2011 ARO IN REVIEW

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ARO IN REVIEW 2011

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CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY

This report is intended to be a single-source document describing the research programs of the U.S. Army Research Office (ARO) for fiscal year 2011 (FY11; 1 Oct 2010 through 30 Sep 2011). This report provides:

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

I. ARO MISSION

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

II. ARO INVESTMENT STRATEGY

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

A. Requirements Pull

The requirements pull strategy supports the National Security Strategy by following Joint Capabilities Integration and Development System (JCIDS) processes, in which ARO promotes research in response to a wide variety of published requirements and needs, including the Army Science and Technology Master Plan, Science and Technology Challenge Areas, Training and Doctrine Command Warfighter Outcomes, and Quadrennial Defense Review (QDR). This strategy can also be referred to as needs-driven research, which emphasizes long-term efforts to improve existing capabilities or overcoming identified technology barriers.

B. Technology Push

ARO also invests heavily in discovery research targeted at extraordinarily novel and innovative science that may not be focused on a specific application, but promises tremendous value across many technologies and applications, some of which may be fundamentally new. This technology push strategy emphasizes opportunity-driven research aimed at developing and exploiting scientific breakthroughs to produce revolutionary new capabilities.

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

C. Specific Strategies

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

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

III. IMPLEMENTING ARO INVESTMENT STRATEGY

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

A. Program Snapshot

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

B. Coordination for Program Development and Monitoring

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

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

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

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

IV. ARO Organizational Structure

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

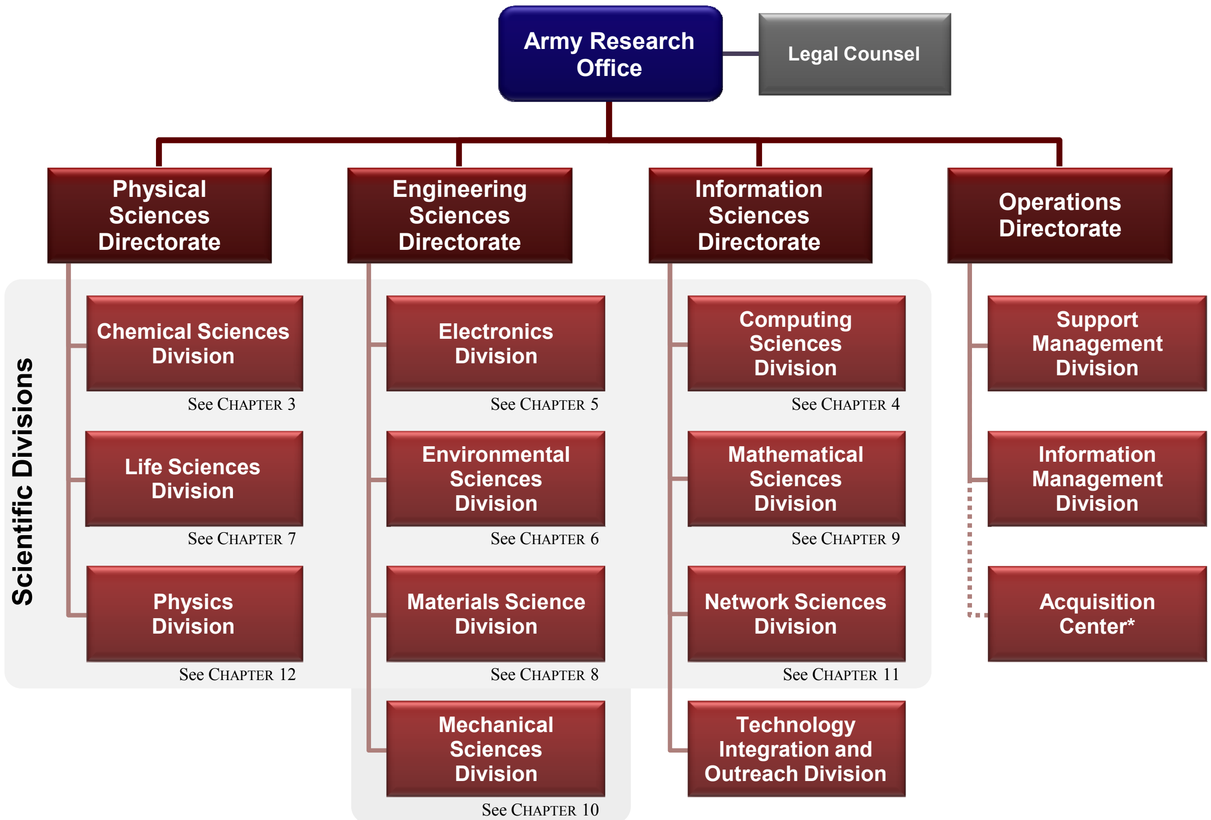

Figure 1

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

CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES

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

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

I. OVERVIEW OF PROGRAM FUNDING SOURCES

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

A. Army Funding

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

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

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

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

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

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

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

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

C. Other Funding Sources

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

II. ARO CORE (BH57) RESEARCH PROGRAM

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

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

A. Single Investigator (SI) Program

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

B. Short Term Innovative Research (STIR) Program

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

C. Young Investigator Program (YIP)

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

D. Conferences, Workshops, and Symposia Support Program

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

E. Special Programs

Although the ARO SI, STIR, YIP, and conference-support programs constitute the primary use of BH57 funds, the ARO Core Research Program also supports a variety of special programs. These special programs include 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), funding for in-house staff and research activities, and matching funds applied to the ARO Core-funded HBCU/MI program.

