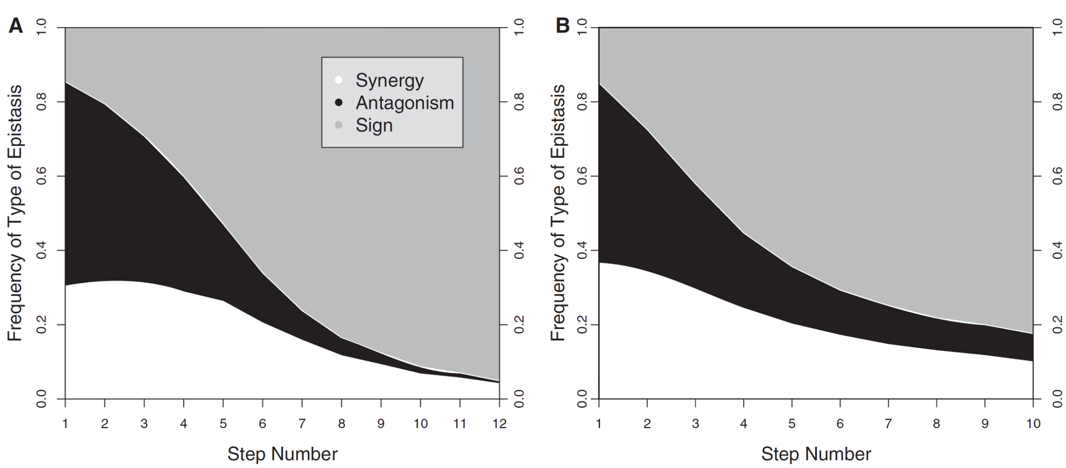

FIGURE 3

Prevalence of epistasis. The panels illustrate the prevalence of synergy, antagonism, and sign epistasis among pairs of consecutive substitutions along adaptive walks on NK landscapes, (A) K=1, (B) K=5, which are characterized by an abundance of antagonism early in adaptation and sign epistasis late in adaptation. For both panels, N=20 and A=2, where N defines the number of sites, each of which can assume any of A alleles. When K > 0, the fitness contribution of a site depends on its own allele as well as the alleles at K other sites.

These results are important because they challenge two standard ways of thinking about evolution. First, although most studies in the literature on the genetics of adaptation declare by fiat that deleterious fixations cannot occur, this work shows that a general theory of adaptation must accommodate deleterious substitutions to achieve predictions that are even qualitatively correct. Second, the literature persistently assumes that fitness is expected to increase when a population is below the equilibrium mean fitness and decrease when a population is above the equilibrium mean fitness; in fact, fitness is expected to decrease when a population starts at its equilibrium mean fitness. The standard intuition fails because it erroneously treats the approach to equilibrium as a deterministic process around the equilibrium mean, whereas in fact a stochastic treatment is required.

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, which 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 in these studies. 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 has been focusing 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. An application of optimal quantum control to canonical phase measurement via a contour plot of the Wigner wave function is shown in FIGURE 4.

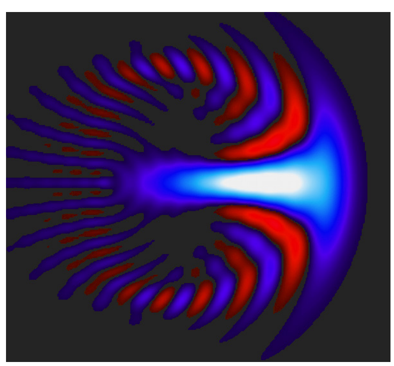

FIGURE 4

Contour plot of the Wigner function for a canonical phase state with 20 photons/phonons. This image illustrates an application of optimal quantum feedback control to canonical phase measurement, enabling state measurements in an open quantum system.

Initial studies are underway in all aspects of the research, theoretically and in the laboratory. Specifically, the initial steps were implemented to develop an experimental and theoretical program that addresses the dynamics of open quantum systems in the presence of coherent feedback control. 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.

In FY13, significant advances in efficient entanglement generation using stochastic control were achieved. In particular, computational verification of proposed algorithmic improvements using super-operator algebra were performed to study the effects of correlated randomness. Powerful multi-parameter optimization tools were used to beat the effectiveness of the random unitary approach. It had been proven that complete control can be exerted (even without complete controllability) if and only if the initial state of a two level quantum system is pure in a coherent feedback scheme. It was also established during FY13 that it is possible to protect an arbitrary, unknown, encoded quantum state against the environment arbitrarily well via a Zeno effect with arbitrarily weak measurements. It was also shown that the concept of entanglement susceptibility can lead to the emergence of area laws for bi-partite quantum entanglement in systems ruled by local gapped Hamiltonians. In future years, it is expected that realistic coherent control schemes will be identified that would be aggressive enough for de-coherence control. 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. Robust Multi-Sensor Classification via Jointly Sparse Representation

Professor Trac Tran, Johns Hopkins University, Single Investigator Award

The goal of this research is to develop a sparse-representation classification (SRC) framework that can capture the rich complex correlation structures existing in real-world data from physics-based sensors. The correlation structures between sensors are captured via structured sparsity priors by assuming the underlying sparse vectors associated with these data signals share a common sparsity pattern (a realistic assumption in practice). Three specific models have been explored thus far: (i) kernel-based joint sparsity; (ii) bilinear mixture models via joint sparse and low-rank representation; (iii) probabilistic graphical model to explicitly mine the conditional dependencies between distinct sparse features from multiple sensors.

For the kernel-based joint sparsity model, the PI has demonstrated that it works exceptionally well for hyperspectral imaging. On the basis of this result, he proposed a new hyperspectral imaging (HSI) classification technique based on sparse representations in a nonlinear feature space induced by a kernel function. The spatial correlation between neighboring pixels is incorporated through a joint-sparsity model. Experimental results on Airborne Visible/Infrared Imaging Spectrometer (AVIRIS) and Reflective Optics System Imaging Spectrometer (ROSIS) HSIs show that the kernelization of the sparsity-based algorithms improves the classification performance compared to the linear version. The proposed algorithm has comparable or better performance in comparison to recent spectral-spatial single classifiers such as state-of-the-art Support Vector Machine with Composite Kernels. The PI extended the current linear mixture model (LMM) sparse regression methods to bilinear mixture model (BMM) methods. The BMMs introduce additional bilinear terms in the LMM in order to model second-order effects. To solve the abundance estimation problem for the BMMs, the PI proposed sparsity-based abundance estimation using two dictionaries: a linear dictionary containing all the pure endmembers and a bilinear dictionary consisting of all the possible second-order endmember interaction components. The abundance values are estimated from sparse codes associated with the linear dictionary. To exploit spatial data structure when adjacent pixels are nearly homogeneous, the PI has employed a joint-sparsity (row-sparsity) model to enforce structured sparsity of the abundance coefficients (see FIGURE 5). Since the joint-sparsity model is a strict assumption that can cause aliasing artifacts in pixels that lie on the boundaries between regions, a low-rank-representation model, which seeks the lowest rank representation of the data, was introduced to capture the spatial data structure. Simulation results demonstrate that the proposed algorithms provide much enhanced performance compared with state-of-the-art techniques in the field.

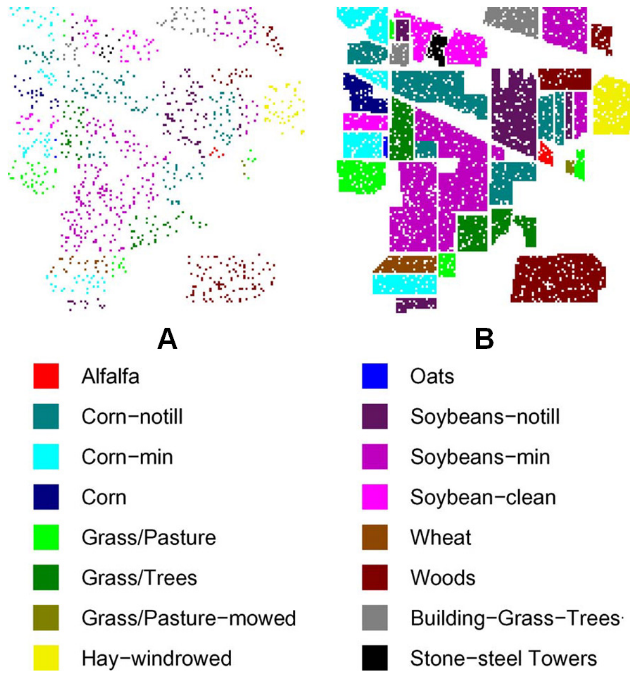

FIGURE 5

Training situation for hyperspectral imaging (HSI). These maps illustrate (**A**) available data, containing only 5% of the content of (**B**) ground truth. After training on data of this genre, full reconstructions can be created using very limited samples (common in practical situations).

D. Multiscale Modeling of Cementitious Materials

Professor Ram Mohan, North Carolina A&T University, PIRT Award

Advanced cementitious materials such as mortar and concrete, both in original construction and as protective retrofitted quick pour concrete panels combining traditional cementitious mortar or concrete with additional functional materials (*e.g.*, nanomaterial fillers and fibers), have the potential to provide effective protection against deadly force and insurgent attack that includes direct projectiles and shock from blast waves. Further enhancement to the design, development, and understanding of the shock and impact resistant properties of cementitious materials requires "materials by design" techniques/concepts rather than a trial-and-error approach to material processing. Macroscopic constitutive models, both empirical and mechanistic, fail to quantify the effects of various nanostructures on blast and ballistic-resistant characteristics of advanced concrete. Advanced computational algorithms and appropriate physics-based simulations are required that effectively include the representative material constitutive behaviors at each length scale, from the lowest length scale and building and bridging to the next length scale for the macroscopic structural configurations.

The objective of this research is to evolve a multi-scale nano to continuum modeling methodology that links and transcends the different length scales from the nano length scale material constituents to the macroscopic deformation and failure behavior through appropriate length scale models and their coupling; these will drive the multi-scale modeling, design, and development of advanced cement material for force and materiel protection from direct, ballistic, and shock threats in theater and homeland security. The technical approaches have focused on multi-scale computational predictive property modeling and multi-scale computational modeling of deformation and failure with a focus on multi-scale computational modeling methodology, coupling the modeling analysis at the different length scales.

A robust molecular dynamic (MD) modeling framework has been developed with necessary parameters for both unhydrated and hydrated cement molecular structures. Material stiffness properties have been successfully computationally predicted for unhydrated and hydrated cement components. Mechanical stiffness properties obtained from MD modeling have been validated against other computational and experimental literature data at various length scales. Scale effects have been studied and documented across mechanical properties at different length and size scales. The effect of high thermodynamic pressure states on mechanical stiffness has also been successfully studied and compared. The researchers developed the first-ever computational material modeling analysis methodology that assesses the compressive, adiabatic effects, and deformation for cementitious materials based on molecular structure (see FIGURE 6).

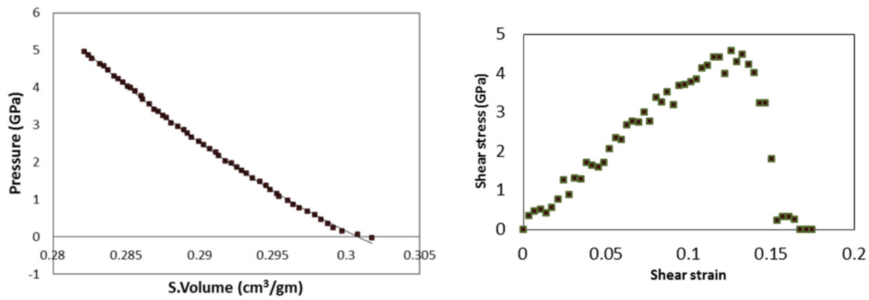

FIGURE 6

Computational modeling analysis methodology based on cement molecular structures to understand the compressive, adiabatic, and deformation effects. This methodology provides an improved understanding of the influence of changes on the expected deformation behavior of materials, and the computational determination of such changes based solely on the material molecular structure at the nanoscale level.

Using computational modeling, the researchers successfully analyzed and demonstrated the methodology to develop isothermal pressure–density (specific volume) dynamic effects in CSH Jennite. Computational modeling has successfully demonstrated the methodology to model the shearing deformation and shear strength–shear strain behavior, and has determined the ultimate shear strength for CSH Jennite. At the microscale, the effect of degree of hydration on material bulk properties has been successfully modeled. Representative Volume Element (RVE) Methods have been developed and have been matched to simulations from the Asymptotic Expansion Homogenization (AEH) code at ARL-CISD, that indicated reasonable agreement in simulating the mechanical response of traditional cements (see FIGURE 7). Further work is ongoing to explore the use of NIST's digital micro-structure generator for non-traditional cements and nano-silicate based cements.

	AEH		RVE (KBC)		RVE (PBC)	
	Uniform Strain Bound	Uniform Stress Bound	Uniform Strain Bound	Uniform Stress Bound	Uniform Strain Bound	Uniform Stress Bound
K	30.8315	30.8315	28.6356	28.6666	29.6804	29.6804
G	9.8585	9.8505	9.5208	9.5133	9.4398	9.4329
λ	24.2592	24.2645	22.2884	22.3244	23.3872	23.3918
E	26.7270	26.7073	25.7127	25.6973	25.6048	25.5878
ν	0.3555	0.3556	0.3503	0.3506	0.3562	0.3563

FIGURE 7

Effectiveness of AEH methodology and good comparisons to RVE methods for highly heterogeneous cement paste. AEH has been traditionally employed for regular, ordered microstructures. Results show the effectiveness and correctness of the AEH method and code developed by ARL for highly heterogeneous cement paste microstructures.

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. Network-based Hard/Soft Information Fusion

Investigator: Professor Rakesh Nagi, The State University of New York - Buffalo, MURI Award
Recipient: ARL-CISD

The goals of this research are to develop a generalized framework, mathematical techniques, and the design and evaluation methods for fusion of hard and soft information in a distributed (networked) Level 1 and Level 2 data fusion environment. The MURI team has developed and refined the 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.

In FY13, the counter-insurgency (COIN) inspired synthetic hard/soft data set ("SYNCOIN") that was developed for testing and evaluation of results produced by this research team transitioned to several government organizations, including ARL-CISD, the U.S. Navy Space and Naval Warfare Systems Center, and AFRL (see Figure 8).

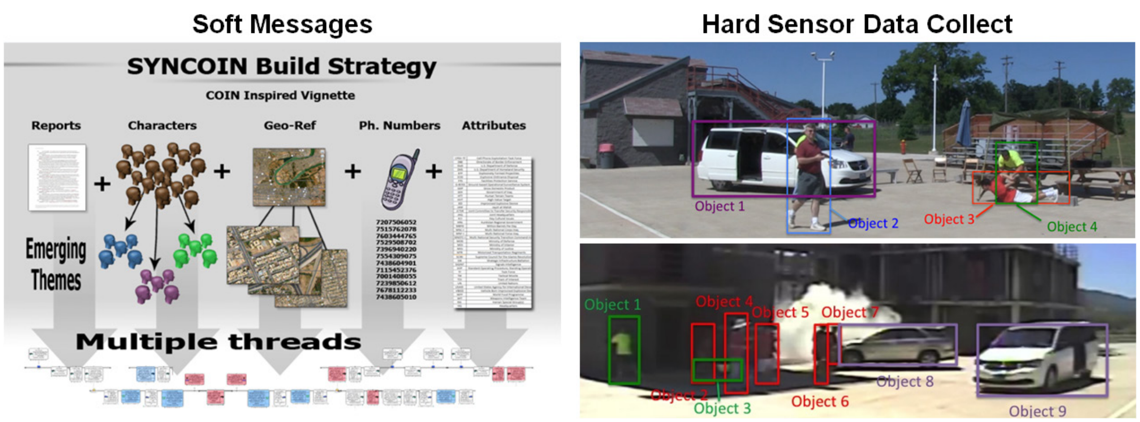

FIGURE 8

Synthetic counter-insurgency data set SYNCOIN. This data set is a combined hard and soft data set, including interlaced scenarios, 600 text messages, and synthetic hard data, the content of which is realistic counter-insurgency situations modeled on actual events. SYNCOIN has non-linear, intertwined, out-of-sequence data and realistic confounding elements (background noise). Linguistic and human observational uncertainty have been built into the data set.

Through the defense contractor Qinetiq, the U.K. Ministry of Defense is using SYNCOIN for testing algorithms for fusion of electro-optical (EO)/infrared (IR) data and text. Defence Research and Development Canada (DRDC) is using SYNCOIN along with additional results on uncertainty representation (conversions between probability theory and possibility theory) provided by this MURI for testing DRDC-developed algorithms for fusion of text. The software package "Tractor" for processing text messages in multiple stages and common referencing has been transitioned to ARL-CISD for the Network Science CTA and for in-house use and to SPAWAR (Navy), San Diego, which are using it to convert text data into semantic propositional graphs (semantic descriptions of entities, events and relationships).

B. Complex Simulations: Accurate Prediction and Fast Computation
Investigators: Professors Chien-Fu Wu and Roshan Vengazhiyil, Georgia Institute of Technology, Single Investigator Award
Recipients: ECBC, ARL-CISD, ARL-WMRD, AFRL

The objective of this research is to develop methods to approximate complex computer simulations by easy-to-evaluate metamodels with the potential long-term application of providing faster evaluations and decisions in combat situations. Kriging is the most commonly used metamodel to approximate complex simulation. However, it is computationally intensive and can be numerically unstable for large problems (see FIGURE 9). The approach is to develop an alternative technique using regression models, basis function approximations, and inverse distance weighting (IDW) that can circumvent these problems. The resulting method is called regression-based inverse distance weighting (RIDW). Simulations show that the accuracy is as good as that of kriging (see FIGURE 9A). On the other hand, RIDW is about three times faster than kriging (see FIGURE 9B), which makes it a potentially useful method for large-scale problems. Another new method is being investigated, called overcomplete basis surrogate models (OBSM), which uses powerful tools in approximation theory and machine learning to obtain metamodels for situations in which the response functions are highly oscillatory and thus cannot be adequately approximated by kriging, which is based on stationary Gaussian process assumption.

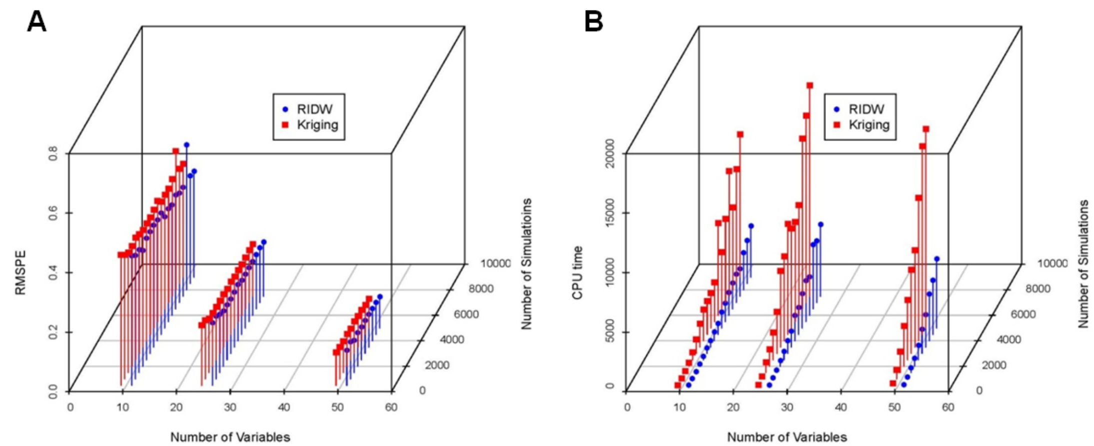

FIGURE 9

Regression-based inverse distance weighting predictor (RIDW). The panels show a comparison of kriging with RIDW: (**A**) RMS prediction error and (**B**) computation time. It can be seen that the prediction performance of RIDW is as good as kriging, yet is about three times

The research team is developing an underlying theory for both RIDW and OBSM, and for the latter to improve the numerical algorithm so that a usable code can be developed. Unlike kriging, these methods are not based on a probabilistic framework and thus, cannot easily generate confidence intervals around the predictions. This is a challenging problem. The research team investigated the possibility of using some heuristic methods using cross-validation errors for constructing confidence intervals. Given that the approach is nonparameteric, the performance and coverage of the confidence intervals were better than those of kriging when dealing with nonstationary problems. Simulations of complex systems have been widely used in physical science, engineering and military applications. Advances in computing, mathematical and physical modeling have allowed very complex systems to be simulated quite accurately but the required computation can be daunting and time-consuming. In situations where an accurate and timely decision has to be made such as in epidemic breakout and urban warfare (*e.g.*, counter-measures for IEDs), an accurate computer output that will take hours or days to produce is rendered irrelevant or useless. Several computationally efficient techniques known as RIDW and OBSM have been developed, which can accurately approximate the simulation code, thus producing the output much faster and enabling real time evaluations and decision making.