III. MULTIDISCIPLINARY UNIVERSITY RESEARCH INITIATIVE (MURI)

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

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

Management oversight of the MURI program comes from the Research Office of ASDR&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 ASDR&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 ASDR&E under a formal acquisition process.

The following topics resulted in eight newly-funded Army MURI awards for FY11. The program managers (PMs) and corresponding scientific division for each award are listed following the award titles.

1. *Controlling the Abiotic/Biotic Interface*, Dr. Jennifer Becker, Chemical Sciences and Dr. Stephanie McElhinny, Life Sciences
2. *Quantum Stochastics and Control*, Dr. Harry Chang, Mathematical Sciences and Dr. TR Govindan, Physics
3. *Qubit Enabled Imaging, Sensing and Metrology,* Dr. TR Govindan, Physics and Dr. Harry Chang, Mathematical Sciences
4. *Flex-Activated Materials*, Dr. David Stepp, Materials Science and Dr. Douglas Kiserow, Chemistry
5. *Game Theory for Adversarial Behavior*, Dr. Purush Iyer, Network Sciences and Dr. Harry Chang, Mathematical Sciences
6. *Light Filamentation*, Dr. Richard Hammond, Physics
7. *Novel Free-Standing 2D Crystalline Materials (Oxides/Nitrides)*, Dr. Pani Varanasi, Materials Science
8. *Value of Information for Distributed Data Fusion*, Dr. Liyi Dai, Computing Sciences

In FY 11, the following topics were published in the FY12 MURI BAA in anticipation of future funding. The PMs for each topic are listed following the topic titles.

9. *Quantized Chemical Reactions of Ultracold Molecules*, Dr. James Parker, Chemistry and Dr. Paul Baker, Physics
10. *3D Topological Insulators with Interactions,* Dr. Marc Ulrich, Physics and Dr. Pani Varanasi, Materials Science
11. *Translating Biochemical Pathways to Non-Cellular Environments*, Dr. Stephanie McElhinny, Life Sciences and Dr. John Prater, Materials Sciences
12. *Revolutionizing High-Dimensional Data Integration for Microbial Forensics*, Dr. Virginia Pasour, Mathematical Sciences and Dr. Wallace Buchholz, Life Sciences
13. *Predictive Models of Culture and Behavioral Effects on Societal Stability,* Dr. Jeffrey Johnson, Life Sciences, Dr. Virginia Pasour, Mathematical Sciences, and Dr. Bruce West, Information Sciences
14. *Multivariate Heavy-Tailed Statistics: Foundations and Modeling*, Dr. Harry Chang, Mathematical Sciences and Dr. John Lavery, Mathematical Sciences
15. *Novel Nanostructures for the Controlled Propagation of Electromagnetic Energy*, Dr. Jennifer Becker, Chemistry and Dr. Richard Hammond, Physics
16. *Simultaneous Multi-synaptic Imaging of the Interneuron,* Dr. Elmar Schmeisser, Life Sciences and Dr. Dwight Woolard, Electronics

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 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, or community outreach.

Of the candidates nominated in FY10 by ARO for consideration in the PECASE program, four investigators were selected in FY11 to receive PECASE awards. These awards began as "new start" projects in FY11 and are listed in this section, with the project title followed by the principal investigator (PI), performing organization, ARO PM and corresponding scientific division. Additional details for each of these projects can be found in the corresponding scientific division's chapter.

1. *Precision Controlled Carbon Materials for Next-generation Optoelectronic and Photonic Devices*.
   PI: Professor Michael Arnold, University of Wisconsin – Madison
   ARO PM: Dr. Michael Gerhold, Electronics Division
2. *New Microstructures for Old Monomers: Syntheses of Gradient Pi-Conjugated Copolymers*.
   PI: Professor Anne McNeil, University of Michigan
   ARO PM: Dr. Douglas Kiserow, Chemical Sciences Division
3. *Nanofluidic Analysis of Protein Transport, Adsorption and Kinetics*.
   PI: Professor Sumita Pennathur, University of California - Santa Barbara
   ARO PM: Dr. Stephanie McElhinny, Life Sciences Division
4. *Single-nanoparticle Transducer.*
   PI: Professor Lan Yang, University of Washington
   ARO PM: Dr. Dwight Woolard , Electronics Division

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 FY11, the Army awarded 62 awards at $10 million total, with the average award being $160K.

VI. UNIVERSITY AFFILIATED RESEARCH CENTERS (UARCS)

The University Affiliated Research Centers (UARCs) are strategic DoD-established research organizations at universities. The UARCs were formally established in May 1996 by DDR&E (currently ASDR&E), OSD in order to advance DoD operations 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 ASDR&E to be the primary sponsor for each UARC. The primary sponsor ensures the DoD UARC management policies and procedures are properly implemented. Collaborations among UARCs and the educational and research resources available at the associated universities can enhance each UARC's ability to meet the long-term goals of DoD.