In FY13, computer simulation codes for generating experimental designs and fitting blind kriging models were transitioned to ECBC, which is using the code for computer experimental design for sensitivity testing. In addition, a computer code for a new class of designs called nested Latin hypercubes was transitioned to ARL-WMRD, ARL-CISD, and AFRL.

C. Understanding Optimal Decision Making Using Neurophysiological Measures
Investigator: Professor Quinn Kennedy, Naval Postgraduate School, Single Investigator Award
Recipient: U.S. Army Training and Doctrine Command (TRADOC)

While the importance of effectively training decision-makers has increased, current understanding of how military decision-makers arrive at optimal decisions is not well understood and the measurement of decision-making performance lacks objectivity. The use of neurophysiological measures in human-in-the-loop wargames has the potential to fill this gap in knowledge and provide more objective measures of decision-making performance.

In FY13, the PIs developed simulations that measure cognitive flexibility and reinforcement learning. This system was used to explore the development of learning optimal decision-making when all participants begin as naïve individuals. Researchers then used the approach to better understand the transition from exploring the environment as a naïve decision-maker to exploiting the environment as an experienced decision-maker, as assessed by statistical and neurological measures. In addition, the researchers examined decision-making in a dynamic and complex environment using gaze controls and monitoring of brain activity. The team has successfully implemented and synchronized EEG to wargames, with preliminary results of pilot data indicating the validity of the wargames and successful collection of neurophysiological markers (see FIGURE 10).

FIGURE 10

The convoy task simulation. In the simulation, the subject seeks to determine which route to select on the next turn through repeated sampling of routes. The images are screen shots of the convoy task in piloting, a typical subject's view of the task. In these snapshots, the player's last choice caused 100 damage to the enemy (Damage to Enemy Forces) and a loss of -250 to friendly forces (Damage to Friendly Forces), resulting in a trial loss of -150 (not shown). The Accumulated Damage is 2750 (a positive Accumulated Damage value is desirable to the player). The assumption is that the subject maintains some estimate of the value similar to Accumulated Damage for each route and updates the estimate after each trial. The accuracy of the estimate will vary between subjects as will the manner in which the subjects incorporate information into their estimate.

Results from these studies have transitioned to TRADOC to explore a potential means of refining procedures supporting more efficient learning and task accomplishment. The work is also of interest to the VA War Related Illness and Injury Study Center (WRIISC) in helping to identify PTSD and TBI. In FY13, transitions to TRADOC and the VA include wargames that measure cognitive flexibility and reinforcement learning, statistical methods to identify optimal decision-making and objectively define and assess the transition from the exploration to exploitation stage, and improved training methods. As examples of the latter, eye-tracking is being exploited to determine which particular information is being used in decision-making and EEG components are clarifying possible reasons for not making the right decision (*e.g.*, boredom, inattention).

D. Designing and Prescribing an Efficient Natural-like Language for Bots

Investigator: Professor Mitch Marcus, University of Pennsylvania, MURI Award
Recipients: ARL-CISD; ARL - Human Research and Engineering Directorate (ARL-HRED)

The goal of this research 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. The SUBTLE program has developed a prototype software system to investigate human-robot interaction using English, to support military designers developing human-bot communication methods.

In FY13, the MURI team successfully demonstrated the operation of an end-to-end prototype 'Bot Language' system and modularized the components of the processing pipeline for rapid re-use and augmentation. The system interprets natural language instructions from a commander (human system user) and converts them into robot actions, and then enables the robot to send video of its view back to the commander with natural language messages describing its activities (demo video at *http://www.youtube.com/watch?v=xTKPUQsGoCA*).

Various results from this research were transitioned to ARL-HRED and ARL-CISD in FY13. A student from the university MURI team visited HRED and did an initial integration of the basic natural language processing (NLP) components into HRED's Symbolic and Subsymbolic Robotic Intelligence Control System (SS-RICS) as a proof of concept. ARL-CISD implemented the Linear Temporal Logic MissiOn Planning (LTLMoP) toolkit from the MURI team into their PackBot running their ROS.

V. ANTICIPATED ACCOMPLISHMENTS

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

A. Robust Multi-Sensor Classification via Jointly Sparse Representation

Professor Trac Tran, Johns Hopkins University, Single Investigator Award

The goal of this research is to develop a sparse-representation classification (SRC) framework that can capture the rich complex correlation structures existing in real-world data from physics-based sensors. It is anticipated that in FY14, the PI will extend his new hyperspectral imaging classification technique to the sparse representation classification (SRC) framework using more sophisticated data models and more discriminative recovery algorithms in the following way. The data models will be improved by designing class-specific dictionaries, one for each type of sensor data. The sparse recovery algorithms will be made more discriminative by incorporating structured priors into the SRC framework. Using class-specific priors, specifically, the spike-and-slab prior widely applied in Bayesian sparse regression in conjunction with class-specific dictionaries is expected to yield an improvement that is greater than the sum of the improvements of each of the two individual items. The anticipated framework will reduce the demand for large samples of training images that are necessary for the success of current sparsity-based classification schemes. The PI will extend his hierarchical dictionary learning method by incorporating structural information in the learning process using the Hi-Lasso norm. The expected benefits of this are two-fold: the label consistency between dictionary atoms and training data is enforced by the group structure and the classification performance is robust to small dictionary size. Using a subspace model, he expects to be able to derive conditions for the hierarchical dictionary learning method that guarantee classification performance and show theoretically the benefit of employing structured sparsity in the dictionary learning. Computational experiments will be performed for both simulated and real applications, including face recognition, digit recognition and object classification.

B. Optimal Control of Stochastic Systems Driven by a Fractional Brownian Motion

Professor Tyrone Duncan, University of Kansas, Single Investigator Award

The objective of this research is to solve stochastic control problems by obtaining explicit optimal controls for linear stochastic systems that are driven by fractional Brownian motions or more generally other stochastic processes with continuous sample paths and that have cost functionals that are quadratic in the state and the control. The solution of control problems for discrete time linear systems with quadratic cost functionals with arbitrary correlated noise is also an objective. These general noise processes both in continuous and discrete time are important in models for many physical phenomena (e.g. turbulence, cognition, telecommunications, and medicine). The continuous time linear system models are obtained from ordinary differential equations, hereditary equations, and partial differential equations. The approach to these problems is a direct method which is relatively elementary and avoids the well known, but difficult methods of Hamilton-Jacobi-Bellman partial differential equations or backward stochastic differential equations. The major scientific challenges for the construction of explicit optimal controls are to determine effective mathematical tools to obtain the optimal controls. The personnel on this grant have developed methods to achieve explicit optimal controls by a direct method. The significance of this research is the construction of explicit optimal controls for a variety of basic models. These results allow for the physical implementation of optimal controllers for such problems as turbulence and telecommunications which should be important applications for the U. S. Army.

It is anticipated that in FY14, an explicit optimal control is expected to be obtained for a quadratic cost and a linear controlled system driven by an arbitrary fractional Brownian motion or more generally, by an arbitrary finite second moment process with continuous sample paths. This will be a significant generalization of the well known results for deterministic systems or systems with Brownian motion that were verified a half century ago.

C. Modeling Subconscious Vision
Professor Daniel Forger, University of Michigan, Single Investigator Award

The objective of this research is to undertake the first detailed modeling study of subconscious vision. For many years, scientists were puzzled at how many "blind" subjects could have subconscious physiological responses to light; for example, light could cause pupil restriction or shift the internal daily (circadian) timekeeping system. About ten years ago, the source of this subconscious vision was discovered; some retinal ganglion cells (RGCs) are intrinsically photosensitive (ipRGCs), even in the absence of inputs from rods or cones. A novel photo pigment, Melanopsin, which has different properties from the pigment controlling conscious vision, causes this photoreception in ipRGCs. Understanding this subconscious vision will lead to treatments to ameliorate the condition of the blind, better adjustment of the body's circadian clock, and a better understanding of vision in general.

It is anticipated that in FY14, the PI will fit and compare several preliminary mathematical models for phototransduction in ipRGCs and will compare these models with responses of ipRGCs to pulses of light, leading to the first biochemical model for ipRGC phototransduction. In addition, the PI will study how Melanopsin is inactivated by light (photoreversal), allowing for novel signaling in the mammalian retina. Furthermore, new model identifiability techniques will be developed and used to form an overall model of the electrical activity of ipRGCs.

D. Globally Convergent Methods for Coefficient Inverse Problems
Professor Michael Klibanov, University of North Carolina - Charlotte, Single Investigator Award

The objective of this research is the development of a globally convergent numerical method for coefficient inverse problems. The fundamentally new feature of this method that distinguishes it from all others is the rigorous guarantee of obtaining a good approximation for the unknown coefficient without any advance knowledge of a good first guess. The PI has proven that initial iterants are guaranteed to contract toward a global solution. Work on this project has established the result theoretically, and work is progressing on implementing it on experimental data, including the case of blind data for objects buried in sand. In FY14, accomplishments are expected in mathematical theory of global convergence and computation of unknown coefficients using this theory.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Joseph Myers
Division Chief
Program Manager, Numerical Analysis

Dr. Harry Chang
Program Manager, Probability and Statistics

Dr. John Lavery
Program Manager, Modeling of Complex Systems

Dr. Virginia Pasour
Program Manager, Biomathematics

B. Directorate Scientists

Dr. Randy Zachery
Director, Information Sciences Directorate

Dr. Bruce West
Senior Scientist, Information Sciences Directorate

Ms. Anna Mandulak
Contract Support

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 2013* is to provide information on the programs and basic research supported by ARO in FY13, 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 FY13.

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, chemically reacting flows, explosives and propellants, and the dynamics 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 mechanical 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 through co-funded efforts with the ARO Chemical Sciences, Materials Science, Mathematical Sciences, Computing Sciences, and Life Sciences Divisions. 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). International research is also coordinated through the International Science and Technology (ITC) London and Pacific offices.

B. Program Areas

The Mechanical Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of projects. In FY13, the Division managed research 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 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 develop new scientific understanding in three major thrusts: (i) multi-dimensional flows in high-dimensional dissipative dynamical systems, (ii) non-smooth and nonequilibrium dynamics, and (iii) creating quantitative understanding of the principles underlying biological agility and force generation. 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. The program considers Army-relevant problems in rigorous approaches to high-dimensional dynamical systems, nonsmooth mechanics, biological agility and force generation, and exploitation of nonlinear and stochastic dynamic interactions at the nanoscale through leveraged DoD programs. High-dimensional nonlinear systems underlie a wide range of Army-relevant research programs from neuroscience to NEMS/MEMS frequency sources to networks, where there is a resounding need for the establishment of a non-perturbative approaches in distributed 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.

This Program Area is spearheading novel exploitation of nonlinear interactions, feedback, information theory, and noise at the nanoscale to enable next-generation infinitesimal information-processing and force generation systems. New research in biomechanics stem from shortcomings in the state-of-the-art in engineered movement systems, in particular intelligent mobility and manipulation systems. At present, engineered capabilities fall far short of organismal systems with regards to (1) exploiting nonlinear amorphous materials and emergent dynamics from active material microstructures, (2) distributed control, information processing, and power density through functional morphology and neuro-muscular-mechanics, (3) dexterity and ease with nonsmooth and nonlinear environmental interactions and locomotion transitions, and (4) balance between energetic efficiency, stability, and robustness in locomotion. Achieving analogous functionality requires new, mathematically rigorous frameworks for nonequilibrium phenomena that not only quantitatively explicate fundamental mechanisms by which organisms achieve integrated functionality but also breaks the state-of-the-art out of the descriptive realm toward a synthetic regime by which such principles may be artificially exploited for a broad range of applications. Thus, the objective of this research thrust is to develop mechanistic understanding to enable synthetic emulation of the principles governing the motion of nature's most remarkably efficient, powerful, and dexterous organismal systems. Mathematically rigorous approaches toward integrative understanding of natural systems is sought to elucidate and emulate principles by which complex yet precisely controlled, multiscale spatiotemporal motion emerges from actuator morphology, hierarchical interaction of heterogeneous and soft active materials, nonlinear neuronal dynamics, large deformation continuum dynamics, and environmental coupling. Broadly, the inception and promulgation of a new mathematical integrative systems theory stemming from recent advances in quantifying the modularity and retroactivity of interconnected bimolecular signal networks will be necessary. A common mathematical language will significantly advance delineating new engineering principles of integrative dynamics while translating novel understanding of biological motion from the perspective of nonequilibrium physics. 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 current knowledge 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 FY13 were $19.0 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY13 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 $2.7 million to projects managed by the Division. The Division also managed $6.9 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 $0.2 million for contracts. Finally, $2.0 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 creation, leadership, and management of 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 FY13 (*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.

The following subsections summarize projects awarded in FY13 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 FY13, the Division awarded 21 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to develop a new approach based on spectral operator theory for determining the global stability and nonlinear dynamics of very high dimensional systems, to determine why the scaling law for size dependence on burning rate decreases below unity and how this guides design of new materials, and to develop a basic understanding of the physical and numerical behavior of the phase-field shear band model. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Itai Cohen, Cornell University; *Investigating Maneuverability, Stability and Control of Flapping Flight*
- Professor Thomas Daniel, University of Washington; *Multiscale Physics and the Dynamics of Muscle*
- Professor Dana Dlott, University of Illinois - Urbana; *Fundamental Mechanisms of Impact Initiation of Reactive Materials*
- Professor Max Donelan, Simon Fraser University; *Control of Energy Minimization in Human Locomotion*
- Professor Maria Fonoberova, AIMdyn, Inc; *Application of Koopman Mode Decomposition Methods in Dynamic Stall*
- Professor Ashok Gopalarathnam, North Carolina State University; *Theoretical and Computational Modeling of Two-Dimensional and Three-Dimensional Dynamic Stall for Rotorcraft Applications*
- Professor Kenneth C. Hall, Duke University; *Minimum Power Requirements and Optimal Rotor Design for Conventional and Compound Helicopters Using Higher Harmonic Blade Root Control*
- Professor Ronald Hanson, Stanford University; *Fuel Studies Using Shock Tube/Laser Absorption Methods*
- Professor David Hu, Georgia Institute of Technology; *Multi-Dimensional and Dissipative Dynamical Systems: Exploration of the Soft-matter Phase Transitions of Fire Ant Aggregations*
- Professor Karl Iagnemma, Massachusetts Institute of Technology; *Measurement and Analysis of Granular Soil Beneath Lightweight Robotic Running Gear*
- Professor Sinan Keten, Northwestern University Evanston Campus; *Validated Predictive Modeling of Engineered Cellulose Materials*

- Professor Chad Landis, University of Texas at Austin; *An Integrated Experimental and Modeling Study of Ductile Fracture*
- Professor J. Michael McCaffery, Johns Hopkins University; *High Resolution Electron Microbeam Examination and 3D reconstruction of Alligator Gar Scale*
- Professor Michael Roukes, California Institute of Technology; *Nanoelectromechanical Oscillator Arrays: a Laboratory for Synchronization on Lattices and Networks*
- Professor Jayant Sirohi, University of Texas at Austin; *Detailed Measurements of the Aeroelastic Response of a Rigid Coaxial Rotor in Hover*
- Professor Jayanarayanan Sitaraman, University of Wyoming; *Advanced Overset Grid Methods for Massively Parallel Rotary Wing Computations*
- Professor Marilyn Smith, Georgia Institute of Technology; *Nonlinear Aeroelastic Analysis of Two- and Three-Dimensional Dynamic Stall*
- Professor Anthony Waas, University of Michigan - Ann Arbor; *Progressive Failure Modeling of Multi-Layered Textile Composites*
- Professor Haim Waisman, Columbia University; *High Strain Rate Failure Modeling Incorporating Shear Banding and Fracture*
- Professor Qingda Yang, University of Miami - Coral Gables; *Augmented Finite Element Method For High-Fidelity Analysis of Structural Composites*
- Professor Michael Zachariah, University of Maryland - College Park; *Towards a Mechanistic Understanding of What makes a Good Oxidizer, and the Size Dependence of NanoEnergetic Reactivity*

2. Short Term Innovative Research (STIR) Program. In FY13, the Division awarded three new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to develop a focused schlieren optical system for flow visualization, to develop topologically interlocked materials for energy dissipation under quasi-static and dynamic conditions, and to develop a mathematical model that represents the spatial and temporal behavior of thermoacoustic perturbations. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Sivaram Gogineni, Spectral Energies, LLC; *Development of Focused Schlieren Based Seedless Velocimetry for Boundary Layer, Transition, and Wake Studies*
- Professor Thomas Siegmund, Purdue University; *Mechanics of Multiscale Energy Dissipation in Topologically Interlocked Materials*
- Professor Kunihiko Taira, Florida State University; *Active Flow Control with Thermoacoustic Actuators*

3. Young Investigator Program (YIP). In FY13, the Division awarded one new YIP project. This grant is driving fundamental research to develop a new paradigm for the control of energy and information flow in molecular networks. The following PI and corresponding organization received the new-start YIP award.

- Professor Elad Harel, Northwestern University; *Complex Dynamics and Systems: Controlling Energy Flow in Colloidal Nano-Networks*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY13 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Information in Dynamical Systems and Complex Systems Summer 2013 Workshop*; Burlington, VT; 18-19 July 2013
- *Challenges in Integrated Computational Structure-Material Modeling of High Strain-Rate Deformation and Failure in Heterogeneous Materials*; Baltimore, MD; 5-6 September 2013

5. Special Programs. In FY13, 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. 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.

2. Nanoscale Control, Computing, and Communication Far-from-Equilibrium. One MURI in this topic area began in FY13. The team is led by Professor James Crutchfield of the University of California at Davis. The objective of this MURI is to develop fundamental understanding to enable new synthetic nanoscale systems capable of behaving as information engines, performing tasks that involve the manipulation of both information and energy. Ultimately, a unified framework for understanding, designing, and implementing information-processing engines will be developed by a team of experts in information processing by dynamical systems, nonequilibrium thermodynamics, control theory, and nanoscale devices to search for and articulate the basic principles underlying the manipulation of information and energy by synthetic nanoscale systems. Theoretical predictions will be empirically validated in experimental nanoscale devices.

This research will enable new capabilities to (i) quantify the intrinsic computation in nanoscale thermodynamic systems, (ii) to produce a thermodynamic theory for control and optimization of out-of-equilibrium nanoscale processes, and (iii) to accomplish experimental validation of the resulting thermodynamic principles of optimization and control of molecular agents. The results will provide a scientific foundation for future nanoscale devices with groundbreaking capabilities, ranging from efficient computation on microscopic substrates to the generation of directed motion. In the long term, this research may enable devices that can coordinate the molecular assembly of materials and novel substrates for information processing on radically smaller and faster scales. This research may lead to a new generation of faster, cheaper, and more energy efficient computing devices capable of manipulating large-scale, complex data structures, as well as self-organizing nanoscale motors capable of interfacing with the physical world with maximum power and efficiency.

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

No new starts were initiated in 2013.

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 FY13, the Division managed one new-start STTR Phase I contract, in addition to active projects continuing from prior years. This new-start contract aims to bridge fundamental discoveries with potential applications, including the development of novel hierarchical structures capable of achieving disparate mechanical properties for enhanced multifunctionality.