ARO is the primary sponsor for two UARCs:

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

VII. MINERVA RESEARCH INITIATIVE (MRI)

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

Minerva projects are funded up to a five-year base period with one five-year renewal option, with awards ranging from small, single investigator grants for 2-3 years to large multidisciplinary projects for $1-2 million per year for 5 years. The program is tri-service managed, with ARO managing projects dealing with the Baathist regime in Iraq, vulnerability of political and social stability in Africa in the face of environment stressors, the relation of the growth of science and technology with the defense transformation in China, and the effects of energy issues on societies. ARO also provides managerial support to OSD for other parts of the program focused on the defense universities.

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

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

A. Purpose and Mission

The purpose of the SBIR and STTR programs is to (i) stimulate technological innovation, (ii) use small business to meet Federal R&D needs, (iii) foster and encourage participation by socially and economically disadvantaged small business concerns (SBCs) that are 51 percent owned and controlled by women, 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 an academic or other qualifying 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. These programs employ a three-phase structure. 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, $70K – $150K max • 4-month option (at Government's discretion), $50K max, to fund interim Phase II efforts	• 6 months, $100K max • No options
Phase II	• 2 years, $1 million max	• 2 years, $750K
Phase III	• No time or size limit • No SBIR set-aside funds	• No time or size limit • No STTR set-aside funds

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

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

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

C. Contract Awards

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 FY11 and funded by the Army, CBD, OSD and other sources with FY11 or FY10 funding is shown in TABLE 2.

TABLE 2

Total Funding for ARO-managed SBIR and STTR contracts awarded in FY11. Total funding (FY11 and FY10) 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	$2,704K	$6,038K
Phase II	$4,936K	$9,045K
Phase II Enhancement	$1,739K	-
CPP	$4,335K	-
Phase III	$13,514K	$99K
TOTAL	**$27,228K**	**$15,182K**

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

Programs for HBCU/MIs are a significant part of the ARO portfolio. Historically, total funding for the HBCU/MI programs has collectively exceeded $38 million, but totaled approximately $57.2 million in FY11, including funding for programs that were programmed for FY10 and were awarded in FY11.

These programs are discussed in the following subsections, as is the ARO (Core) HBCU/MI Program, which is part of ARO's BAA.

A. ARO (Core) HBCU/MI Program

The ARO began its HBCU/MI program in 1980 with $0.5 million designed to encourage greater participation of HBCUs and MIs in basic research. The initiative has continued and in recent years has been funded at $1.2 million annually. These funds are made available to the ARO scientific divisions as co-funding opportunities to support HBCU/MI research proposals submitted under the ARO Core Program BAA. In FY11, the ARO HBCU/MI program supported 18 grants and 4 conferences with a total value of approximately $2.1 million. 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. Seven institutions were funded under HSAP/URAP in FY11, totaling approximately $45K. Additional information regarding HSAP/URAP can be found in Section XI: *Youth Science Activities*.

B. Partnership in Research Transition (PIRT) Program

The PIRT Program is 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. Funding for this program totals approximately $2.5 million per year. A total of 22 research proposals were received from 12 HBCUs. Five awards were made during 2Q FY11. Approximately $4 million (cumulative FY10 and FY11 funding) was awarded to support these selected Centers of Excellence:

- *Center of Advanced Algorithms*
  Delaware State University, Dover, DE
  Co-Cooperative Agreement Manager (Co-CAM): Dr. Dev Palmer, Engineering Sciences Directorate
- *Bayesian Imaging and Advanced Signal Processing for Landmine and IED Detection Using GPR*
  Howard University, Washington, DC
  Co-CAM: Dr. Dev Palmer, Engineering Sciences Directorate
- *Extracting Social Meaning From Linguistic Structures in African Languages*
  Howard University, Washington, DC
  Co-CAM: Dr. John Lavery, Information Sciences Directorate
- *Lower Atmospheric Research Using Lidar Remote Sensing*
  Hampton University, Hampton, VA
  Co-CAM: Dr. Gorden Videen, Engineering Sciences Directorate
- *Nano to Continuum Multi-Scale Modeling Techniques and Analysis for Cementitious Materials Under Dynamic Loading*
  North Carolina A&T State University, Greensboro, NC
  Co-CAM: Dr. Joseph Myers, Information Sciences Directorate

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

ARO has administered programs on behalf of ASD(R&E) (formerly DDR&E) since 1992. During FY10, approximately $45 million was made available for new awards under the solicitation "*Research and Educational Program for Historically Black Colleges and Universities and Minority-Serving Institutions (HBCU/MI)*." The Research and Educational Program (REP) aims to: (i) enhance programs and capabilities in scientific and engineering disciplines critical to the national security functions of the DoD, (ii) encourage greater participation in DoD programs and activities, (iii) increase the number of graduates, including underrepresented minorities, in the fields of science, technology, engineering and/or mathematics (STEM), and (iv) encourage research and educational collaboration with other institutions of higher education directed toward advancing the state of the art and increasing knowledge.