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 FY13, the Division managed four 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 2013.

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 FY13, the Division managed five 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 dynamic stall in a wide range of mach numbers by plasma actuators with combined energy/momentum action and length scale effects on progressive damage.

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). In FY13, Phase II of the program began, which continued and expanded research efforts. 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 funded and/or monitored by the Mechanical Sciences Division.

A. A Stochastic Approach to Structural Health Monitoring of Advanced Composites

Professor Aditi Chattopadhyay, Arizona State University, Single Investigator Award

The objective of this research is to develop a fundamental understanding of the damage phenomena across multiple scales in composite test structures under various loading conditions. A stochastic multiscale modeling approach is being developed to predict the mechanical response of composite materials and structures. This is to be accomplished by exploring the development of a multiscale structural health monitoring (SHM) framework for polymer matrix composites. The effort is using a three prong approach: (i) stochastic multiscale modeling; (ii) probabilistic damage state awareness and prognosis; and (iii) testing and validation.

In FY13 the team successfully developed a novel thermoelastic constitutive damage relation and implemented it into a multiscale modeling framework to account for the manufacturing-induced residual stresses and strains and resulting matrix microcracking in carbon fiber reinforced ceramic matrix composites (see FIGURE 1).

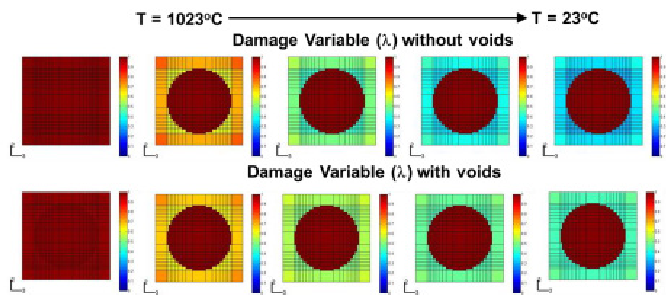

FIGURE 1

Comparison of local damage progression in 2D fiber/matrix subcell RUC for matrix with and without voids during cool-down.

Capturing the as-produced state of the material system requires consideration of the manufacturing phase following the CVI process. As the composite cools during this phase, microcracks form in the matrix material, causing the as-produced state of the composite to be pre-damaged. The thermoelastic damage multiscale matrix damage framework was able to capture the damage progression during the cool-down phase and accurately model the thermal and mechanical behavior of the composite system. In addition, the initiation and progression of damage and the evolution of effective moduli were studied for different fiber architectures and varying void volume fractions. Overall, the model provides important insight into the thermal, elastic, and damage behavior of carbon fiber reinforced ceramic matrix composites.

B. Mechanical and Ferroelectric Response of Highly Textured PZT Films

Professor Ioannis Chasiotis, The University of Illinois - Urbana-Champaign, Single Investigator Award

The objective of this research is to investigate the mechanical and ferroelectric response of highly textured {001} and {111} Lead Zirconium Titanate (PZT) films for microelectromechanical systems (MEMS). Such films hold the promise to increase actuation stresses of existing PZT-based microsystems by as much as 30-50%. This effort aims to obtain the material microstructure-electromechanical property relationships for freestanding textured PZT stacks (500-1,000 nm in thickness) at a broad range of strain rates that are relevant to advanced MEMS applications. The results will provide direct evidence about the mechanical reliability and the high field (but low voltage) ferroelectric response of textured PZT films, and the much needed quantitative inputs for the design and predictive modeling of PZT-based microdevices.

In FY13, the researchers developed microscale Pt thin film specimens which were designed at UIUC in collaboration with ARL, and were fabricated at ARL using DC magnetron sputtering on Si (100) substrate. The fabrication started with the deposition of a base layer of Ti on SiO_2 by DC magnetron sputtering at 50˚C to serve as an adhesion layer. The Ti films had a strong {0001} texture with basal plane of HCP structure lying in plane of substrate. The Ti films were then converted to titanium dioxide (TiO2) through oxygen annealing for 15-30 minutes inside a tube furnace at 800˚C. X-Ray diffraction studies showed {100}-texture for TiO_2. The original Ti {0001}-texture was maintained during oxidation and oxygen penetrated the Ti lattice forming rutile structure with {100} texture. 1-µm thick Pt films were then sputter deposited onto the TiO_2 with a 99.9% pure target at a substrate temperature of 500^{o}C. Patterning of the Pt film to specified geometry and dimensions was done using Ar ion milling. Prior to etching, the wafer was exposed to a 20 s reactive ion etching to remove the surface oxide developed on the exposed silicon surfaces. Next, the film was subjected to xenon difloride (XeF_2) isotropic etching to remove the Si underneath and then treated with wet hydrofluoric acid (HF) to remove the SiO_2 and TiO_2 layers (see FIGURE 2). After release, the wafer was stealth diced to prepare individual dies containing 10 tensile specimens. Following manufacture, the Pt surface was qualitatively characterized by electron dispersive spectroscopy, indicating a grain size of 100-300nm. The films were then mechanically characterized at low and high strain rates using a strain gauge load cell at the low strain rates and a piezoresistive load cell at the high strain rates. A random speckle pattern was placed on the films and on optical microscope equipped with a CCD camper was used to acquire images of the specimen surface during loading. Strain was computed from the resulting image contour plots to obtain the mean strain in the axial and transverse directions.

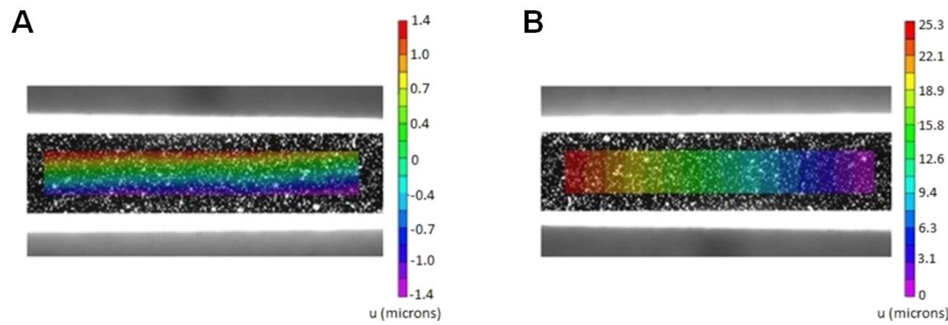

FIGURE 2

Layers in the deposition scheme of Pt thin film. (**A**) u and (**B**) v displacement contour plots obtained via DIC.

This approach was repeated for different thickness Pt films (see FIGURE 3). Although the elastic modulus remained unchanged, the yield stress of Pt films increased as film thickness decreased. This increase in yield stress with decreasing film thickness is explained in the discussion section later in this report. Moreover, the strain at failure remained low (~1%) and was same for the two films of different thickness. In comparison, the Pt films tested elsewhere using the same methods as in this research program were not only stiffer but also had higher strength and ductility. Furthermore, they were not textured and, thus the differences in measured properties between the two types of Pt call for an explanation and will be investigated further.

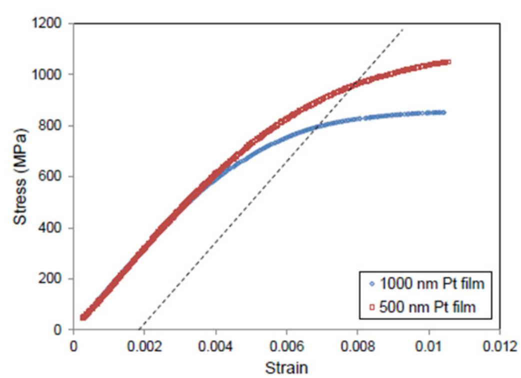

FIGURE 3

Strain-strain response of Pt films for two film thicknesses. Engineering stress-strain curves for Pt freestanding films as a function of thickness at the strain rate of 3×10^{-4} s^{-1}.

C. Studying Electron Transport in Nanowires using Fluctuations of Nano-mechanical Structures

Professors Mark Dykman and Steve Shaw, Michigan State University, Single Investigator Award

The goal of this research is to reveal important features of coupled systems of electrons and vibrations in nano-electro-mechanics. Insights into these features can be gained from the studies of the backaction, wherein mechanical vibrations change the electron transport across contact barriers and the charge distribution on the resonator, which in turn affect the vibrations. Fundamentally important are vibration fluctuations, as they carry information about the interaction with the electron system and the spectral properties of the system response. Studying fluctuations and linear and nonlinear response of the coupled electron-vibrational systems should provide important investigative tools and reveal difficult-to-access information about the properties of the contacts between the resonators and the conductors that support them, and about mechanisms of decay and dephasing of the resonator vibrations. This will significantly enhance the fundamental understanding of the dynamic response of nano-electro-mechanical devices, and will be of use in their development for a variety of applications, both electronic and mechanical.

Several novel research contributions were made in FY13. First, the PIs demonstrated ultrasensitive force detection with a nanotube mechanical resonator. Mechanical resonators are attracting considerable interest as ultra-sensitive detectors of force. Their force sensitivity offers numerous opportunities for various scientific and technological applications, such as resonant magnetic imaging with individual spin resolution and magnetometry measurements of individual magnetic molecules. Pushing the sensitivity towards the ultimate limits greatly increases the range of possible applications and paves the way for new scientific discoveries. The PI's demonstrated a force sensitivity of 12 $zN/Hz^{1/2}$, a factor of 43 lower than that achieved in previous measurements (see FIGURE 4). A 12 zN force corresponds to the force of an individual nuclear spin in the magnetic field gradient that is typically used in magnetic resonance force microscopy. Comparably, 12 zN also corresponds to the gravitational force between two persons separated by a distance of 4,500 kilometers. This force sensitivity was achieved with a resonator based on a carbon nanotube. The low mass of the nanotube is pivotal to reducing the limit on the force sensitivity imposed by the fluctuation-dissipation theorem. Over the last decade, force sensitivity has been improved by only a modest amount (*i.e.* a factor of 1.5). This is especially low when considering the intensive activity in the field. Thus far, the researchers have been actively searching for novel strategies without noticeable success. This finding marks a major step forward and proves that force sensing with nanotube resonators is a very promising route to take. A major tool for achieving the high force sensitivity is the coupling of the vibrations to the electron transport in a carbon nanotube. Because of this coupling, the conductivity of the nanotube is modulated by the vibrations. If a voltage applied to the nanotube is at frequency ω close to the vibration eigenfrequency ω_0, the current through the nanotube is modulated by the fluctuations of the vibrations, and there emerges a fluctuating current at frequency close to $|\omega - \omega_0|$. This is cross-correlation based down-conversion and shifts detection of the fluctuations to much lower frequencies than ω_0. The detector sensitivity is significantly higher in this range.

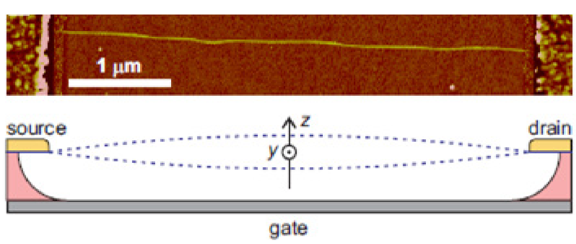

FIGURE 4

Ultrasensitive force sensing. Force sensing experiments with a sensitivity of 12 zN/√Hz at a temperature of 1.2 K using a resonator made of a carbon nanotube (the micrograph). The detection method enables measuring the Brownian vibrations of the nanotube down to cryogenic temperatures.

Second, the researchers demonstrated thermal transport and quench relaxation in nonlinear Luttinger liquids. Electron systems in nanowires are essentially one-dimensional (1D), as the motion in the direction normal to the nanowire is strongly quantized. 1D systems are special, since several exact solutions are known even where the electron-electron interaction is not weak. The corresponding integrability ensures that scattering of the particles of an *N*-body system is equivalent to a sequence of pair-particle collisions, and thus the set of incoming momenta for any scattering event coincides with the set of outgoing momenta. Such scattering does not alter the distribution function and is unable to drive the system towards thermal equilibrium. A quantum Newton's cradle, realized with trapped 1D Bose gas, gives the best example for such long-lived out-of-equilibrium quantum states unaffected by binary collisions. When interaction in the 1D electron liquid becomes very strong, the electron liquid start to crystallize, and forms a 1D Wigner crystal. Vibrations of such crystal are intrinsically anharmonic. Such anharmonicity leads to a finite lifetime of the elementary excitations, which correspond to plasmons of the Luttinger liquid, and thus to plasmon thermalization. It modifies the thermal conductance in a nontrivial way. The leading-order relaxation process is two-plasmon collisions; however, complete equilibration is achieved by inelastic scattering that does not conserve the number of plasmon modes. Interestingly, both scattering rates have the same temperature dependence $\propto T^5$. Based on this evidence, the investigators concluded that at the time scales exceeding the interaction-induced lifetime of plasmons, thermal currents displayed nonexponential decay, which can be rooted in the fact that the eigenvalues of the collision integral for the plasmon scattering cover a continuous spectrum of excitations.

D. Flexoelectricity in Nanoribbons and Biomembranes

Professor Prashant Purohit, University of Pennsylvania, Single Investigator Award

The objective of this research is to gain a fundamental understanding of flexoelectricity in PZT, biomembranes and non-piezoelectric solids. Flexoelectricity represents curvature or strain-gradient induced polarization of a material, as opposed to piezoelectricity, which is strain-induced polarization. Although, flexoelectric phenomena have been known for a few decades they are not as well understood as piezoelectricity because of the difficulty of producing and measuring very large strain gradients. However, in nanoscale specimens, such as thin films and cell membranes, it is possible to produce strain gradients (or curvatures) large enough that flexoelectric effects can be measured. The investigators are constructing theory and using it (i) to solve boundary value problems in one and two dimensions that will become a benchmark for testing computational methods and interpreting experiments, (ii) to determine and analytically solve the shape equation for vesicles and cells accounting for flexoelectric contributions, and (iii) to interpret electromechanical experiments on cells and PZT nanowires.

In FY13, major progress has been made in a number of areas. First, the PI proved a flexoelectric reciprocal theorem and solved several flexoelectric boundary value problems (see FIGURE 5). The literature on flexoelectricity, which is a few decades old, primarily addresses the origins of the phenomenon in the electronic structure of the materials or its measurement in solids and membranes. Unlike the well-developed theory of piezoelectricity in solids there has been little, if any, effort to solve boundary value problems. To fill this gap the PI formulated a theory for flexoelectric solids starting with an energy function that can depend on strains, strain gradients and polarization. The PI worked with small strains so that the energy function can be treated as quadratic in the kinematic variables and use the variational methods of Mindlin and Toupin to derive the field equations and boundary conditions. For a linear flexoelectric material the PI proved a reciprocal theorem and then verified it in a one-dimensional beam bending problem. Several 2D flexoelectric boundary value problems were solved which are similar to those solved for piezoelectric materials and are described in textbooks. An interesting boundary value problem where the flexoelectric solution is different from the piezoelectric case is that of shearing a flexoelectric cylinder or disk. This results in an azimuthal polarization, an effect that is not seen in a piezoelectric cylinder under the same loading. Researchers plan to continue this line of research in the next year by solving for stresses and electric fields near point defects and edge dislocations in solids.

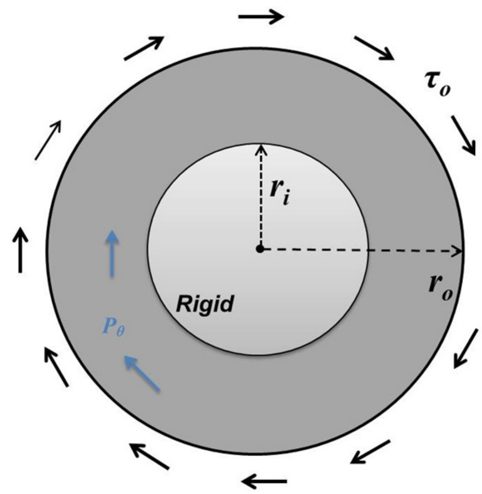

FIGURE 5

Flexoelectric boundary value problems. Researchers solved several 2D flexoelectric boundary value problems which are similar to those solved for piezoelectric materials and are described in textbooks. An interesting boundary value problem where the flexoelectric solution is different from the piezoelectric case is that of shearing a flexoelectric cylinder or disk. This results in an azimuthal polarization, an effect that is not seen in a piezoelectric cylinder under the same loading.

Second, researchers developed a new model for the growth of neurons under applied pressure differences and shown (in collaboration with Professor Mike McAlpine at Princeton) that can account for the experimental observations. Earlier research on biomembranes give an expression for the membrane tension (and spontaneous curvature) in terms of the potential difference across it. Starting with this expression for the tension it is possible to solve for the shape of a cell that is placed under mechanical constraints with a prescribed potential difference across its membrane. The solutions are in terms of elliptic functions. The PI computed these shapes and described them in detail in a paper published last year in Nature Nanotechnology. An extension of this line of research was to understand the growth processes in neuronal cells in response to pressure differences imposed by microfluidic devices. The mathematical models in the literature are unable to capture the effects of this pressure difference even though they account for the chemistry and transport processes involved in growth. The key assumption of these models is that the growth process is reaction limited. The PI showed instead that a diffusion limited model can account for the growth of a neuron under pressure differences. A paper describing this model has been published in *Lab on a Chip*. It has been shown in earlier work that the main effect of the potential difference across a membrane is to change the spontaneous curvature. The PIs preliminary research suggests that this changes the shape equation of the vesicle, but it can still be solved in 2D using elliptic functions. The PI's solutions will serve as benchmark for more complex problems.

E. Efficient and Safe Chemical Gas Generators with Nanocomposite Reactive Materials

Professor Evegny Shafirovich, University of Texas - El Paso, REP Award

The objective of this research is to determine the characteristics and reaction mechanisms of gas-generating compositions involving novel nanocomposite and mechanically alloyed reactive materials, produced by arrested reactive milling, a technique developed recently at the New Jersey Institute of Technology (NJIT). In the long term, such reactive materials will be used to develop chemical gas generators that will exhibit improved effectiveness, process stability, and fire safety.

In FY13, the researchers completed construction of a laser ignition facility for gas-generating mixtures and begun testing various materials to determine ignition characteristics. Several materials have been tested to date including pure metal powders (Fe and Mg), mechanically alloyed powders (Fe/Mg [3:1], B/Ti [2:1], Al/Mg [4.7:5.3], Al/Mg [7:3], Al/Mg [4:1], Al/Mg]9:1]) and reactive nanocomposites (Al/$NaNO_3$ [5:3], and Al/$NaNO_3$ [2.1:1]; mole ratios indicated). The materials tested were chosen based on thermodynamic calculations completed in the previous year.

Combustion experiments with oxygen-generating mixtures revealed that the B/Ti additive leads to numerous sparks during combustion, which is generally undesired. The mixtures with Al/$NaNO_3$ additives were found to be not combustible. Mechanically alloyed Al/Mg materials may be advantageous as compared to the currently used Fe and Sn. Lower amounts of these materials were needed, which increases oxygen yield. At equal concentrations, Al/Mg additives lead to a steadier propagation of the combustion wave over the mixture pellet. Pure Al could not be used in oxygen generators because it does not ignite at the desired low operational temperatures. Use of the pure Mg was also problematic because it rapidly ages during its storage. The Al/Mg alloys were designed to overcome the above drawbacks of the pure Al and Mg; they provide a promising alternative to the currently used Fe and Sn.

As another approach to hydrogen generation, combustible mixtures of gelled water and mechanically alloyed Al/Mg material were studied (see FIGURE 6). To prevent sedimentation of particles, 3 wt% polyacrylamide was added to water. The mixtures were placed into quartz tubes and ignited by the laser. A steady propagation of the combustion wave over the sample was observed.