Under this program, qualifying institutions were able to submit proposals to compete for Centers of Excellence (three focused on STEM education and three focused on STEM research) and approximately 25 basic research grants. Proposals were received in late FY10 and awards were made in 2Q FY11. Collectively, fifty-two grant awards totaling approximately $45.7 million were made to 32 HBCUs; 19 HSIs and one other Minority Institution. Six Centers of Excellence were awarded to:

- *DoD HBCU/MSI ED Center*
  University of Texas-Pan American, TX, Edinburg, TX
  Co-Program Manager: Ms. Peggy Lacewell, Information Sciences Directorate
- *Central State University DoD Center of Excellence in STEM and STEM Education*
  Central State University, Wilberforce, OH
  Co-Program Manager: Ms. Peggy Lacewell, Information Sciences Directorate
- *Jackson State University Center of Excellence in Science, Technology, Engineering, and Mathematics Education*
  Jackson State University, Jackson, MS
  Co-Program Manager: Ms. Peggy Lacewell, Information Sciences Directorate
- *The Center of Excellence in Infection Genomics*
  University of Texas – San Antonio, San Antonio, TX
  Co-Program Manager: Dr. Micheline Strand , Physical Sciences Directorate

- *Center of Excellence in Advanced Nanomaterials and Devices*
  Norfolk State University, Norfolk, VA
  Co-Program Manager: Dr. Pani Varanasi, Engineering Sciences Directorate
- *UPR-UGA Partnership for a Research Center for Excellence in Renewable Energy*
  University of Puerto Rico – Rio Piedras, Rio Piedras, PR
  Co-Program Manager: Ms. Peggy Lacewell, Information Sciences Directorate

In 2Q FY11, Broad Agency Announcement W911NF-11-R-0007 was issued for the FY11 DoD REP for HBCU/MI. More than 160 proposals were determined to be eligible under the solicitation. It is anticipated that awards totaling approximately $17 million will be made by 2Q FY12.

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

As Congressional set-aside program for TCUs, this instrumentation program aims to enhance science, mathematics, and/or engineering education programs and/or research capabilities through the acquisition of equipment and/or instrumentation that will augment existing facilities, enhance curricula, or help develop new laboratories, programs and capabilities in these areas. This includes basic equipment for laboratory and classroom use as well as sophisticated instruments and computers (including software) for advanced studies and research important to DoD. Fifteen proposals were submitted in response to the solicitation published in 2Q FY10. Thirteen were selected for awards totaling approximately $3.5 million. Awards were made in 1Q FY11.

E. Other DoD Programs

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

In addition, the John H. Hopps Scholars Program at Morehouse College (funded in FY08) continued to serve more than twenty scholars during FY11.

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

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

With approximately $5 million available to the Army in FY11, ARO selected 63 NDSEG Fellows from eleven categories relevant to the Army fundamental research priorities. These awardees began their fellowships in the fall of 2011. Each of ARO's divisions reviewed the applications assigned to NDSEG topic categories within their particular areas of expertise, and selected fellows whose doctoral research topics most closely align with the Army's missions and research needs. The number of Fellows chosen from each discipline was based on the percentage of applicants who submitted topics in that category. The number of fellows chosen from each scientific discipline for the FY11 NDSEG program is shown in TABLE 3.

TABLE 3

FY11 NDSEG fellows by discipline. The table displays the number of NDSEG Fellows chosen in FY11, according to the eleven topic categories relevant to the designated Army research priorities.

Scientific Discipline	NDSEG Fellows Selected in FY11
Biosciences	11
Chemistry	8
Physics	5
Computer and Computational Sciences	4
Mathematics	4
Aeronautical and Astronautical Engineering	5
Civil Engineering	3
Electrical Engineering	7
Geosciences	2
Materials Science and Engineering	5
Mechanical Engineering	9
TOTAL	**63**

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 tutorial classes during the summer, showcasing talented young high school scientists at symposia, and student science fair support.

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, 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 $30K, and expense-paid trips to international programs.

During the summer of FY11, 217 students served as interns and worked in university laboratories with selected mentors though the High School Apprenticeship Program (HSAP), Undergraduate Research Apprentice Program (URAP), and the Research and Engineering Apprenticeship Program (REAP). In FY11, 440 students engaged in research experiences in military laboratories through the Science and Engineering Apprentice Program (SEAP) and College Qualified Leaders (CQL) program, and 438 students participated in programs that offered enrichment classes in engineering at universities through the UNITE program. Over 100 teams of fourth-eighth grade students learned engineering and alternative energy concepts as they designed, built, and raced solar cars through the Junior Solar Sprint (JSS) Northeastern Regional Championship. These programs are described further in the following subsections.

A. Junior Science and Humanities Symposium (JSHS) Program

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

B. Research and Engineering Apprenticeship Program (REAP)

REAP is designed to offer high school students the opportunity to expand their background and understanding of scientific research. While originally chartered as a program to identify and support under-represented students in STEM, the program has been expanded to accept applications from all students seeking a first time experience in research. This is accomplished by offering the student an internship during the summer months to participate in a work/study atmosphere with a mentor in a laboratory setting. The experience serves to motivate the student towards a career in STEM by providing a challenging science experience that is not readily available in high school. In FY11, 144 apprentices were placed at 53 hosting universities throughout the U.S.

C. UNITE Program

The UNITE Program is an aggressive and effective initiative that encourages and assists under-represented students in preparing for entrance into engineering schools. High school students are provided the opportunity during the summer months to participate in college-structured summer courses that provide hands on applications, participation in lectures, problem solving as well as tours of laboratories and private and governmental 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. Nine sites were funded in FY11 serving 438 students.

D. Army Awards Program (AAP)

The Army Awards Program provides Army sponsored special awards to students at regional, state, and the International Science and Engineering Fair (ISEF). Each year, ROTC units, Recruiting Battalions, Army Reservists, Army Corps of Engineers Personnel, and Army command/laboratory personnel serve as judges of student projects at more than 275 science fair competitions held throughout the United States and Puerto Rico. By participating in science fairs, the Army is able to encourage and stimulate talented students to consider careers in science and technology while simultaneously exposing these students to Army R&D professionals.

E. Junior Solar Sprint (JSS) Program

The JSS Program provides 4^{th}-8^{th} grade students in the northeast 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. Top winners from each local competition are invited to race in the Northeastern championship in Springfield, MA.

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

HSAP/URAP funds the STEM apprenticeship of promising high school juniors and seniors, and undergraduates to work in university-structured research environments under the direction of existing ARO-sponsored PIs serving as mentors. In FY11, HSAP/URAP awards provided 73 students with research experiences at 31 different universities. ARO invested approximately $300K in the FY11 effort.

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

The U.S. Army sponsors high school and college student internships in research laboratories throughout the Army. Students receive a stipend to spend their summer conducting meaningful research. ARO supports this unique vehicle for hiring student apprentices using research funding from participating Army laboratories. In FY11, 173 high school students participated in SEAP and 267 college students participated in the CQL program.

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

The GEMS program provides middle and high school students with a unique hands-on science experience in an Army laboratory. Students spend 14 weeks learning about Army research and conducting STEM experiments guided by Army scientists and engineers. In FY11, 1,425 students participated at GEMS programs held at White Sands Missile Range (WSMR), Army Research Lab (ARL) in Adelphi and Aberdeen Proving Ground, MD; Walter Reed Army Institute of Research (WRAIR), Redstone Arsenal, and Engineer Research and Development Center (ERDC) in Vicksburg, IL and Champaign, IL.

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

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

Virginia Polytechnic Institute and State University has led the consortium of non-profits and academic institutions to execute a collaborative STEM education and outreach program focusing on these core objectives.

- Increase the number of STEM graduates to address the projected shortfall of scientists and engineers in National and DoD positions
- Expand the involvement of students in ongoing DoD research
- Provide STEM educational opportunities for students at all stages of their K-12, undergraduate, graduate, and post-graduate education
- Entice students into college-level DoD programs
- Inform students about military or civil service career opportunities in STEM

XII. SCIENTIFIC SERVICES PROGRAM (SSP)

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

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

SSP awards tasks in a wide variety of technical areas, including mechanical engineering, computer sciences, life sciences, chemistry, material sciences, and military personnel recruitment/retention. In FY11, in addition to the more traditional use of the program, new tasks were initiated to support Warfighters and Combatant Commanders engaged in the Global War on Terror, Operation Iraqi Freedom, and Homeland Security. In FY11, there were a total of 106 new SSP tasks awarded and a modification of the scope and/or funding of 413 ongoing tasks. A summary of the agencies served under this program and the corresponding number of FY11 new SSP tasks is provided in TABLE 4.

TABLE 4
FY11 SSP tasks and sponsoring agencies.

Sponsoring Organization	SSP Tasks
Army Research, Development and Engineering Command (RDECOM)	
Army Research Laboratory (ARL)	10
Army Research Office (ARO)	3
Research, Development, and Engineering Centers (RDECs)	
Army Missile RDEC (AMRDEC)	9
Army Material Systems Analysis Activity (AMSAA)	3
Armaments RDEC (ARDEC)	13
Communications-Electronics RDEC (CERDEC)	2
Natick Soldier RDEC (NSRDEC)	2
Space & Terrestrial Communications Directorate	1
Tank Automotive RDEC (TARDEC)	9
TOTAL: RDECOM	**52**
Army Medical Research and Materiel Command (MRMC)	
Aeromedical Research Laboratory (AARL)	8
Medical Research Institute of Chemical Defense (ICD)	8
Medical Research Institute of Infectious Diseases (IID)	1
Office of Research and Technology Applications (ORTA)	1
Walter Reed Army Institute of Research (WRAIR)	6
TOTAL: MRMC	**24**
Other DoD	
Headquarters Department of Army (HQ DA)	2
Army Corps of Engineers	11
Navy	6
Air Force	6
TOTAL: Other DoD	**25**
Department of Health and Human Services (DHHS)	**5**
TOTAL FY11 SSP Tasks	**106**

XIII. SUMMARY OF PROGRAM FUNDING AND ACTIONS

A. FY11 Research Proposal Actions

The FY11 extramural basic research proposal actions according to each ARO Division are summarized in TABLE 5, below.

TABLE 5

FY11 ARO Research Proposal Actions. The status of FY11 research proposals (*i.e.*, proposals received within the period 1 Oct 2010 through 30 Sep 2011) is listed based on proposal actions reported through 17 May 2012. The table reports actions for extramural proposals in the 6.1 basic research categories only: SI, STIR, YIP, MURI, PECASE, and DURIP.

	Received	Accepted	Declined	Pending	Withdrawn
Chemical Sciences	81	26	24	31	0
Computing Sciences	37	9	6	22	0
Electronics	66	15	2	49	0
Environmental Sciences	38	13	2	23	0
Life Sciences	98	40	15	42	1
Materials Science	71	24	3	44	0
Mathematical Sciences	36	16	5	15	0
Mechanical Sciences	103	25	31	42	5
Network Sciences	60	20	14	25	1
Physics	65	18	7	40	0
Tech Integration and Outreach	1	0	1	0	0
TOTAL	**656**	**206**	**110**	**333**	**7**

B. Summary of ARO Core Program Budget

The ARO FY11 Core (BH57) Research Program budget is shown in TABLE 6, below.