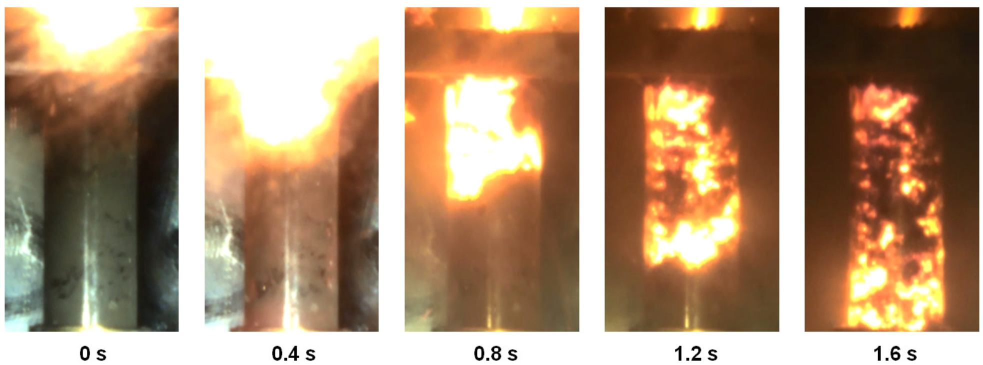

FIGURE 6

Study of combustible mixtures of gelled water and mechanically-alloyed Al/Mg. Combustion propagation over the mixture of gelled water and Al/Mg powder placed in a quartz tube and ignited with a CO2 laser.

The team sought to ignite a mixture of water, ammonia borane, and an activated aluminum powder fabricated from foil using high-energy ball milling. To obtain information on the mechanisms of the involved reactions, isotopic tests were conducted. Specifically, heavy water (D_2O) was used instead of H_2O in these experiments. Upon laser ignition, self-sustained propagation of the reaction front was observed. Mass-spectrometric measurements have revealed significant amounts of H_2 and HD in the product gas, with no D_2. XRD analysis of the condensed products has shown that it contains Al but no Al_2O_3. Thus, the process involved thermolysis of NH_3BH_3 (produces H_2) and hydrolysis of NH_3BH (produces HD), while Al could play a role of a catalyst for the hydrolysis.

F. Investigations of the Flowfield Characteristics on a Retreating Rotor Blade

Professor Narayanan Komerath, Georgia Institute of Technology, Single Investigator Award

Dynamic stall and reverse flow occurring on the retreating rotor blades of a helicopter rotor or a yawed wind turbine limit performance, fatigue life and safety. Uncertainties persist in the pitching moment signature, partly because the sharp radial flow gradients induced by rotation have not been accessible to detailed measurement or computation. The objective of this research is to identify the mechanisms of retreating-blade stall on a helicopter rotor blade. Stereoscopic Particle Image Velocimetry (SPIV) captures the 3-component velocity field in planes, to derive explanations. Previous results on a teetering 2-bladed rotor in forward flight showed that discrete, quasi-periodic vortical structures break away from the radial jet layer caused by centrifugal effects in the stalled region, thus limiting jet growth and the resulting 3D effects on the accompanying airloads (see FIGURE 7).

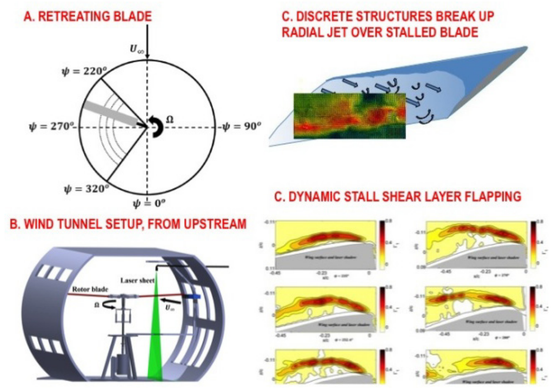

FIGURE 7

Rotor in dynamic stall and its rotating disc analogy for shear layer structures. Results on a teetering 2-bladed rotor in forward flight showed that discrete, quasi-periodic vortical structures break away from the radial jet layer caused by centrifugal effects in the stalled region, thus limiting jet growth and the resulting 3D effects on the accompanying airloads.

In FY13, a rotating disc experiment was used to capture the radial jet layer for comparison with analytical solutions. When an edgewise flow at angle of attack was superposed, very similar structures appeared (see FIGURE 8). This suggests that a breakthrough can be achieved: the spacing and strength of such structures that limit the radial flow effects on airloads in rotor dynamic stall can be estimated using a modified analytical formulation for a rotating disc.

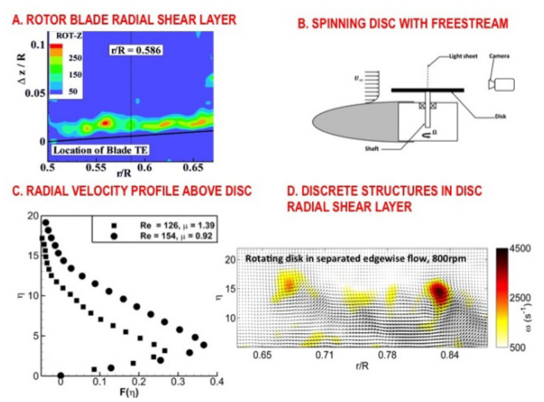

FIGURE 8

Identifying the mechanisms of retreating-blade stall. The results of a rotor in dynamic stall and its rotating disc analogy for shear layer structures are shown.

The process of 3-D dynamic stall on a rotating blade was captured in detail from inception through reattachment using SPIV. The spanwise progression of separation is again influenced by the radial flow, with the dynamic stall vortex trajectory much closer to the blade surface. A strong radial flow persists over the blade, especially within the discrete structures in the separated shear layer. The link between these structures and those seen in the radial jet downstream is yet to be established. The separated shear layer also shows a low-frequency, quasi-periodic flapping. The cause and the effect on airloads are not yet known; however it means that phase-resolved ensemble averaged measurements would seriously underestimate the vorticity and strength of the discrete structures in the shear layer. The Normalized Angular Momentum technique was used to locate vorticity centers in the velocity field, and the method of Proper Orthogonal Decomposition was used to obtain better-resolved measurements of the vorticity field.

The reverse flow occurring over part of the retreating blade at high advance ratios is important as rotorcraft venture into the high speed flight regime. The airloads on a yawed blade were studied in fixed-wing mode in forward and reverse flow. The results supported the hypothesis of an analogy with delta wing leading edge vortex (LEV) models, and tuft visualizations proved it. In rotor mode, the velocity field under corresponding flow conditions showed that rotation delayed separation to a higher angle of attack. Measuring the pitching moment through stall is difficult even for a fixed wing, and to do this at high rate demands a large dynamic range of transducers. A pitch-plunge oscillating wing experiment in the School's 1.07m wind tunnel was used to extract excursions in lift and pitching moment through dynamic stall, using only kinematics without direct load sensors. The pitching wing experiment has yielded a powerful and elegant new method to extract aerodynamic coefficients and study flows through large-amplitude dynamic stall motions.

G. Heavy Alkane and Cyclohexane Reduced Oxidation Kinetics and Flame Modeling

Professor Josette Bellan, California Institute of Technology, Single Investigator Award

The objective of this research is to explore the possibility of computationally efficient chemistry modeling for heavy alkanes and cyclohexane using the concept of self similarity identified in the detailed oxidation kinetics database of n-heptane and iso-octane**.** Using this concept, the researchers have previously been successful to obtained reduced models for *n*-heptane, iso-octane, primary reference fuels and mixtures of iso-octane with *n* -pentane or iso-hexane**.** Having recently gained experience in using this methodology for *n*-heptane and iso-octane laminar flame prediction, they have undertaken the heavy alkanes and cyclohexane work.

In FY13, the researchers demonstrated that the chemical kinetic reduction model based on local self-similarity applied to *n*-heptane, iso-octane, *n*-decane and *n*-dodecane reduces the number of computed species from 160, 857, 2115 and 2115, respectively, to 20 light species without loss of accuracy to: ignition time, equilibrium temperature (for lean or stoichiometric mixtures), maximum temperature (for rich mixtures), or species timewise evolution**.** Additionally, they demonstrated that by judiciously selecting the light species from the previous set of 20, the reduced mechanism can be further reduced for *n*-dodecane to 15 or even 6 progress-variable species with no loss of accuracy**.** This decrease by a factor of over 100 in the number of species that needs to be tracked should lead to a significant reduction in computational time for calculations of these reacting systems**.** Importantly, the researchers also used the method to model a steady, quasi one-dimensional premixed laminar flame developing unopposed into a uniform flow**.** Results from this simulation compared favorably with the data, considering the different configurations**.** Results from parametric studies not associated with experimental data showed that at stoichiometric conditions the flame temperature, flame velocity and strain rate are not sensitive to the pressure, although flames become increasingly thinner with increasing pressure and the yield of the unsteady light species is different**.** Computations conducted at 40 bar for various equivalence ratios and for velocities differing with the equivalence ratio showed that the maximum flame velocity, flame strain and flame temperature were obtained at stoichometric conditions.

To achieve this objective, Professor Bellan capitalized on a previous kinetic reduction model that relied upon constituents and species and identified a local and full self similarity between a properly scaled global-constituent molar density and a normalized temperature. By definition, constituent radicals are those composing species with a carbon number larger than or equal to three. Any of these species are called ‘heavy’, and the species which are their complement in the ensemble of species are called ‘light’. For any fuel, it is possible to determine an optimal set (*i.e.*, a set containing the smallest number) of constituents. A thorough examination of the LLNL skeletal mechanism for *n*-heptane over a wide range of pressures and stoichiometries revealed that it is possible to empirically define a similarity variable which is a normalized temperature and is function of the initial temperature, initial pressure and equivalence ratio, and for which a scaled global-constituents' molar density exhibits a self-similar behavior across initial temperatures in the cold ignition regime, initial pressures and equivalence ratios. The significance of this finding is that there is a reduction in the dimensionality of the problem. Therefore, going from n-heptane to heavier hydrocarbons, the number of constituents may increase, but if as for *n*-heptane they can all be bundled into a single total constituent mole fraction that is the single representative progress variable of the constituents, the computational time should essentially remain the same. Evaluation of this hypothesis was successfully performed by applying the n-heptane methodology to iso-octane chemical kinetics, and to mixtures of iso-octane with *n*-pentane, iso-hexane or *n*-heptane. Thus, by construct this model is hierarchical because the progress variables are not necessarily species, but also include species ‘constituents’, defined very much like in Benson’s classical group additivity theory.

The goal of the chemical reduction process is to retain only a very small number of species, which are denoted as “major” (*i.e.*, important) and model the influence of the other species, denoted as “minor” on the major species. The retained species are known as “computed” and the modeled species “non-computed,” very much in concert with the concept of Large Eddy Simulation for computing turbulent flows. The fact that the state vector obeys local self similarity does not guarantee that the non-computed part of a function will be self similar: a judicious choice of the computed species is necessary to ensure local self-similarity for the non-computed part of the functions. Similar to the investigator's previous work, the light species was chosen as the computed species and the heavy species as the non-computed species. With no assumptions made regarding quasi-steadiness of some species, the light species ensemble consists of 20 species.

N-heptane and iso-octane oxidation at stoichiometric condition over a pressure range of [1, 40] bar was simulated. The simulations were performed within a range of initial velocities differing by less than 1% according to pressure and showed that the flame temperature, flame velocity and stretch rate were all insensitive to pressure. However, the width of the flame decreased with increasing pressure and the yield of unsteady light species was different.

A study of iso-octane oxidation at a pressure of 40 bar was conducted over a range of equivalence ratios varying in [0.75, 1.5]. Each simulation was initiated with a different velocity, and the velocity decreased away from the stoichiometric condition in accord with known information about flammability limits. Since a single simulation was performed for each equivalence ratio, it is most likely that by varying the initial velocity at a fixed equivalence ratio value, results different from those presented here will be found. Thus, the comparisons only have a qualitative aspect, but with this caveat the results revealed that the maximum flame velocity and temperature are obtained at stoichiometric conditions. Results of these simulations at an atmospheric and elevated pressure of 40 bar are shown in FIGURE 9.

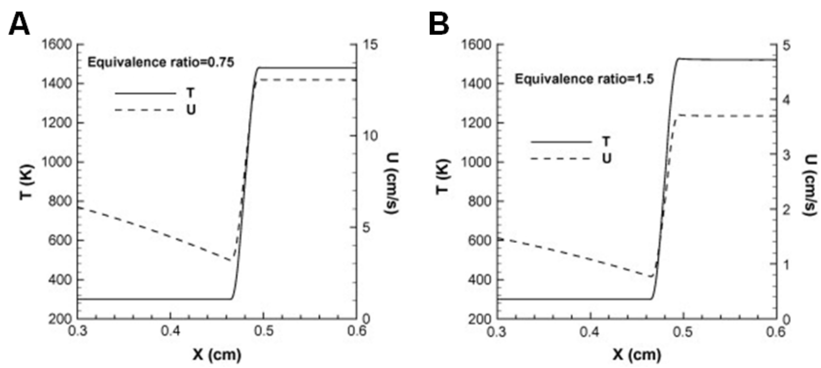

FIGURE 9

N-heptane and iso-octane oxidation at stoichiometric condition. Steady-state profiles of temperature (T) and flame speed (U) for iso-octane flame propagation for (A) p = 1 bar and (B) and p = 40 bar. YF is not indicative of the fuel, but of the mass fraction of the constituents: YF ≡ Ncmc/(cm) where c is the molar density.

H. Modeling of Two-Dimensional and Three-Dimensional Dynamic Stall

Professors Ashok Gopalarathnam and Jack Edwards, NC State University, Single Investigator Award

The objective of this research is to develop complementary low-order and high-order prediction methods for airfoils and rotor blades undergoing dynamic stall. Research efforts supported by this grant have focused on (i) development of a low-order model for airfoils undergoing dynamic stall and (ii) RANS and LES/RANS simulations of a NACA 0012 airfoil undergoing dynamic stall.

The low-order method builds on an existing approach that augments unsteady thin airfoil theory with a criterion for intermittent leading-edge vortex (LEV) shedding. The existing model worked well for airfoils undergoing motions having high reduced frequencies (k = 1.0–4.0) in which LEV formation occurs without significant separation at the trailing-edge of the upper surface. Unsteady motions of this type are of interest to MAVs and insect-flight analyses. In contrast, at very low reduced frequencies, of which steady flow (k = 0) is a subset, the PI expects the airfoil to stall due to progressive trailing-edge separation without any LEV formation. Helicopter dynamic stall occurs at intermediate values of k (k = 0.1–0.3) where progressive trailing-edge separation often precedes LEV formation, affecting forces and LEV onset. For this reason, it is necessary to develop modeling approaches for predicting trailing-edge separation. In FY13, the investigator developed an approach that uses steady-flow results from CFD and experiment along with a time-lagged decambering approach to determine progressive trailing-edge separation in unsteady flow. Early results from the low-order model for a pitch-up and pitch-down motion were compared with results from high-order CFD (RANS) predictions (see FIGURE 10).

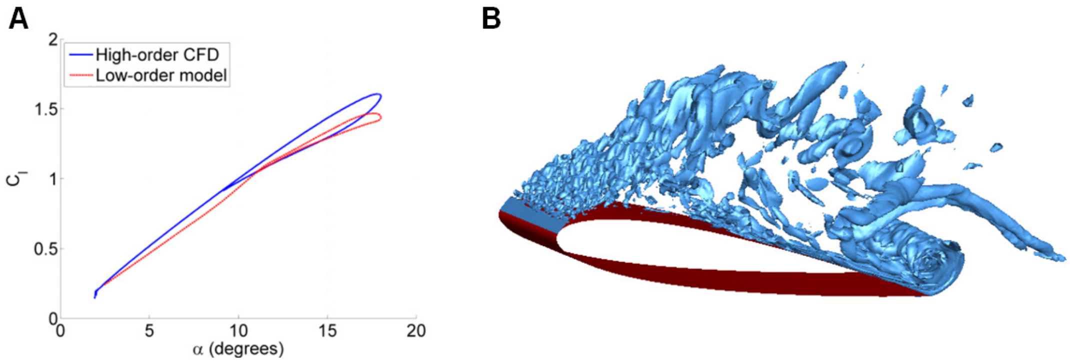

FIGURE 10

Results for lift hysteresis and LES/RANS analysis. (A) The lift hysteresis of a low-order decambering model compared to high-order CFD results for pitch-up and pitch-down motion. (B) The Swirl-strength iso-surfaces of LES/RANS computations of NACA 0012 airfoil undergoing dynamic stall is highlighted.

In addition, a companion research effort is focused on the development of a hybrid LES/RANS techniques suitable for airfoils and wings undergoing dynamic stall. The current approach embeds the Menter/Langtry transition model into the LES/RANS method of Gieseking, et al. which utilizes ensemble-averaging techniques to model specific turbulence length scales. New ensemble-averaging methods suitable for moving domains were developed and tested for a dynamic stall experiment conducted by Bowersox and colleagues at Texas A&M. A snapshot of swirl-strength iso-surfaces during upstroke is shown in FIGURE 10B.

I. Active flow Control with Thermoacoustic Actuators

Professor Kunihiko Taira, Mechanical Engineering, Florida State University, STIR Award

The objective of this research is to numerically investigate the effectiveness of thermoacoustic actuators as potential controllers for turbulent separated flow. If successful, this effort will provide an alternative technique for modifying turbulent flows. This new technique will complement the mass and momentum injection concepts that have been examined in past flow control studies. The use of near-field acoustic excitation has not been explored deeply in the past due to the absence of surface-compliant actuators capable of delivering high-intensity acoustic waves. This study examines the possible use of a novel thin-layer speaker made with carbon nanotube/graphene membranes that generate high intensity acoustic waves over a broad range of frequencies with low power input.

In FY13, the researchers performed large eddy simulations to predict the turbulent flow field over a wall-mounted hump from a NASA Validation Workshop. This geometry was chosen to facilitate the assessment of control effectiveness against other actuators, such as steady mass injection, synthetic jets, and plasma actuators. Due to the moderate Reynolds number of $Re = O(10^6)$ and Mach number of M=0.25, the computational domain required a fairly large number of grid points to resolve the small scale turbulent structures and the acoustic waves. While the prediction of this particular flow is known to be challenging, the flow field predicted by the simulation agreed well with those reported by other simulations and experiments.

To simulate the effect of the thermoacoustic actuator, the PI has developed a boundary condition model that generates the thermoacoustic waves consistent with experimental findings. This boundary condition model for the thermoacoustic actuator was implemented in the large eddy simulation (see FIGURE 11). Ongoing numerical studies are examining the fundamental role that acoustic waves play in modifying the dynamics of turbulent separated flows and reducing the drag. Close collaboration is carried out with a research group at the Aberdeen Proving Ground that is fabricating the thermoacoustic actuators. Computational support for this project was provided by the DoD High Performance Computing Modernization Program.

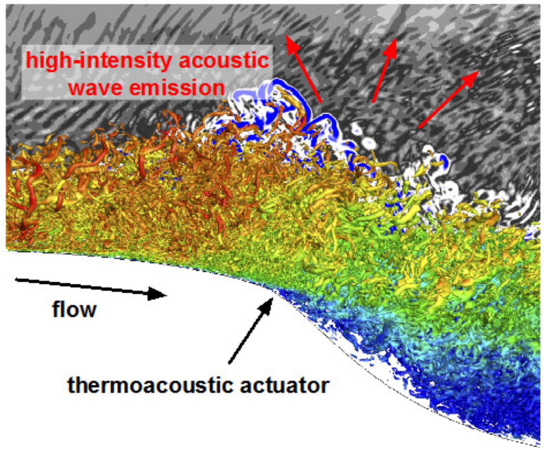

FIGURE 11

Separation control with locally mounted thermoacoustic actuator. The turbulent flow structures are shown with modifications by the high-intensity acoustic waves generated at high frequency over a wall mounted hump. The spanwise slice and insert image are the numerical Schlieren illustrating the wave-turbulence interaction

J. Rail Plasma Actuator for High-authority Aerodynamic Flow Control at Atmospheric Pressures

Professors Laxminarayan Raja and Jayant Sirohi, The University of Texas - Austin, STIR Award

Plasma actuators are attractive for aerodynamic flow control applications due to the absence of moving parts, extremely fast response times, and conformability to aerodynamic surfaces. In particular, there has been significant research on non-equilibrium surface dielectric barrier discharges (DBD) that are based on electrohydrodynamic forcing. However, the effectiveness of this mechanism is inherently limited; the plasma Debye length determines the size of the net space-charge region, which is inversely proportional to the plasma density, and therefore, to the induced flow velocity. The objective of this research project was to develop and experimentally validate a novel magnetohydrodynamic Rail Plasma Actuator (“RailPAc”). Preliminary results indicated that the actuator preserves most of the desirable properties of existing plasma actuators such as DBDs, but it is capable of inducing a significantly larger flow velocity.

The RailPAc comprises two rail electrodes flush mounted on an aerodynamic flow surface (see FIGURE 12A). A pulsed arc is propelled down the length of the rails by Lorentz forces supported by a self-induced magnetic field. The arc induces a high-velocity pulsed air wall jet due to the pushing and entrainment actions. A proof-of-concept RailPAc, comprising two parallel copper strips each measuring 150 mm long, 10 mm wide, and 1.6 mm thick, separated by a distance of about 10 mm and bonded to a fiberglass plate, was constructed and tested (see FIGURE 12B). The right ends of the rails are connected to a pulse forming network that initiates an arc, which is later propelled down the rails by Lorentz forces as it drags the flow along with it.

Experiments were performed on the proof-of-concept RailPAc in quiescent air, and on a RailPAc embedded in a two-dimensional, 14.5 in chord airfoil section in a wind tunnel at zero angle of attack and a free stream velocity of 16 m/s (Reynolds number ~0.45 million). High-speed video of the arc motion indicated that the plasma arc achieves a peak velocity of around 100 m/s for discharge energy on the order of 300 J per pulse. A Laser Doppler Anemometer was used to measure time-averaged velocities over a grid extending along the airfoil chord and up to around 13% chord above the airfoil surface. These measurements indicated that the RailPAc induced a velocity of up to 16 m/s at a height of 7.5 mm above the airfoil surface; the RailPAc affects the velocity profile up to 45 mm above the airfoil surface. These induced flow velocities are significantly greater than what is demonstrated in typical DBD actuators.

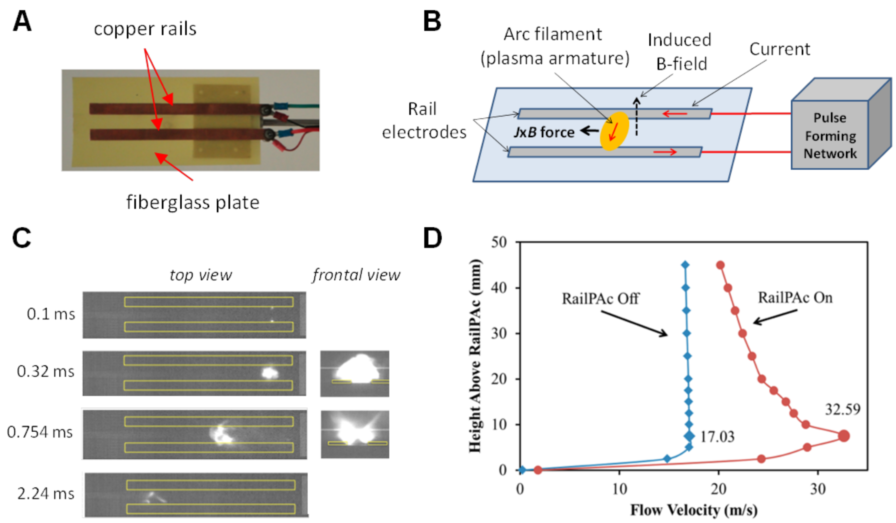

FIGURE 12

RailPAc plasma actuator. The figure illustrates the (**A**) top-down picture of prototype bench-scale RailPAc with 150 mm long copper rails, (**B**) schematic illustration of the rail plasma actuator (RailPAc) concept, and (**C**) high-speed imaging of the arc propagation down the length of the rails from right to left and velocity profile comparison over the airfoil surface at 60% chord with and without RailPAc activation.

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. Hierarchical Scales, Information Reduction Efficiency and Inference in Complex Systems

Investigator: Professor Erik Bollt, Clarkson University, Single Investigator Award
Recipient: Aviation and Missile Research, Development and Engineering Center (AMRDEC)

The objective of this research is to study interactions across spatial and temporal scales in complex dynamical systems. The PI is working to develop analysis of analysis for insight to better understand spatiotemporal and functional structures in complex systems from components of simple elements, how such structures emerge, how information moves, and how this occurs across scales. The PI seeks to understand "hierarchically efficient" dynamical networks to develop a theory to define hierarchy relationships of averaged models across scales.

Closely connected to these questions is the notion of inference and inverse problems where the PI has developed a information based inference analysis called Causation Entropy, a new theory that could allow one to untangle complex causal interactions, make better predictions, and ultimately design improved intervention strategies in social, biological, or physical complex networks. Earlier theories for this problem have failed to account for information transfer, which has often led to erroneous inferences of relationships and interconnections in a network. This research transitioned to AMRDEC in FY13, which is working with Clarkson University to extend the theory to include estimates of confidence levels for optimal placement and resolution of sensors that may enable inference of adversarial networks, malicious intrusion, and strategies for eavesdropping deception.

B. Electro-Static Discharge Sensitivity

Researcher: Professor Edward Dreizin, New Jersey Institute of Technology, Single Investigator Award
Recipient: Armaments Research Development and Engineering Center (ARDEC)

The objective of the research is to understand and describe quantitatively the mechanisms of ignition in reactive powders as a result of their stimulation by electrostatic discharge (ESD). Specific focus is on ignition mechanisms for novel reactive nanocomposite materials and on correlations between thermally initiated reactions and ignition mechanisms in such materials. Understanding ESD sensitivity is important as there are various applications of these reactive materials and mechanically alloyed powders for pyrotechnics work being conducted by ARDEC. In FY13, the researchers identified several Al-Mg alloys as first materials to explore for pyrotechnics. While continuing to explore ESD sensitivity, the team mechanically alloyed powder samples to ARDEC. The samples had different Al/Mg ratios, ranging from 50/50 to 90/10, for testing of suitability by ARDEC. ARDEC is examining these samples in the M127A1 white light-emitting signal formulations. These powders will be a replacement for the Mg currently used, which has issues with aging and performance. Further plans include testing the materials in the IM-28 armor-piercing incendiary configuration.

C. Multi-length Scale Material Model Development for Armor-grade Composites

Investigator: Professor Mica Grujicic, Clemson University, Single Investigator Award
Recipient: ARL-WMRD

The objective of this research is to develop and validate a continuum-level, large deformation, high rate, large strain, high pressure material model for ultra high molecular weight polyethylene (UHMWPE) reinforced composites. The study has involved three phases: (i) a comprehensive atomic-level computational investigation of the filament/matrix bonding/de-bonding behavior in the UHMWPE filament-reinforced ballistic-grade composites with different polymeric matrices (e.g., Kraton, poly-urethane, etc.); (ii) incorporate the results in a meso-scale finite-element mechanical-testing computational procedure in order to determine the unit-cell effective mechanical response (including damage/de-bonding induced material degradation and failure), when subjected to a variety of deformation modes; and (iii) validate the developed model by carrying out a series of transient non-linear dynamics calculations of the impact/penetration of UHMWPE reinforced armor-grade composite armor panels of different areal densities by a variety of bullets and fragment simulating projectiles (FSPs). Both single-threat and multi-hit scenarios were considered. The computational results obtained through this effort transitioned to ARL-WMRD for comparison with their experimental counterparts.

D. Quantitative 3D Imaging for Characterizing Spray in the Near-field of Nozzle Exits

Investigators: Professors Rebecca Fahrig and John Eaton, Stanford University, Single Investigator Award
Recipients: ARL-VTD, USMA

The objective of this research is to advance the understanding of the dense near-field liquid sprays by using cost-effective X-ray computed tomography. To accomplish this objective, ARL-VTD and Stanford University have partnered in a cooperative research and development agreement (CRADA) to implement an innovative three-dimensional imaging technique (that was recently developed at Stanford) in conjunction with a new X-ray computed tomography technique to study dense sprays. The first set of tasks associated with this project involved the redesign of the air co-flow in a CT compatible nozzle. These efforts were geared towards the reduction of liquid accumulation on the internal surfaces and to validate the explicit assumptions of 'no co-flow system effects' on spray redistribution.

The design and construction of the new system along with the nozzle were successful and transitioned to ARL-VTD. Numerous experiments aimed at investigating the properties of the spray from this nozzle using povidone iodine (with higher CT attenuation coefficients) are being conducted. Preliminary results were encouraging and may provide improved asymmetric nozzle geometry (see FIGURE 13). Parametric studies geared toward optimizing the performance parameters for the CT system, in terms of enhanced resolution, noise reduction and reproducibility, are also being conducted. At this stage in its development, the signal-to-noise ratio was insufficient to visualize further than 5 times the nozzle diameters downstream of its exit. The next step is to improve the sensitivity of the x-ray imaging system. Research efforts are focused on: improved data acquisition hardware to permit averaging over many seconds; the use of appropriate reconstruction filters to improve resolution and sensitivity; and the integration of new frame grabber driver for improved image acquisition.

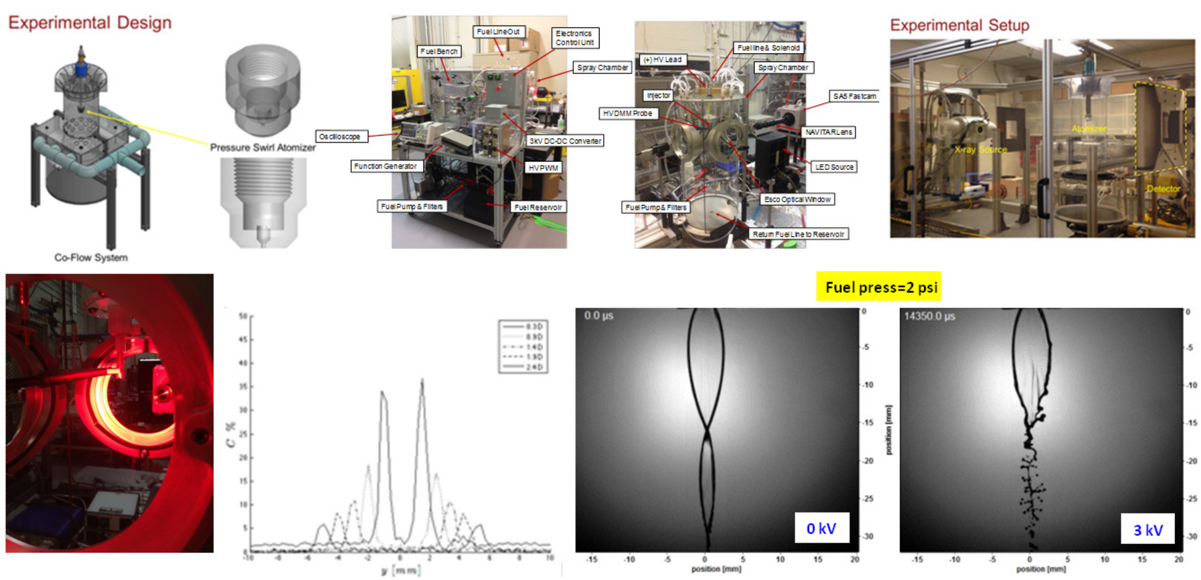

FIGURE 13

Improved asymmetric nozzle geometry. The panels display a schematic of the experimental design and setup. Images of povidone iodine from the 'scaled up' nozzle using 3D CT, Stanford University table-top experimental setup, a cut through of the 3D volume image of the nozzle exit, reconstructed with resolution of 0.3x0.3 mm, contrast as a function of distance plotted in 3D, and profiles through the symmetric nozzle as a function of distance from the nozzle exit.

V. ANTICIPATED ACCOMPLISHMENTS

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

A. Progressive Failure Modeling of Multi-Layered Textile Composites

Professor Anthony Waas, University of Michigan - Ann Arbor, Single Investigator Award

The objective of this research is to conceive and develop a multi-scale computational mechanics framework for progressive failure modeling of multi-layered composites, and then validate through experiments and analysis. These composites, which include 3D woven textile composites, are a relatively new class of lightweight, hierarchical engineered material systems designed to mitigate effects due to high intensity short duration loads, such as blast. The computational framework will specifically consider applications that expose the textile composite structures to loads of high intensity and short duration. It is anticipated that in FY14, the research team will develop a progressive damage and failure modeling framework for analyzing textile composites subjected to static and dynamic external loading. A new modeling strategy that combines mechanics of the constituents, the interaction amongst them at different scales, and how these interaction changes as a function of loading rate for textile composites will be used in the development of this framework. In addition, experiments using split Hopkinson pressure bar tests will be performed to provide characterizing data for the constituents.

B. Exploiting Transient High-Dimensional Nonlinear Dynamics for Spatiotemporal Data Processing

Professor Daniel Gauthier, Duke University, Single Investigator Award

The objective of this research is to develop a new form of information processing, known a reservoir computing (RC), to map input data into a high-dimensional phase space to understand spatiotemporal pattern formation. Recently, physicists revisited this problem and have proposed the use of complex transient dynamics displayed by time-delay systems built with electronics and optoelectronic components to realize reservoir computers. It is anticipated that in FY14, Professor Gauthier will develop methods to generate transient dynamics using a simple autonomous Boolean network (ABN) comprising an XOR function with delayed feedback loops. Such ABNs possess a stable steady state corresponding to a low voltage. However, if seeded by an external perturbation, such a network can produce very complex transients on the edge of chaos that can last up to several seconds. Such transients have time scales several orders of magnitude larger than the typical time-scale of the Boolean dynamics, which could allow for a mechanism to reset artificially the dynamical state of the ABN after a given period of time. This would be a first step towards a fully integrated autonomous Boolean reservoir computer.

C. Fundamental Mechanisms of Impact Initiation of Reactive Materials

Professor Dana Dlott, University of Illinois, Urbana-Champaign, Single Investigator Award

The objective of this research is to develop techniques to study impact-induced emission from nanotechnology reactive materials (RM) and use them to elucidate the fundamental mechanisms involved in impact ignition. For this study, tiny laser-launched flyer plates will impact reactive material samples and high-speed emission spectroscopy will be used to measure their dynamics. The time dependence of emission from exploding RM is usually limited by the size of the charge. The research will use such a small charge that the time dependence is limited by fundamental processes such as initiation and ignition.

It is anticipated that in FY14, the development, initial testing, and characterization of the laser flyer plate technique will be completed, with a target flyer plate velocity in excess of 5km/s. Additionally, test instrumentation will be used to perform basic shock compression science and shock spectroscopy measurements, and study RM impact ignition with an initial selection of a variety of interesting and useful RMs. These measurements will help to better understand the relationships between nanostructure and impact response to aid the development of future multifunctional RM.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Ralph Anthenien
Division Chief
Program Manager, Propulsion and Energetics

Dr. Samuel Stanton
Program Manager, Complex Dynamics and Systems

Dr. Larry Russell, Jr.
Program Manager (Acting), Solid Mechanics

Dr. Frederick Ferguson (IPA)
Program Manager, Fluid Dynamics

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 2013* is to provide information on the programs and basic research supported by ARO in FY13, 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 FY13.

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 research 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, 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 its research portfolio 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

The Network Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY13, the Division managed research 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 to pursue the program's long-term goal. The Wireless Communications Networks Thrust supports research 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 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 Sciences Division for FY13 were $43.1 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY13 ARO Core (BH57) program funding allotment for this Division was $4.9 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 $7.0 million to projects managed by the Division. The Division also managed $28.5 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 $0.3 million for contracts. Finally, $2.3 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 creation, leadership, and management of 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 FY13 (*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 FY13 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 FY13, the Division awarded nine 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 the theoretical underpinnings for a computational model that supports scalable reasoning, create new source/channel coding strategies for communicating in the presence of adversarial attacks, and to determine new methods for online learning of novel forms of locomotion in autonomous vehicles and robots by developing methods for global optimization. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Howard Choset, Carnegie Mellon University; *Distributed Learning for Complex Policies*
- Professor Christopher Davis, University of Maryland - College Park; *Free Space Optical and Hybrid Communication Systems for Robotics and Situational Awareness*
- Professor Subbarao Kambhampati, Arizona State University; *Long-Term Continual Planning for Remote Human-Robot Teaming in Open Worlds*
- Professor Thomas Malone, Massachusetts Institute of Technology; *How Does Unit Size Affect Collective Intelligence in Online Groups?*
- Professor Nicholas Ouellette, Yale University; *Laboratory and Modeling Studies of Insect Swarms*
- Professor Anna Squicciarini, Pennsylvania State University; *Game Theoretic Approach to Modeling and Detecting Deviant Users in Online Social Networks*
- Professor Joshua Tenenbaum, Massachusetts Institute of Technology; *Fundamental Theory and Parallel Inference for Probabilistic Programming*
- Professor Aaron Wagner, Cornell University; *Communicating Under Adversarial Attacks: Models, Codes, and Fundamental Limits*
- Professor Lei Ying, Arizona State University; *Searching Information Sources in Networks*

2. Short Term Innovative Research (STIR) Program. In FY13, the Division awarded four new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to create novel algorithms to learn the structure of social networks, investigate the use of analog signal processing to cancel co-site interference to create a full duplex radio, and to determine the universal laws that support a unified theory of interdependent networks with cascading failures. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Animashree Anandkumar, University of California - Irvine; *High-Dimensional Learning in Social Networks*
- Professor Yingbo Hua, University of California - Riverside; *Online Tuning of All-Analog Radio Interference Cancellation*
- Professor Gabriel Silva, University of California - San Diego; *Information Flow and Capacity in Geometric Networks*
- Professor H. Stanley, Boston University; *Robustness of Inter Dependent Networks Subject to Cascading Failures*

3. Young Investigator Program (YIP). In FY13, the Division awarded three new YIP projects. These grants are driving fundamental research, such as studies to discover the structure and temporal dynamics of large high dimension social networks to derive tools for analyzing and influencing the networks, determine methods of combining real time functional magnetic resonance imaging with knowledge of the human valuation system to counteract sub-optimal decisions, and to create new machine learning algorithms by combining both data driven and knowledge driven methods. The following PIs and corresponding organizations were recipients of the new-start YIP award/awards.

- Professor Animashree Anandkumar, University of California - Irvine; *Learning, Dynamics and Intervention in Large-Scale Social Networks*
- Professor Andrew Brooks, Emory University; *Optimizing Decision Making Using Real Time Functional Magnetic Resonance Imaging*
- Professor Sriraam Natarajan, Indiana University at Bloomington; *Human In the Loop Statistical Relational Learners*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conference was held in FY13 and was supported by the Division. As with other grants in this category, the support was provided via a competitive grant to academic researchers responsible for organizing or leading the scientific conference.

- *2013 Robotics Science and Systems Conference*; Berlin, Germany; 24-28 June 2013

5. Special Programs. In FY13, 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 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 FY11 and was awarded to a team led 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.

4. 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 of the University of Pennsylvania, with participation from researchers at MIT, Stanford, Cornell, and Georgia Tech. The objective of this MURI is to find synergy in methods and models from work in social sciences, engineering, network sciences, and mathematics to develop new techniques and mathematical models that would explain societal events not *posterior* but as they are happening, based on detailed analytical models of social systems. The team hopes to use a unified yet interdisciplinary lens that goes beyond social and political sciences, and adequately covers the full spectrum from rigorous math-based theory and modeling to large scale data extraction and analyses and from multi-agent simulation to controlled lab experiments and field surveys. The results of the MURI may have significant impact on the Army and DoD to understand cataclysmic changes, such as the Arab Spring, as they are about to happen.