TABLE 6

ARO Core (BH57) Program funding. The ARO Core Program FY11 Budget is listed according to each scientific discipline (Division) or Special Program. The FY11 Budget by scientific discipline is reported based on the ARO Director's Budget as of 1 Apr 2012, while the FY11 Budget for special programs is reported based on the Status of Funds Report as of 30 Sep 2011.

ARO Core (BH57) Program Type	Division or Program Title	FY11 Budget
Scientific Disciplines	Chemical Sciences	$6,211,000
	Computing Sciences	$4,116,000
	Electronics	$5,690,000
	Environmental Sciences	$2,726,000
	Life Sciences	$6,345,000
	Materials Science	$6,150,000
	Mathematical Sciences	$4,824,000
	Mechanical Sciences	$5,643,000
	Network Sciences	$4,800,000
	Physics	$5,900,000
	SUBTOTAL: Core Program Funding by Scientific Discipline	**$52,405,000**
Special Programs	Senior Research Scientist Research Programs[1]	$2,273,684
	National Research Council (NRC) Associates Program[2]	$80,000
	HBCU/MI Program[3]	$949,752
	HSAP/URAP	$150,000
	In-House Operations	$15,797,404
	SUBTOTAL: Core Program Funding to Special Programs	**$19,250,840**
TOTAL	**ARO Core (BH57) Program**	**$71,655,840**

[1] This total includes funding for ARL Fellows and unallocated Directorate Director funds.
[2] In addition to the FY11 allotment shown, FY10 funds were received or reallocated for this category in FY11, as specified in TABLE 10.
[3] These HBCU/MI Program funds are allocated at the Directorate level, and are matched with Division Core Program funds on a 1:1 basis.

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

The FY11 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

FY11 allotments for other Army-funded programs. These programs, combined with the ARO Core (BH57) Program elements shown in TABLE 6, represent all of the Army-funded programs managed through ARO. The FY11 allotment values shown here represent the status of funds on the last day of FY11: 30 Sep 2011.

Other Army-funded Program	FY11 Allotment
Multidisciplinary University Research Initiative	$52,328,206
Presidential Early Career Award for Scientists and Engineers	$4,330,000
Defense University Research Instrumentation Program	$10,066,976
University Research Initiative Support	$2,379,000
University Research Initiative (unallocated)[1]	$4,087,317
MINERVA Program (Projects V72 and D55)	$11,153,500
Strategic Technology Initiatives	$100,000
Army Center of Excellence	$956,000
HBCU/MI – PIRT Centers	$2,678,000
Institute for Collaborative Biotechnologies (ICB)	$9,327,000
Institute for Soldier Nanotechnologies (ISN)	$10,113,000
Institute for Creative Technologies (ICT)	$7,598,000
Board of Army Science and Technology (BAST)[2]	$1,029,000
Small Business Innovation Research (SBIR)[2]	$6,109,665
Small Business Technology Transfer (STTR)[2]	$10,147,648
ARO-W Ballston Lease	$70,000
Youth Science Activities	$4,238,000
Research In Ballistics (Project H43)	$924,000
SBIR/STTR Support Services / Contract Support	$1,193,000
TOTAL: Other Army-funded Programs	**$138,828,312**

[1] Based on the status of funds on the last day of the fiscal year (30 Sep 2011), these University Research Initiative funds had not yet been designated for use in a particular URI program (*e.g.*, MURI, PECASE, DURIP).

[2] In addition to the FY11 allotment shown, FY10 funds were received or reallocated in FY11 for this category, as specified in TABLE 10.

TABLE 8

FY11 allotment for externally-funded programs. FY11 funds received from sources other than Army or OSD are indicated below. The Other Customer Funds category includes funding from a variety of customer sources, such as the Joint IED Defeat Organization (JIEDDO) and the Joint Project Manager, Nuclear, Biological, and Chemical (JPMNBC). The FY11 allotment values shown here represent the status of funds on the last day of FY11: 30 Sep 2011.

External Program	FY11 Allotment
Defense Advanced Research Projects Agency (DARPA)	$113,986,696
Scientific Services Program (SSP)	$19,370,555
Other Army	$35,687,422
National Security Agency (NSA)	$16,150,185
Defense Threat Reduction Agency (DTRA)	$8,021,740
Simulation and Technology Training Center	$9,634,772
Joint Program Manager NBC Contamination Avoidance	$9,451,787
Other Customer Funds (*e.g.*, JIEDDO and JPMNBC)	$56,163,248
TOTAL: External Programs	**$268,466,405**

TABLE 9

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

OSD Direct-funded Programs	FY11 Allotment
SBIR/STTR[1,2]	$0
Historically Black Colleges and Universities / Minority Institutions (HBCU/MI)	$20,090,000
Chemical and Biological Defense (CBD) Programs[2]	$3,405,786
CBD SBIR[1,2]	$127,052
TOTAL: OSD Direct Funding	**$23,622,838**

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

[2] In addition to any FY11 allotments shown, FY10 funds were received or reallocated in FY11 for this category, as specified in TABLE 10.