5. Control of Complex Networks. This MURI began in FY13 and was awarded to a team led by Professor Raissa D'Souza of the University of California at Davis. The goal of this MURI project is to develop rigorous principles to predict and control behaviors of systems made of interdependent networks. This will be accomplished through an interdisciplinary approach synthesizing mathematical theories from statistical physics, control theory, nonlinear dynamics, game theory, information theory, system reliability theory, and operations research. The results will be informed and validated by empirical studies of real-world systems from nanoscale mechanical oscillators, to collections of interdependent critical infrastructure systems, to data on coalitions and conflict in primate societies, to longitudinal data on the evolution of political networks of nation states and task-oriented social networks in open source software. The focus is to develop new approaches that exploit network interdependence for network control, and this diversity of empirical testbeds is central to developing robust theoretical principles and widely applicable methods.

It is expected that this MURI will lead to (i) network interventions that prevent cascades of failure in critical infrastructures, (ii) novel control schemes relying on control actions and local interventions, (iii) rigorous principles for multi-modal recovery of heterogeneous systems, (iv) shaping human social response via designed incentives that align human behavior with the capabilities of technological networks, (v) design of networks of nonlinear nanoelectromechanical oscillators that exploit coupling and nonlinearity to create coherent motion, (vi) new mathematical structures for representing and analyzing networks-of-networks, especially with respect to control theory, and (vii) fundamental bounds on controllability of interdependent networks and rigorous techniques to identify which network layers are easiest to steer.

The anticipated impact on DoD Capabilities is broadly applicable to controlling a disparate collection of autonomous agents interacting through numerous networks in noisy, dynamic environments with a myriad of time-scales and length-scales. Results can be applied to security (and restoration) of critical infrastructures, supply chains, political alliance dynamics (including upheavals such as Arab Spring), conflict, risk, social dynamics, and collective action. It is also reasonable to expect that there will be new levels of nanoscale functionality in the NEMs device developed, enabling new technologies and devices.

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

Research 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 FY13, the Division managed two new-start Phase I 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 a system that integrates and fuses information from disparate sensors to aid command-level decisions, and artificial intelligence technology for building Associate systems.

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

No new starts were initiated in FY13.

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 FY13, the Division managed five 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 FY13.

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 FY13, the Division managed six new DURIP projects, totaling $1.13 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of multi-agent autonomous systems, microrobotics, brain-computer interfaces, and novel wireless networking protocols.

H. DARPA Anomaly Detection at 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 funded and/or monitored by the Network Sciences Division.

A. Dynamics and Control of Discrete State Networks

Professor Daniel Gauthier, Duke University, Single Investigator Award

The objective of this research is to lead an experimental program in fundamental network science to observe and analyze the evolution of complex dynamical networks such as synchronization, pattern formation and control, and emergence of complexity. Specifically, researchers are studying time-delayed Boolean networks implemented experimentally with logic gates on field-programmable gate arrays (FPGAs). This experimental platform has already created diverse networks that display periodic, chaotic, and excitable (neural-like) dynamics. The research approach consists of a devising a Boolean analogy to a given physical phenomenon occurring in networks (e.g., chaos, excitability, phase locking, synchronization patterns), designing an experimental embodiment, and proposing mathematical models (*e.g.*, Boolean delay equations (BDE), Glass models) to analyze and interpret experimental findings.

During FY13, researchers created and analyzed the dynamics of larger and more realistic neural-like networks with similar features (size and topology) to those that are closer to their biological counterparts. These types of networks are promising for possible applications in signal processing. They also developed a novel architecture to create a Boolean analog of a Kuramoto oscillator that will be the basis of future work on large-scale network ensembles of coupled periodic oscillators.

Most importantly, this research experimentally demonstrated a new strategy to potentially control extreme events in complex systems such as financial crises, rogue ocean waves, power blackouts, or epidemics. The technique builds on a recent discovery of intrinsic feedback mechanisms in complex systems, known as Dragon Kings, which continually amplify small disturbances and lead to alarmingly high probabilities for catastrophic extreme events. By examining the dynamics of a class of complex systems, researchers demonstrated that Dragon Kings could be forecasted and suppressed through a feedback method requiring a series of very weak occasional impulses on the order of less than 1% of the system size. This presents a major advance in the controllability of complex systems and networks; however more research is needed to understand if the parameters that most influence emergence of extreme events are reachable (see FIGURE 1).

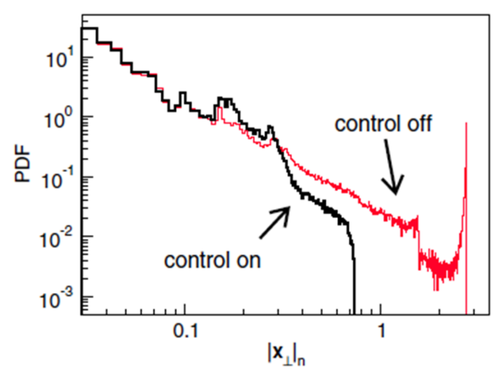

FIGURE 1

Slaying dragon kings. Intrinsic feedback structures in complex networks have shown that rare events can be more common than previously thought. Preliminary results, however, suggested that such events are in fact both predictable and controllable.

B. Cognitive Protocol Stack Design

Professor Ramesh Rao, University of California - San Diego, Single Investigator Award

The goal of this research is to investigate the interactions of a wireless communications network using stochastic graphical models. In FY13, the research team derived models that model the interactions between network layers in the protocol stack, as well as the interactions between the network protocols and the environment (including both load from the user and changes in the radio propagation environment) using Bayesian network analysis. Using this modeling technique, retransmission strategies were investigated for multi-user detection decoding schemes that can be applied to secondary users of cognitive radio network. The Bayesian network approach was demonstrated in a protocol design, which employed different retransmission schemes, with the aim of successfully delivering the data packet with limited impact on the rest of the network. The Bayesian analysis approach was also utilized to analyze cooperation between two collocated multihop networks, such as may exist between two government entities or in a coalition scenario. During a learning phase, the probabilistic relationships among all the parameters are learned from the data and summarized in a Bayesian network. This model was utilized to calculate a cost metric that is used to model the interaction between the two networks using a game theoretic approach. The results from these analyses show that even when only a small fraction of the nodes is shared, a significant gain can be obtained. In particular, for both lightly and heavily loaded scenarios, the selection scheme based on game theory can achieve almost the same performance as a full cooperation scheme for the different cost metrics considered.

C. Integrative Perception and Action

Professor Ashutosh Saxena, Cornell University, Single Investigator Award

Research in robotics and integrated intelligence depends upon bringing together studies in vision, knowledge representation, reasoning, learning, and control aspects. While vision plays a central role in integrated intelligence, it is mostly used as a separate component of the system and, thus. not tightly integrated with the control or learning. The objective of this research is tight integration of perception and control using deep learning as the main mechanism, starting with a lower dimensional percept and then learning successively more refined information until as needed by the controller and planner.

One goal of this project is to get robots to be able to perform actions in an unstructured human environment with objects, such as opening doors or grasping objects. The approach used is one of discovering representations that enable the robot to go from perceiving its environment to performing meaningful actions. To achieve this, in FY13, the Cornell team used multi-modal RGB-D (video with dimensional space data) to create a new representation using deep learning. Using conditional random fields, which allow one to represent the actions of humans, environment, and robots, the team created new planning algorithms for anticipating future human actions (see FIGURE 2).

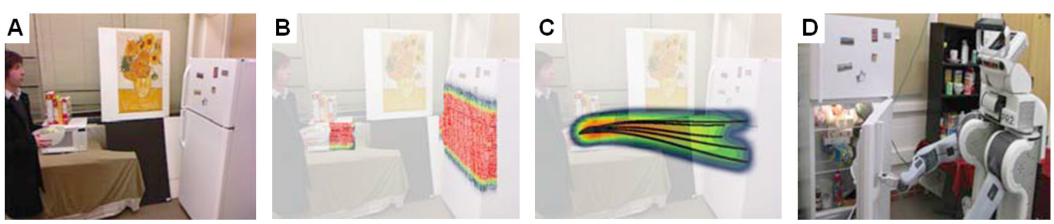

FIGURE 2

Integrative perception and action of robots. This research is integrating perception and control to ultimately enable robot actions in unstructured human environments. The panels illustrate (A) the test robot's RGB-D view, (B) the affordance heatmap, (C) the trajectory heatmap, and (D) the robot successfully opening the door.

D. Biophysical Model of Cortical Network Activity

Professor Stan Anderson, Johns Hopkins University, Single Investigator Award

The objective of this research is to perform cortical mapping using electrical stimulation to define function and behaviors, such as decision behaviors. In FY13, a large-scale neural network simulation with realistic cortical architecture was initiated to investigate the effects of external electrical stimulation on the propagation and evolution of ongoing seizure activity. The model includes seven neuron classes organized by cortical layer, inhibitory or excitatory properties, and electrophysiological characteristics. The cell dynamics are governed by a modified version of the Hodgkin-Huxley equations in single compartment format. Axonal connections were patterned after histological data and published models of local cortical wiring. Stimulation-induced action potentials take place at the axon initial segments, according to threshold requirements on the applied electric field distribution, and stimulation-induced action potentials in horizontal axonal branches are also separately simulated. Clear differences in seizure evolution are presented for stimulated versus undisturbed rhythmic activity. Data is provided for frequency dependent stimulation effects demonstrating a plateau effect of stimulation efficacy as the applied frequency is increased from 60 Hz to 200 Hz. Timing of the stimulation with respect to the underlying rhythmic activity demonstrates a phase-dependent sensitivity. Using a dipole stimulation electrode arrangement, clear orientation effects of the dipole with respect to the model connectivity has also been demonstrated. A sensitivity analysis of these results as a function of the stimulation threshold is also provided.

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. Information-Driven Blind Doppler Shift Estimation and Compensation Methods

Investigator: Professor Paul Cotae, University of District of Columbia, HBCU/MI Award
Recipient: Naval Research Lab

The goal of this research is to explore different methods for blind Doppler shift estimation and compensation in underwater acoustic wireless sensor networks by analyzing experimental data. Methods of analysis have included power spectrum analysis, autocorrelation, and squaring time phase recovery to estimate Doppler shift in collaborative distributed underwater sensor networks. Optimum sensor locations were found using the Karush–Kuhn–Tucker (KKT) conditions considering the interference between the sensor nodes. During the Spring of 2013, Professor Cotae received a ONR Summer Faculty Fellowship and spent ten weeks at the NRL Center for High Assurance Computing. During this time, Professor Cotae transitioned his research findings to NRL, using the Matlab simulation code that has been transferred to NRL.

B. GraphLab - Middleware for Machine Learning on Distributed Systems

Investigator: Professor Carlos Guestrin, University of Washington, MURI Award
Recipient: GraphLab.com and In-Q-Tel

GraphLab is a graph-based, high performance, open source distributed computation framework written in C++. GraphLab was originally developed for Machine Learning tasks, but has found great success at a broad range of other data-mining tasks and has out-performed other abstractions, such as those based on Map-Reduce, by orders of magnitude. This software was developed as part of the Abductive Inference MURI (see Section II-B.1). In FY13, this software transitioned as an open source software to In-Q-Tel and GraphLab.com.

C. Aggressive Maneuvering Algorithms

Investigator: Professor Panos Tsiotras, Georgia Institute of Technology, MURI Award
Recipient: Ford Motor Company

The objective of this research is to develop neuro-inspired control theory that may ultimately apply to the aggressive motion of autonomous ground vehicles. In the course of this investigation, researchers began to study aggressive maneuvering of ground vehicles using low-level control actions in a control hierarchy. In particular, researchers examined the problem of vehicle posture control to create a yaw instability to enable a vehicle to rotate in a very short time interval. Optimal control theory was used to generate several solutions for a variety of speeds and friction coefficients. The approach was implemented to mitigate unavoidable T-bone collisions between two automobiles at an intersection. The maneuvering vehicle is assumed to possess torque vectoring technology at the rear wheels, allowing the generation of a direct yawing moment. In FY13, these results transitioned to Ford Motor Company. Future work will try to eliminate this restriction and execute these aggressive maneuvers with conventional controls (*e.g.*, steering and acceleration/braking).

V. ANTICIPATED ACCOMPLISHMENTS

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

A. Learning, Dynamics, and Intervention in Large-Scale Social Networks

Professor Anima Anndkumar, University of California - Irvine, Young Investigator Award

The objective of this research is to understand the structure and temporal dynamics of large, high dimension social networks and from this understanding derive tools for analysis and influence of these networks. The goals of the project fall naturally into three thrust areas. The first is learning the network structure including indirect interactions and hidden influences. The second is modeling and estimating the dynamical evolution of the network. The third is influencing the network to a more adventitious state or outcome.

In general, learning an unknown social network graph and parameters is an NP hard problem. It is anticipated that in FY14, techniques for learning hidden tree models will be applied to small world models, which are relevant to social networks. Exponential random graph attributed models (ERGAMs) will be used to model and understand network dynamics and equilibrium. Game theory techniques will be applied to ERGAMs in order to understand influencing the state of social networks. Tensor analysis will be utilized to model the higher dimensionality relationships of the networks that are not captured by conventional second order analysis.

B. Probabilistic Perception and Control

Professor Mark Campbell, Cornell University, Single Investigator Award

Current and future Army missions will require autonomous robotic systems for supply missions, information collection, decision aids, and warfare support. While current research in autonomous systems has made great strides in select areas such as perception algorithms or cooperative control, few robotic systems can operate intelligently, for months at a time, in complex and new environments without heavy human supervision. In FY14 researchers will develop a control and planning theory that not only enables planning in the presence of complex uncertainties, but also allows for continual improvement in performance over time. The approach will consist of the development of an evolving closed loop system that will be a mixture of parameterized controllers (*e.g.*, an *a priori* human derived controller that guarantees closed loop stability), along with non-parametric controllers (*e.g.*, developed using a Gaussian Process based model, which enables learning via data/experiences). The latter model allows uncertainties to be easily captured, and enables learning even in sparse data conditions. This research will explore (i) how to guarantee closed loop stability and continually improve performance, (ii) how to learn controllers that are computationally efficient, and will also (iii) develop a fundamental understanding of the relationship between the learned controller and model learning.

C. Domain Adaption for Intelligent Systems in Changing Environment

Professor Fei Sha, University of Southern California, Young Investigator Award

Autonomous systems and machine learning algorithms are typically trained on a class of examples before being deployed. Unfortunately, far too often, the probability distribution of the training set does not coincide with the distribution of the actual data that arise in practice leading, perhaps, to catastrophic failure of the autonomous system. The goal of this research is to exploit the intrinsic structure of the data to learn kernels, which can then be used to measure similarity between two different domains leading to discovery of maps between prior experience and new domains. During FY14 Professor Sha's laboratory will investigate the use of the discriminative clusters to build logical characterization of domains. Furthermore, he will also consider the problem of characterizing non-stationary domains using the history of changes. Finally, the research team will apply the resulting algorithms to vision problems in the context of robotics.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Purush Iyer
Division Chief
Program Manager, Intelligent Networks

Dr. Janet Spoonamore
Program Manager (Retired), 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

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 2013* is to provide information on the programs and basic research supported by ARO in FY13, 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 FY13.

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 this research 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 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 research 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 research with the Electronics Division is 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 its research portfolio 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

The Physics Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY13, the Division managed research within these four Program Areas: (i) Atomic and Molecular Physics, (ii) Condensed Matter Physics, (iii) Optical Physics 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 is cooled the quantum nature dominates and the atoms behave 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. Optical Physics 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) Extreme Light and (ii) Meta-optics. 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. Research in the Meta-optics Thrust includes studies of optical angular momentum (OAM) beams, interactions with metamaterials, and novel optical physics. An example is the study of OAM beams and how they interact with metamaterials, or how they can be used to induce new kinds of interactions or physics. Another area of interest regards overcoming losses in metamaterials. Cloaking is a well-known ideal, but losses and the dispersion must be oversome before this is a reality in the practical sense. In addition, other fields which may be used in place of electrodynamics are of interest to this program.

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 FY13 were \$57.8 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY13 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 \$11.5 million to projects managed by the Division. The Division also managed \$3.2 million of Defense Advanced Research Projects Agency (DARPA) programs, and \$36.0 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided \$0.4 million for contracts. Finally, \$0.7 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes \$0.2 million provided through the ARO Core (BH57) allotment, in addition to funding for 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 creation, leadership, and management of 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 FY13 (*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.

The following subsections summarize projects awarded in FY13 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 FY13, the Division awarded ten 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 the infrared and optical responses of electrostatically induced effects in correlated oxides, to investigate new synthetic physics in cold quantum gases, and to discover radically new techniques and materials to control the manipulation of light. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Dimitri Basov, University of California - San Diego; *Electric Field Control of Phase Transitions in Correlated Oxides*
- Filippo Capolino, University of California - Irvine; *Linear and Nonlinear Properties of Loss-Compensated Metamaterials*
- Jonathan Dowling, Louisiana State University and A&M College; *From Quantum Computing to Quantum Sensing*
- Victor Galitski, University of Maryland - College Park; *New Synthetic Physics in Ultracold Quantum Gases*
- David Hsieh, California Institute of Technology; *Optical Spectroscopy and Imaging of Correlated Spin-Orbit Phases*
- Ramki Kalyanaraman, University of Tennessee at Knoxville; *Ferroplasmons: Theory and Experimental Investigations of Visible Light Plasmons in Ferromagnets*
- Steven Olmschenk, Denison University; *Laser Cooling Trapped Ions With Telecom Light*
- Alexander Rimberg, Dartmouth College; *Quantum Limited Electrometry and Ultra-Strong Photon-Phonon Coupling using a Cavity-Embedded Single Cooper Pair Transistor*
- Vladimir Shalaev, Purdue University; *Flat Photonics with Metasurfaces*
- Martin Zwierlein, Massachusetts Institute of Technology; *Strongly Correlated Quantum Gases of Atoms and Dipolar Molecules*

2. Short Term Innovative Research (STIR) Program. In FY13, the Division awarded six new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to explore nonequilibrium floquet states in topological Kondo insulators, and to explore ultra-low loss optomechanics using diagmagnetically levitated drops of liquid helium. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Alexander Burin, Tulane University; *Theoretical Investigation of the Non-equilibrium Dielectric Response of Two-level Defects Within the Superconducting Qubits.*
- James Davis, Cornell University; *Visualizing Quantum Critical Electronic Matter*
- Jack Harris, Yale University; *Ultralow Loss Optomechanics Using Diagmagnetically Levitated Drops of Liquid Helium*
- Anantharaman Kumarakrishnan, York University; *Grating Echo Atom Interferometer for Inertial Sensing Using Ultracold Atoms*
- Johnpierre Paglione, University of Maryland - College Park; *Nonequilibrium Floquet States in Topological Kondo Insulators*
- Qimiao Si, William Marsh Rice University; *Spin-Orbit Coupling and Novel Electronic States at the Interfaces of Heavy Fermion Materials*

3. Young Investigator Program (YIP). No new starts were initiated in FY13.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY13 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 Novel Topological Quantum Matter*; Dallas, TX; 25-26 February 2013
- *Workshop on the Development of Man Made Electronic Materials and Devices: Past and Future*; Charlotte, NC; 5-7 May 2013
- *International Conference on Laser Spectroscopy*; Berkeley, CA; 9-14 June 2013
- *Conference on Coherence and Quantum Optics and the Quantum Information and Measurement Meeting*; Rochester, NY; 17-20 June 2013
- *Atomic Physics Gordon Research Conference*; Newport, RI; 23-28 June 2013
- *Majorana Fermions in Condensed Matter Physics Conference*; Erice, Italy; 12-18 July 2013
- *Quantum Control of Light and Matter Gordon Research Conference*; South Hadley, MA; 28 July - 2 August 2013
- *Complex Oxide Interfaces Workshop*; Stanford, CA; 6-8 August 2013

5. Special Programs. In FY13, 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 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.

9. 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.

10. Non-equilibrium many-body dynamics. This MURI began in FY13 and was awarded to a team led by Professor Cheng Chin at the University of Chicago. The goal of this MURI is to study fundamental non-equilibrium dynamics using cold atoms in optical lattices.