D. Summary of FY10 Funds Received or Reallocated for Use in FY11

TABLE 10

FY10 funds received or reallocated for FY11. In addition to the FY11 allocations listed in TABLES 6-9, these programs were also supported through FY10 funds received or reallocated for use in FY11.

Program Category	FY10 Funds Received in FY11
NRC Associates Program (BH57 funds)*	$259,688
BAST (Army funds)	$204,015
Army SBIR (Army funds)	$5,946,078
Army STTR (Army funds)	$937,118
SBIR/STTR (OSD direct funds)	$1,575,623
CBD Programs (OSD direct funds)	$2,919,413
CBD SBIR (OSD direct funds)	$1,797,362
TOTAL: FY10 Funds Received or Reallocated in FY11	**$13,639,297**

* These NRC funds were FY10 carry-over reallocated for use in FY11.

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

TABLE 11

Summary of FY11 allotment for all ARO managed or co-managed programs. This table lists the subtotals from TABLES 6-9 and the grand total FY11 allotment for all ARO managed or co-managed programs. These totals do *not* include FY10 funds received or allocated in FY11 for certain programs (refer to TABLE 10).

Program Category	FY11 Allotment
Core (BH57) Programs	$71,655,840
Other Army-funded Programs	$138,828,312
External Program Funds	$268,466,405
OSD Direct-funded Programs	$23,622,838
GRAND TOTAL: (all sources)	**$502,573,395**

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 2011* is to provide information on the programs and basic research efforts supported by ARO in FY11, 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 FY11.

A. Scientific Objectives

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

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

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

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

B. Program Areas

To meet the long-term program goals described in the previous section, the Chemical Sciences Division engages in the development, identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, that provide a framework for the identification, evaluation and monitoring of research projects. In FY11, the Division managed research within these four Program Areas: (i) Polymer Chemistry, (ii) Molecular Dynamics, (ii) Electrochemistry, and (iv) Reactive Chemical Systems. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

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

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

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

The research supported by this Program Area will likely enable many future applications for the Army and general public. These applications include more efficient and clean combustion technology, the development of new tools to study condensed phases of matter, the capability to accurately predict the properties of theoretical molecules, and the development of novel molecules for use in energy storage.

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.

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

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

C. Research Investment

The total funds managed by the ARO Chemical Sciences Division for FY11 were $48.6 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY11 ARO Core (BH57) program funding allotment for this Division was $5.9 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $7.2 million to projects managed by the Division. The Division also managed $6.5 million of Defense Threat Reduction Agency (DTRA) programs, $8.0 million of Defense Advanced Research Projects Agency (DARPA) programs, and $3.0 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.7 million for contracts in FY11. The Institute for Soldier Nanotechnologies received $12.6 million in FY11. Finally, $3.7 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

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

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). 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. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. Coatings Workshop (Arlington, VA: 16 December 2010). This was a follow-up workshop to the 2009 Control of Coatings Properties for Hazard Containment Workshop (held in the UK). Many of the participants from the UK workshop and new participants representing academic, government, and industry organizations presented the current state of their coatings related research, including challenges and strategies to overcome these and other technical obstacles. In addition, an overview was provided by the JPM-Decon on various coating concepts and potential integration into future systems. During the course of the day, a variety of key challenges were identified, stimulating prospective basic research focus areas in the understanding of chemical agent resistant coating (CARC), responsive materials, fundamental adsorption and diffusion, and novel coatings including peelable, passive, and active coatings.

2. Workshop on Advanced Energetic Materials Synthesis (College Park, MD; 3-5 April 2011). This workshop brought together leading synthetic chemists from the USA and Europe to discuss current challenges in the area of synthesis of advanced energetic materials. Approximately thirty scientists participated and represented both academic and government institutions. The most promising emerging chemistries and technology challenges for synthesis of advanced energetic materials were discussed. The participants provided recommendations for speeding up transition paths from lab scale to production while minimizing costs. The workshop clearly demonstrated that the energetic materials focus in the DoD during the past 5 years has been driven by near-term needs to meet environmental needs and support insensitive munitions requirements. The workshop clearly demonstrated the need for underpinning basic research that will lead to the development of the next generation of high-performance energetic materials.

3. 31st Free Radicals Symposium (Port Douglas, Australia; 24-29 July 2011). Molecular free radicals play a vital role as intermediates in diverse chemical reactions including those involved in combustion, detonation, chemical synthesis, and even atmospheric and interstellar phenomena. The International Free Radicals Symposium was established to bring together scientists at the frontier of research in a wide variety of areas of free radical chemistry with particular emphasis on the spectroscopic identification, characterization and dynamics of radicals. Topics covered included combustion, atmospheric chemistry, spectroscopy, chemical kinetics, molecular ions, ultracold radicals, and reaction dynamics. Many topics addressed by the symposium are central in determining the inherent roles that radicals play in processes such as detonation, deflagration, and combustion; all of which are of interest to the Army.

4. Flow Battery Workshop (Arlington, VA; 8-9 August 2011). The focus of the workshop was to discuss DoD needs and relevant research for high energy density storage devices to support small footprint, self-sufficient operations around the world. Flow batteries may be an important contributor in addressing this need. The goals of the workshop were to understand the state of the art across several different flow battery technologies (including the challenges and limitations for each), to explore the near-term R&D opportunities for flow batteries to overcome their respective challenges, and to identify basic research needs that can contribute to flow batteries. In addition to high energy density, key considerations are safety, cycle life, charge/discharge rates, ruggedness, transportability, scalability, and manufacturability. Attendees included technical representatives from ARL, industry, university professors, National Laboratory researchers, DARPA, the intelligence community, and Department of Energy (DOE). Five speakers from industry, four from academia, and two from national laboratories gave technical presentations.