Dynamics far from equilibrium is of great importance in many scientific fields, including materials science, condensed-matter physics, nonlinear optics, chemistry, biology, and biochemistry. Non-equilibrium dynamics recently has taken on significance in atomic physics, where new tools will enable breakthroughs. In particular, optical lattice emulation is allowing one to gain insight, and potentially solve, traditionally intractable problems, including non-equilibrium. Breakthroughs in other disciplines are also enabling a new look at non-equilibrium. In materials science, a recent pump-probe experiment enabled dynamical control of material properties.[2] Another example is in biochemistry, in determining the role that non-equilibrium phase transitions play in driven biochemical networks, e.g., canonical phosphorylation-dephosporylation systems with feedback that exhibit bi-stability.[3-4] Despite the ubiquitous nature of non-equilibrium dynamics, little scientific progress has been made due to the many challenges, such as the difficulty in finding many-body systems that remain far from equilibrium on experimentally accessible time scales.

The objective of this MURI project is to discover how many-body systems thermalize from non-equilibrium initial states, and explore the dynamics of far-from-equilibrium systems. Given that non-equilibrium dynamics plays an important role in many scientific and engineering areas, such as quantum sensing and metrology, atomtronics, and quantum chemistry, this research could ultimately lead to the development of dynamic materials, and devices for improved computation, precision measurement, and sensing.

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

[2] Goulielmakis E, Yakovlev VS, Cavalieri AL, et al. (2007). Attosecond control and measurement: lightwave electronics. *Science*. 317:769-775.

[3] Qian H. (2006). Open-system nonequilibrium steady state: statistical thermodynamics, fluctuations, and chemical oscillations. *J. Phys. Chem. B*. 110:15063-15074.

[4] Ge H and Qian H. (2011). Non-equilibrium phase transition in mesoscopic biochemical systems: from stochastic to nonlinear dynamics and beyond. *J. R. Soc. Interface*. 8:107-116.

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

No new starts were initiated in FY13.

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 FY13, 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 developing a high-speed single-photon counter for potential use in quantum communications, hyperspectral imaging, and florescence spectroscopy.

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 FY13, the Division managed one new ARO (Core) HBCU/MI project and six 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. Non-equilibrium Dynamics with Ultracold Atoms. The objective of this PECASE, led by Professor David Weld at the University of California – Santa Barbara, is to investigate non-equilibrium many-body quantum dynamics using ultracold lithium atoms in an optical trap.

The behavior of non-equilibrium many-body quantum systems is not well understood; therefore, predicting and controlling the behavior of these systems is a major challenge of modern physics. Existing theoretical and experimental tools for addressing many-body systems far from equilibrium are limited. Due to their experimentally accessible timescales and exquisite controllability in both space and time, optically trapped ultra cold atomic gases are an ideal context in which to study many-body non-equilibrium dynamics in the quantum regime. This research is pursuing the development of an experimental platform using ultracold lithium atoms in dynamically-configurable optical traps to investigate two broad classes of non-equilibrium phenomena: quantum quenches and driven systems. Major advances in knowledge and control of non-equilibrium many-body quantum dynamics may enable the development of novel materials and computational abilities beyond classical computers.

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 FY13, the Physics Division managed nine new DURIP projects, totaling $1.3 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of topological insulators and spin-dependent optical lattices.

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 ARO-supported research 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 funded and/or monitored by the Physics Division.

A. Ferromagnetism In a 2D Electron Gas

Professor Susanne Stemmer, University of California - Santa Barbara, MURI Award

The MURI team led by Professor Stemmer is investigating methods for the control of correlations at complex metal oxide interfaces, with the ultimate goal of predicting, understanding, and controlling the many-body properties of complex oxide heterostructures. In FY13, the research team reported that correlations in an ultra-high density electron gas at a complex oxide interface induced a magnetic state in an otherwise insulating and non-magnetic oxide.[5]

Complex oxides represent a class of materials which can hold extreme electron densities compared to semiconductors, with the ability to support electron densities at which Coulomb correlations may dominate the electronic characteristics of the material. Accordingly, correlated electron effects such as high temperature superconductivity (copper oxides) and colossal magnetoresistance (manganese oxides) are readily observed in complex oxides. Roughly a decade ago, interfaces between complex oxides were shown to exhibit characteristics foreign to either oxide that formed the interface, setting off a research endeavor to discover new correlated electron effects or to otherwise control these phenomena in oxides. In $LaAlO_3/SrTiO_3$ (LAO/STO) interfaces, the most well known complex oxide heterostructure, a 2D electron gas (2DEG) is formed at the interface. An exciting discovering in such interfaces would be the observation of exchange-induced ferromagnetism in a 2DEG. Ferromagnetism has been observed in the LAO/STO interfaces; however, the relatively low free electron density and non-uniformity suggest that impurities rather than the exchange mechanism between free electrons is the origin.

Recently, Professor Stemmer investigated $GdTiO_3/SrTiO_3$ (GTO/STO) interfaces with exceptional success. The researchers discovered that the band alignment and charge discontinuity between these two oxides was favorable for inducing a 2DEG in the STO at the interface. In single interfaces and superlattices, the team found that unlike the LAO/STO interface, GTO/STO supports ~3×10^{14} cm^{-2} free carriers per interface in accordance with the simplistic polar discontinuity model. In layers of $SrTiO_3$ with only a few unit cells, the carrier concentration approaches one electron per unit cell where correlation effects are expected to occur. This density is well over an order of magnitude higher than what has been achievable in LAO/STO to date and should be favorable for ferromagnetic effects. Indeed magnetization was found to appear at low temperatures (see FIGURE 1).

However, $GdTiO_3$ is ferrimagnetic with magnetization as measured by the research team. If this proximity effect is the case, hysteresis in magnetoresistance studies would reflect the orientation of the magnetization of the $GdTiO_3$. If the magnetization were due to exchange interaction in the free electrons in the $SrTiO_3$, the magnetoresistance would have a different relationship to the orientation of an external magnetic field. The two phenomena are distinguishable. Studies in FY13 confirmed the relationship that corresponds to exchange interaction-induced ferromagnetism in the $SrTiO_3$. Further evidence that the $GdTiO_3$ is not inducing the ferromagnetism is that the onset of the magnetization occurs at a different temperature than that of $GdTiO_3$ and that thicker films of $SrTiO_3$ (thus having roughly half the electron density) do not exhibit the hysteretic effects.

These results give strong evidence that strong correlations can be induced in suitably chosen complex oxide heterostructures. Accordingly, it is hopeful that more exotic correlations – perhaps high temperature superconductivity – may be designed or discovered at complex oxide interfaces.

[5] Jackson CA, Stemmer S. Interface-induced magnetism in perovskite quantum wells. (2013). *Phys. Rev. B* 88:180403(R); See also Moetakef P, et. al. (2012). Carrier-Controlled Ferromagnetism in $SrTiO_3$, *Phys. Rev. X* 2:021014.

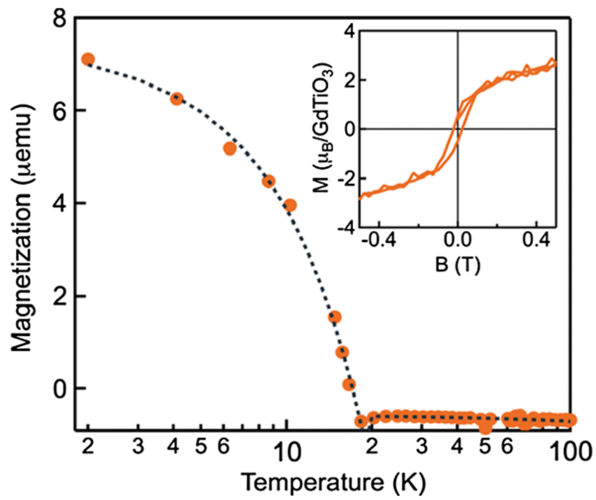

FIGURE 1

Magnetization of a 2DEG in GTO/STO. The magnetization was measured in 10 mT for a 4 nm $GdTiO_3$/1 nm $SrTiO_3$/4 nm $GdTiO_3$ heterostructure. The inset shows the hysteretic characteristics of the sample at a temperature of 2 K.[6]

B. Light Filamentation Science

Professor Martin Richardson, University of Central Florida (UCF), MURI Award

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 phenomenon first observed 18 years ago. When the power of an ultra-short laser beam exceeds a certain critical value (~ 3 GW), the beam begins to self-focus, seemingly defying the laws of diffraction, due to a non-linear increase in the refractive index. The diameter of the beam diminishes with distance, and its intensity consequently increases until it reaches a value of ~5×10^{13} $W \cdot cm^{-2}$, at which point partial ionization of the nitrogen in air begins to provide a compensating negative change to the overall refractive index, thereby stabilizing the beam into a ~100 μm diameter filament, surrounded by a penumbral 'carrier field' propagating for hundreds of meters with these high intensities. Moreover, by adjusting the properties of the outgoing laser beam, one can utilize the dispersion of the air itself to delay the onset of this self-focusing phenomena for at least a kilometer, and most probably several tens of kilometers. Intensities this high are large enough to ionize any material, and can in fact produce high temperature plasmas on solid surfaces. Thus, the filamentation process can enable the projection of laser intensities that are orders of magnitude more intense than can ever be projected by classical optics and linear laser beams. This opens to conjecture new applications of high pulsed power laser intensities projected to intermediate and long-range distances.

The Richardson laboratory and the University of Central Florida (UCF) have been building new Ti:Sapphire laser systems for filamentation studies; however, compact ultrafast fiber lasers have been coming close in performance levels to replace the complex laboratory architecture of Ti:Sapphire lasers. The fiber amplified laser architecture, with hybrid fiber and diode-pumped solid state lasers will eventually enable the fabrication of compact efficient ruggedized filamentation lasers suitable at lower cost for field operations, operating at kHz repetition-rates. UCF has been developing the first of this new breed of filamentation lasers. New phase-control modifying optics have been transforming conventional laser beams into photonic structured light configurations that would have been unimaginable a few years ago.

In FY13, the MURI team demonstrated the effect of these optics on an initially Gaussian beam profile (see FIGURE 2). Organized arrays of multiple filaments like these may permit electric or EM radiation guiding.

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[6] Moetakef P, et. al. (2012). Carrier-Controlled Ferromagnetism in $SrTiO_3$, *Phys. Rev. X.* 2:021014.

In a recent paper, MURI team member Prof. Natalia Litchintiser, in collaboration with UCF, described the microwave guiding effects of a rectilinear array of filaments.[7] The team completed model calculations that showed the propagation of a microwave beam, initially in free space then propagated through a transient photonic structure created in air by a rectangular array of light filaments.

In addition, the Richardson laboratory has been investigating ways to create 'massive arrays' of organized filaments, as many as 100 individual filaments. The potential and outcomes of filamentation in these new regimes are largely unknown at present, but their impact is expected to be profound. A new problem the Richardson team is examining is the effect of filamentation on clouds. Few studies have so far been performed in this area. Cloud aerosol droplets and dust particles in the air are of a similar size to the diameter of a filament. It is known that if a filament hits an obstacle this size head-on, then the majority of the filament intensity, and its carrier field is transmitted past the obstacle and reforms a new filament downstream. If the obstacle was a cloud aerosol, than it would immediate explode into an ionized vapor ball. The investigators have shown this interaction at a laser intensity below that for filamentation to occur, and is currently assembling the optical diagnostics to investigate the explosion that immediately occurs in this case.

A final challenge to the comprehensive study of filamentation in the atmosphere is primarily one of logistics. It must be noted that the longest range over which any filamentation phenomena in air have been studied in detail (in the open literature) is ~ 1.5 km[2]. Indeed many photographs of white light emanating from optical filaments projected 10's km have been shown in the literature. Logistically, it is difficult to obtain access to a secure range has been very limited. Moreover, the available current mobile laser systems have not been available for such studies, but until comprehensive knowledge of the characteristics of a single filament is demonstrated, their application relatively limited. To this end, the MURI team is building up an effort to locate a high power femtosecond laser at the Townes Institute Innovative Science and Technology Experimentation Facility laser range. This facility will ultimately permit laser-ranging tests up to 15 km in distance.

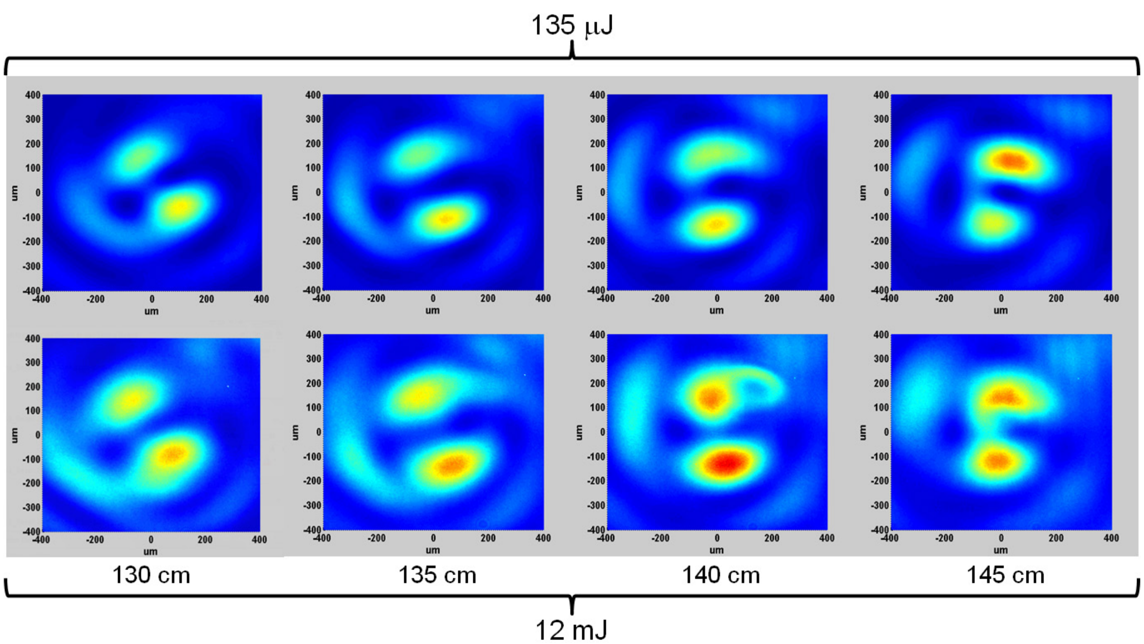

FIGURE 2

Effect of new phase-control modifying optics on an initially Gaussian beam profile. The panels show an anti-clockwise rotation of two helical filaments created with double Bessel function phase-plate axicon diffraction optics.

[7] Kudyshev ZA, Richardson MC, Litchinitser NM. (2013). Virtual hyperbolic metamaterials for manipulating radar signals in air. *Nature Communications*. 4, Article number: 2557.

C. All-Electrical Control of Single Spins in Semiconducting Nanowire Quantum Dots

Professor Jason Petta, Princeton University, PECASE

The goal of this PECASE is to develop an experimental platform that allows "all-electrical" control of spin for quantum information processing. Single-spin control has been achieved using conventional magnetic resonance, but this method has at least two drawbacks: (i) the ac magnetic fields achieved are small, and (ii) the AC magnetic fields are difficult to localize, which limits the ability to address single spins without affecting neighboring spins. In this project, all-electrical control is being achieved using electrically driven spin resonance, where an ac electric field is applied to a depletion gate on an indium arsenide (InAs) nanowire quantum dot. The spin-orbit interaction converts the applied ac electric field into an effective ac magnetic field, resulting in single spin rotations. InAs wires are utilized due to the larger g-factor and shorter spin-orbit length, which will potentially improve speed of operation.

Previously a MOCVD reactor for the growth of high quality, single crystalline InAs nanowires was developed. While the nanowires were of sufficient quality to conduct early experiments, the growth method resulted in significant variation in terms of wire lengths and diameters. This is especially problematic in the bottom-gated qubit architecture that is used in experiments. In the previous process, nanowires are randomly dispersed across a substrate with pre-fabricated gate arrays. Certain number of nanowires land nicely across a gate array. Such nanowires are then used to form double quantum dots. Variations in wire properties decrease yield. To overcome the random growth nature of the prvious process, a templated nanowire growth process has been developed. Here nanowire catalyst particles are deposited on the growth substrate in a regular pattern. Regular arrays of nanowires with homogeneous inter-wire spacing and tightly controlled nanowire diameters are grown using the catalyst template. A typical successful growth chip with a rectangular array of nanowires is shown in FIGURE 3.

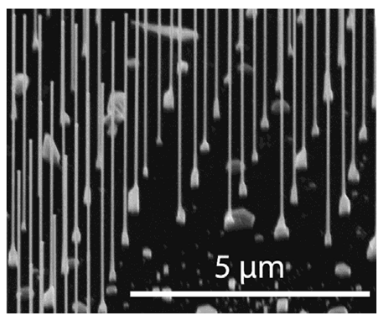

FIGURE 3

Array of nanowires with uniform 2µm spacing grown using a MOCVD process. Gold catalyst particles are defined using electron beam lithography and liftoff.

Utlizing the developed capability to fabricate regular arrays of nanowires, single InAs nanowire were coupled to a low quality factor resonator. Basic charge sensing using the technique of RF-reflectometry was demonstrated. Using this technique, the total charge parity at an interdot charge transition in a double quantum dot was measured. Due to spin blockade, even parity charge transitions are not visible in the dispersive measurement at high magnetic fields, while the RF response is field insensitive for odd parity interdot charge transitions (see FIGURE 4). This not only allows for a direct measurement of the charge parity, but also showcases the spin-sensitive nature of the RF-reflectometry technique.

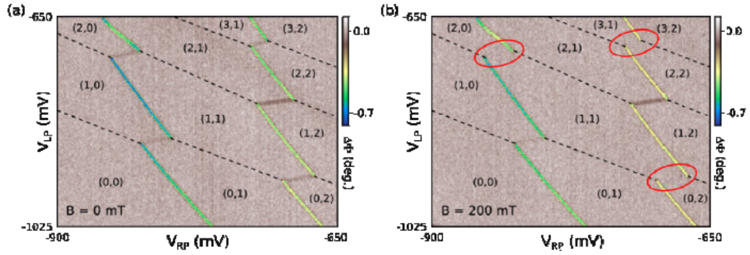

FIGURE 4

Charge sensor response as a function of gate voltages. (A) Zero magnetic field and (B) 200 mT magnetic field. Notice the visibly decreased response for even parity transitions in (B).

D. Quantum-Optical Circuits of Hybrid Quantum Memories
Professor Jacob Taylor, University of Maryland, MURI Award

As part of the MURI team led by Professor Christopher Monroe (refer to Section II.B.2), this research is contributing to studies to convert quantum information from one platform to the other without losing the quantum nature of the information. More specifically, the Taylor laboratory has been exploring the use of photonics to control topological features.

In FY13, the Taylor laboratory demonstrated topological edge states of light in a two-dimensional system (see FIGURE 5). The team's discovery demonstrated the potential of using photonics to control topological order in both non-interacting and many-body regimes.

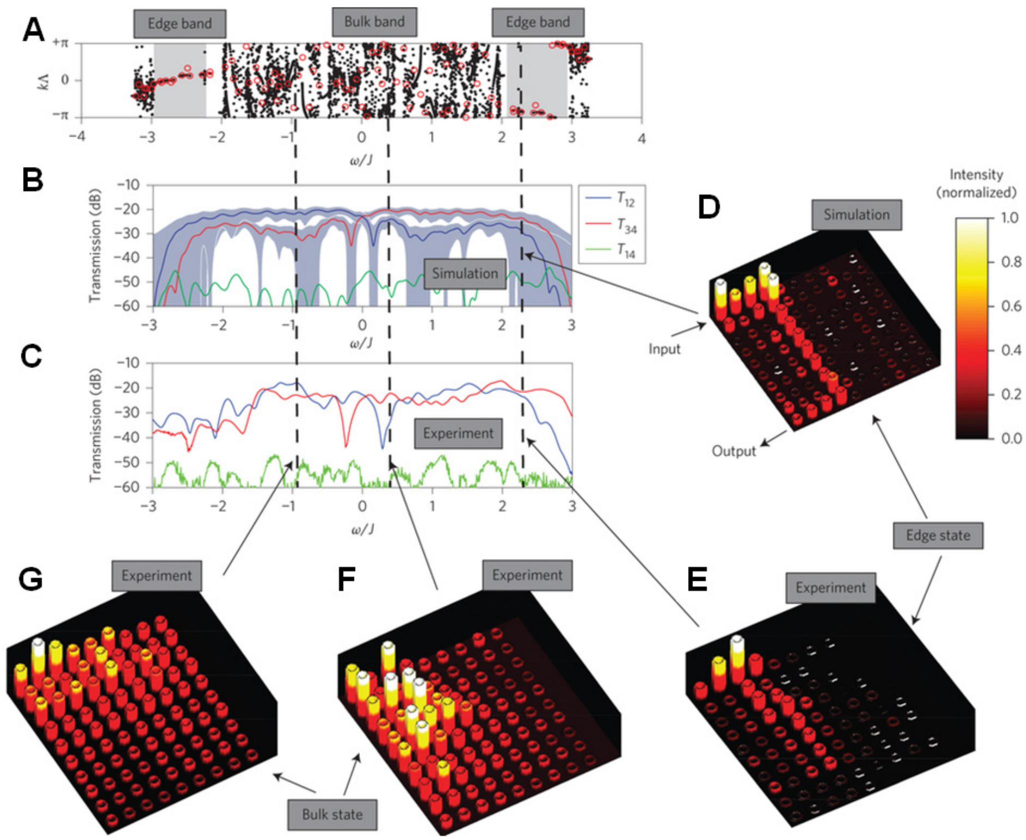

FIGURE 5

Edge states around a magnetic domain. (**A**) Simulated dispersion of the system: kΛ is the relative phase between two adjacent resonators on the edge while ω is the relative detuning of frequency with respect to the band center, in units of the tunneling rate. Red dots represent the dispersion in the system, black dots represent simulation of a longer system (10×400), to better distinguish the bulk band from the edge band. (**B**) Simulated transmission of a 10x10 lattice. T_{ij} is the transmittance between port i and j. T_{14} measures the backscattered light. Simulation parameters are estimated from the experiment. (**C**) Measured transmission spectrum. (**D**) Simulated scattered light from a 2D array of the couple resonators, when the system is pumped at the edge state band (**E**) Image of the edge state; the system is pumped at the frequencies corresponding to edge state band. (**E-G**) Image of bulk states; the state is pumped at frequencies that are in the bulk state band.[8]

[8] Hafezi M, Mittal S, Fan J, Migdall A, Taylor JM. (2013). Imaging topological edge states in silicon photonics. *Nat Photon.* 7:1001-5.

E. Quantum Computing and Control, and Quantized Nonlinear Optics with Superconducting Circuits
Professor Andrew Houck, Princeton University, PECASE

The objective of this research 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. The Houck laboratory has been exploring 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.

In FY13, the research team investigated coupled arrays of microwave cavities for purposes of quantum simulation. The focus has been on the two-dimensional Kagome lattice, the most natural lattice for transmission line cavities due to symmetry of cavity-cavity connections. Arrays of more than 200 cavities have been fabricated and transmission measurements on several arrays of a dozen cavities were performed (see FIGURE 6). Disorder in these lattices has been characterized extensively, finding that the disorder is primarily caused by fluctuations in kinetic inductance due to small device variations. With suitable design, this can be made smaller than two parts in ten million, small enough for quantum simulation. Further, qubits have been added to the cavities with the goal of studying many-body effects. Initially, phase transitions in a two-cavity two-qubit sample with large photon number have been studied. This is a small enough system that can be completely controlled, while still complex enough that many-body effects can be observed. In particular, with strong photon-photon interactions, photons localize to one cavity; with smaller interactions, photons oscillate between these cavities. Because interaction strength varies with photon number, this leads to a dynamical phase transition in which the behavior of the system exhibits one of two possible behaviors depending on starting conditions, with a sharp crossover occurring at a critical photon number.

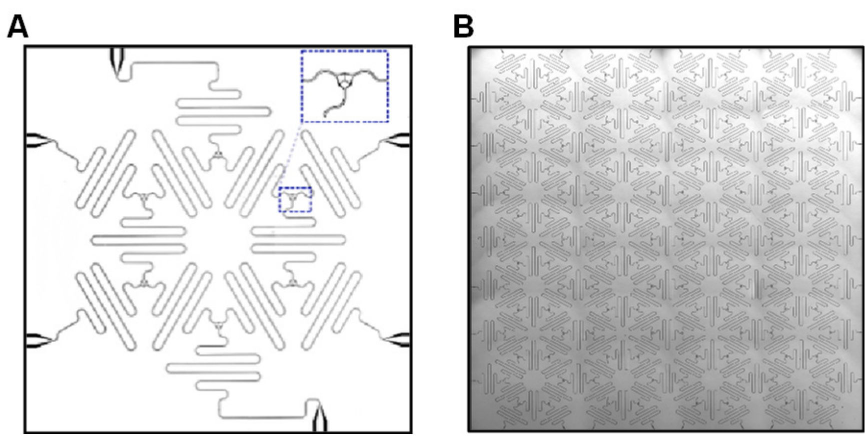

FIGURE 6

Investigation of coupled arrays of microwave cavities for purposes of quantum simulation. Coupled cavity arrays showing (**A**) a dozen cavities in a Kagome star geometry and (**B**) two hundred cavities in an extended Kagome lattice.

F. Evidence for Sympathetic Vibrational Cooling of Translationally Cold Molecules
Professor Eric Hudson, University of California - Los Angeles, Single Investigator Award

Professor Hudson's research group is investigating methods for sympathetically cooling molecular ions through controlled collisions with neutral atoms. The ultimate goal of this research is to obtain is to develop methods of cooling and trapping molecules to take advantage of their non symmetric long range interactions. In FY13, Professor Hudson's research team reported[9] evidence for sympathetic vibrational cooling of molecules, which may lead to critical insights into quantum chemistry (see FIGURE 7).

Several creative methods are being explored to overcome the technical challenges of cooling molecules in an effort to exploit their rich internal structure. Studying this rich structure reveals important insights in quantum chemistry, novel methods suitable for quantum information, and improved tests for fundamental violations and variations. These rich potential features that are the result of complex internal structure also makes molecules more difficult to laser cool compared to neutral atoms. It is desirable to prepare the molecules in the rovibrational ground state. These states are not governed by strict selection rules. Additionally, traditional collisional, or sympathetic, cooling methods are inefficient at quenching molecular vibrational motion. The Hudson group has demonstrated the quenching of the vibrational motion of trapped $BaCl^+$ molecules by collisions with ultracold calcium atoms at a rate comparable to the classical scattering, or Langevin, rate. This result is over four orders of magnitude more efficient than traditional sympathetic cooling schemes.

The high cooling rate, a consequence of a strong interaction potential (due to the high polarizability of calcium), along with the low collision energies involved, leads to molecular samples with a vibrational ground-state occupancy of at least 90%. This demonstration uses a novel thermometry technique that relies on relative photodissociation yields. Although the decrease in vibrational temperature is modest, with straightforward improvements it should be possible to produce molecular samples with a vibrational ground-state occupancy greater than 99 per cent in less than 100 milliseconds. Because sympathetic cooling of molecular rotational motion is much more efficient than vibrational cooling in traditional systems, it is expected that the method also allows efficient cooling of the rotational motion of the molecules. Moreover, the technique should work for many different combinations of ultracold atoms and molecules, making it applicable to several species.

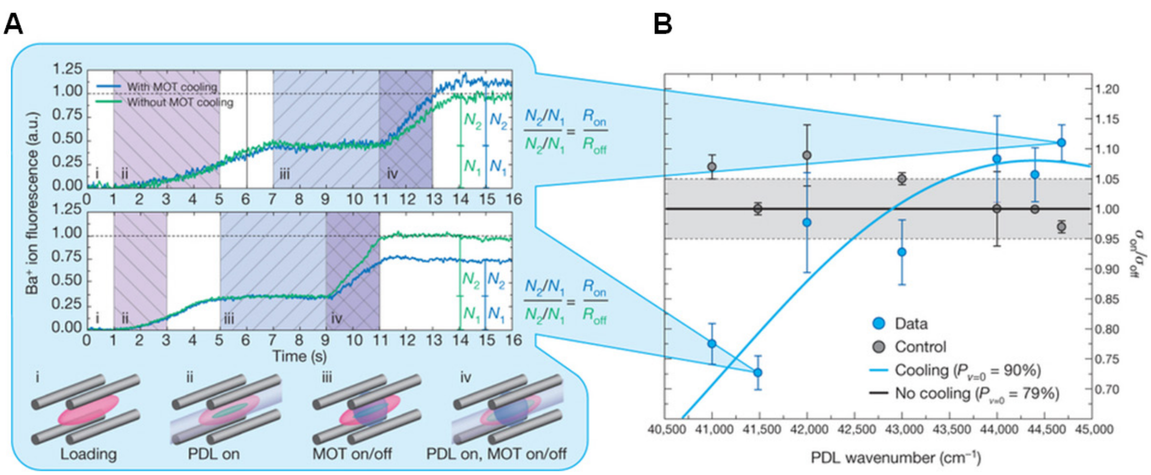

FIGURE 7

Evidence for sympathetic vibrational cooling of molecules. (**A**) Example traces of the Ba^+ ion fluorescence measured during the experimental sequence. Initially the trap is loaded with a pure $BaCl^+$ sample (pink) (i). The PDL is then turned on to create a mixed sample of $BaCl^+$ and Ba^+ ions (green) (ii). Once the Ba^+ ions have been laser-cooled, the MOT (blue) is optionally turned on and the $BaCl^+$ ions are collisionally cooled by the ultracold Ca atoms (iii). Following that, the $BaCl^+$ ions are probed with the PDL to determine the amount of vibrational relaxation due to the MOT (iv). The ratio of the numbers of Ba^+ ions created in each instance of photodissociation with the MOT respectively on or off is then calculated. The top and bottom panels are data for PDL wavenumbers of 41,500 and 44,675 cm^{-1}, respectively. a.u., arbitrary units. (**B**) The average of all data points (errors, s.e.) obtained, as described in Methods, is plotted for various photodissociation wavenumbers. The blue points are cooling data and the grey points are a control analysis that should be consistent with unity. The curves are the expected result from a rate equation model of the experimental sequence described in Methods. The agreement with the data shows that the $BaCl^+$ sample has been cooled to a ground-state vibrational population of ~90% in the average case.[9]

[9] Rellergert, W., Sullivan, S., Schowalter, S., Kotochigova, S., Chen, K., Hudson, E. (2013) Evidence for sympathetic vibrational cooling of translationally cold molecules. *Nature* 450:490-494.

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. Molecular Signatures in Laser-Induced Breakdown Spectroscopy

Investigator: Professor Uwe Hommerich, Hampton University, REP Award
Recipient: ARL-SEDD and Edgewood Chemical and Biological Center (ECBC)

One of the goals of Professor Hommerich's research is to expand an understanding of the processes involved with Laser-induced breakdown spectroscopy (LIBS). This is particularly useful for extending LIBS for remote detection of chemical, biological or explosive materials. This research has transitioned to a collaboration with scientists from ARL-SEDD, ECBC, and Brimrose Corporation. Through this collaboration, Professor Hommerich's laboratory has discovered new long-wavelength infrared (LWIR) LIBS signatures for molecular species associated with chemicals that are commonly found in improvised explosive devices.

The LIBS process is conducted using a near-infrared laser to ablate the surface of a sample. The chemical constituents of the resulting plasma are monitored using a mercury-cadmium telluride LWIR detector and a spectrometer. In addition to the atomic spectral lines observed with near- and mid-infrared detection, additional spectral features associated with molecular components in the plasma were identified. The Army-Industry-University team exploring these processes will further refine the spectral identification process and utilize fundamental studies of the laser-induced plasma and its dynamics in an effort to more fully understand the complex phenomena involved while also enabling enhanced detection capabilities.

B. Mode Division Multiplexing with Higher-order Principle States of Polarization

Investigator: Professor Robert Alfano, The City College of New York (CUNY), HBCU and REP Awards
Recipient: Corning Inc.

The goal of this research is to explore methods to circumvent the scattering obstacle for optical signal propagation and imaging through turbid media, making use the phase singularity and orbital angular momentum of vortex beams. Professor Alfano has extablished a collaboration with Corning Inc. to pursue experimental and theoretical investigations into structuring the wave front of various LG and LP01 modes to study their application as a spatial modulators in fiber optic telecommunication systems.

Exponentially increasing demands on information capacity in fiber optic communication will lead to imminent information "bottlenecks" in coming years. This bottleneck is a direct result of inherent information capacity limits in conventional single mode optical fibers associated with fiber non-linearity. There is great need to develop methods beyond and in addition to wavelength and time division multiplexing to increase information capacity in optical fibers.

Dr. Alfano's team is investigating information capacity increase in optical fibers via the burgeoning method of mode division multiplexing using spatial modes and OAM by utilizing orthogonal spatial modes as new information channels. The team's goal is the integration of their patented novel multi elliptical core fibers and multimode spun elliptical core fibers with theoretical tools, such as a higher-order Poincare Sphere to design components for field implementation of a mode division multiplexing system. The new patent on SU(N) will advance the field of communication highway capacity increase. Implementation of mode division multiplexing requires mitigation of inherent modal dispersion that leads to signal crosstalk. The research team previously addressed this issue theoretically by developing a formalism to establish so-called "higher-order" principal states of polarization. Higher-order principle states of polarization are a direct extension of well-known principle states of polarization in a single mode optical fiber. These are states of polarization that propagate down the fiber without modal dispersion. In contrast to a single mode optical fiber, higher-order principle states of polarization in a multimode optical fiber are comprised of linear combinations of many higher-order modes. Therefore, their physical implementations (*i.e.*, determination of and launching) cannot be carried out with conventional optical elements.

In FY13, this research transitioned to Corning for further study to develop novel optical components for physical implementation of higher-order principle states of polarization for mode division multiplexing. This will include applying novel and patented optical fiber designs of multi elliptical core optical fibers and multimode spun elliptical core fibers in concert with a novel and patented technique to determine and launch higher order principle states of polarization.

V. ANTICIPATED ACCOMPLISHMENTS

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

A. Novel Electronic States in Periodically Driven Systems

Professors Gil Rafael, California Institute of Technology, and Victor Galitski, University of Maryland, DARPA Award

Periodically driven electronic systems has recently emerged as a promising field of study in physics with the application of Floquet theory and recent experimental studies verifying some aspects of this theory. Floquet theory is actually a mathematical precedent to the Bloch theorem that forms the basis for the quantum theory of solids. It is from this theory that the band structure of all electronic materials is derived. The Bloch theorem briefly states that the quantum state of an electron in a periodic potential is described by a plane wave and a function having the periodicity of the potential. This greatly simplified the process of calculating the electronic band structure of crystalline solids and has underpinned virtually all efforts to understand electronic materials for approximately the last 90 years. The Bloch theorem essentially transferred Floquet theory into three dimensions. Today, however, physicists are applying Floquet theory to a potential periodic in time rather than space and the results are fascinating. It is anticipated that in FY14 this research will culminate in experimental verification of the theoretical predictions such as the transformation of a trivial insulator into a topological insulator (an insulator with a conductive edge state that is mathematically protected by the topology of the band structure) or vice versa by the application of periodic strain, electromagnetic fields, electric fields or magnetic fields; all regularly fluctuating in time. While the ability to control the topological protection of a surface state is clearly unique, the field in expected to greatly expand in the near future with farther reaching consequences.

B. Probing Molecular Ions with Laser-Cooled Atomic Ions

Professor Kenneth Brown, Georgia Technical University, Single Investigator Award

The objective of this research is to precisely measure molecular ion spectra by quantum logic and sympathetic heating spectroscopy techniques. These techniques can then be applied to understanding molecular ion spectra in the interstellar medium and to precision measurements of fundamental constants. For example, the relative dependence of molecular transitions on the ratio of the electron mass to the proton mass can be used with atomic spectroscopy to bound possible time variations in the strong force. Three experiments will be pursued in FY14: vibronic spectroscopy of BH^+, vibrational overtone spectroscopy of CaH^+, and control of resolved motional sidebands of sympathetically cooled molecular ions. Anticipated results are the measurement of molecular ion mass with sub-amu precision and the first measurement of vibrational lines of CaH^+.

C. Spin-optics in Metamaterials: Hyberbolic Metamaterials in the Atmosphere

Professor Natalia Litchinitser, The State University of New York (SUNY), Single Investigator Award

The objective of this research 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.

As noted in Section III-B, Professor Litchinitser and colleagues recently found that an array of light filaments can guide a microwave beam without dispersion (see FIGURE 8).[7] This finding revealed the possibility of long range covert communications and disruption of unfriendly electronics. Light filaments, a combination laser beam and plasma, do not diffract due to the self focusing of air. Since filaments have a plasma core they are essentially a conductor and can act as a waveguide for the microwaves, as shown in the figure below. In fact, the conducting elements in the dielectric air form a hyberbolic metamaterial. Professor Martin Richardson at the University of Central Florida, in collaboration with Litchinitser, is now designing an array of laser filaments and acquiring microwave equipment to perform experiments. It is anticipated that in FY14 the theory will be confirmed and for the first time ever it will be shown that microwaves can be guided and controlled by a laser.

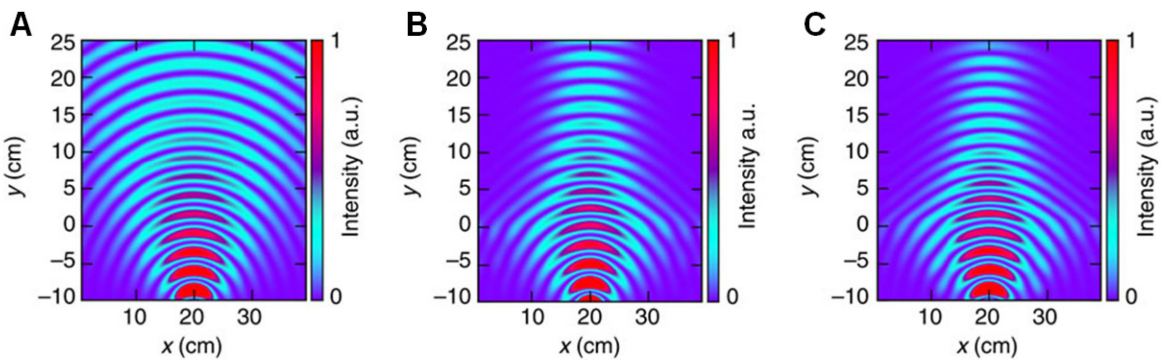

FIGURE 8

Intensity distributions for λ = 7.5cm. Field intensity distributions for a TM-polarized continuous wave Gaussian beam at wavelength λ = 7.5 cm in (a) vHMM with fill-fraction f = 0.2, (b) VHMM with fill-fraction f = 0.3, and (c) vHMM with fill-fraction f = 0.4 for given recombination rate coefficient $\beta_{e+} = 0.12 \times 10^{-13} m^3 s^{-1}$.

D. Quantum Computing, Control, and Quantized Nonlinear Optics with Superconducting Circuits

Professor Andrew Houck, Princeton University, PECASE

The objective of this research 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.

It is anticipated that in FY14, the research team will simulate many-body effects using large arrays of microwave cavities with qubits in them. In particular, experiments will seek signatures of photonic quantum phase transitions in these systems. Experiments with local probes to image photons in the large arrays will be pursued to obtain more information about the internal states of the system. Experiments will also continue on the tunable coupling qubit, focusing on making a qubit with no dispersive shift to the cavity. In addition, a "catch" experiment will be attempted in which the state of one qubit is transferred to a separated second qubit by applying a time reversed set of control pulses. This will be a key component for the communication and distribution of quantum information.

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