5. Chemical/Biological Filtration and Materials Strategies Working Groups (Arlington, VA: 13-15 September 2011). These working groups provided a forum for academic and government experts in chemical and biological materials development to provide the Soldier with enhanced capabilities for future CB protective equipment. Many of the PIs participating in these groups are contracted through ARO, and in some cases, are co-funded by the Edgewood Chemical and Biological Center (ECBC) and ARO. The Chemical/Biological Filtration Strategies Working Group was the fourth in its series. This year's focus included identifying, characterizing, and engendering surface chemistry in substrates; development of novel nanostructured porous materials for toxic chemical removal; and sorbent maturation for ammonia. This was the first year for the Materials Strategies Working Group and included overviews of the current and prospective respirator programs, including current research on dry adhesives, anti-fog coatings, air management concepts, and improved seal developments. Novel materials development progress on nanomaterials, nanosensors, and MEMS, was also presented.

C. Multidisciplinary University Research Initiative (MURI)

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

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

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

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

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

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

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

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

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

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

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

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

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Direct Ethanol Fuel Cell System. Two Phase I SBIR contracts were awarded to Lynntech, Inc., and Tremont Technology, LLC, to develop an alkaline direct ethanol fuel cell (DEFC) capable of converting ethanol fuel into electricity in an efficient, small, lightweight, portable power system. Ethanol offers an attractive fuel-source alternative because it can be produced in large quantities from biomass and is less toxic than methanol. Direct ethanol fuel cells have recently been receiving increased attention in the literature; however, previous studies in acidic media have demonstrated only 2 or 4 electrons are generated per ethanol molecule rather than the 12 that are possible when ethanol is fully oxidized, resulting in poor system efficiencies. The recent development of alkaline membranes that conduct hydroxyl ions (OH-) makes alkaline membrane fuel cells very attractive largely due to more facile kinetics for both fuel oxidation and oxygen reduction reactions. The rapid kinetics makes the use of catalysts with lower noble metal contents feasible and potentially enables the cleavage of carbon-carbon bonds at low temperatures. The ultimate goal of these projects is to develop a high-efficiency alkaline DEFC system with a power density over 150 mW/cm^2, and a system energy density over 1000 Wh/kg. If successful, this research will provide a system that can significantly increase fuel utilization and fuel cell performance, with lower cost and improved safety.

2. Highly-sensitive Plasmonic Nanosensors for Chemical Warfare Agents. Two Phase I SBIR contracts were awarded to Real Time Analyzers, Inc., and MKS Technology, Inc., to develop a prototype sensor based on the phenomenon of localized surface plasmon resonance (LSPR) for the real-time detection of chemical warfare agents (CWAs) at ultra-low concentrations. Recent developments in the study of LSPR in metallic nanodots have shown a possible path toward greatly improved sensitivity of optical sensors based on metal nanoparticle arrays. LSPR, a phenomenon that occurs when light incident on metal nanoparticles induces the conduction electrons to oscillate collectively with a resonant frequency, causes nanoparticles to absorb and scatter light with an extremely high intensity. Research has shown that when molecules adsorb onto a plasmonic nanoparticle, the local electromagnetic fields around the particle can enhance the Raman scattering by as much as 10^{15} for a single molecule. This phenomenon, known as surface-enhanced Raman scattering (SERS), results in a highly specific and sensitive method for molecular identification. The ultimate goal of these SBIR efforts is to develop highly-sensitive and selective sensors that will be able to detect a specific CWA simulant at a vapor-phase concentration equal to or less than 0.0001 mg/m^3 in a response time of less than one minute. If successful, these sensors may be used to support chemical demilitarization efforts and provide protection for personnel in battlefield environments.

3. Spore Viability Detection System. Two Phase I CBD-SBIR contracts were awarded to Physical Optics Corporation and Triton Systems, Inc., to develop a system to rapidly and quantitatively identify the presence of spores. Current fielded biological indicator systems are rapid and offer on-site detection, however they are only qualitative. There is a current need for a bio detection system to rapidly assess the efficacy of decontamination products for inactivating Bacillus anthracis spores on environmental surfaces in a quantitative manner. The goal of these SBIR contracts is to use spore strips made of different materials that are inoculated with Bacillus thuringiensis spores combined with a handheld device to quantitatively determine remaining viable spores. Prototype systems will be developed and validated using quantitative viability tests of the decontaminated spores attached to the spore strips. If successful, this research may lead to a rapid, NIST-certified, quantitative bio-indicator system for decontamination and Soldier protection.

4. Low-power Organophosphate Detector. A Phase II Chemical Biological Defense SBIR (CBD-SBIR) contract was awarded to Lynntech, Inc., to develop and validate a nerve agent detection system that requires little to no operating power. Chemical nerve agents pose a significant threat to the military and civilians. In the case of a hazardous material release, the exact identification of the active agent could enable faster and more effective medical and environmental responses. The ultimate goal of this SBIR project is to develop an inexpensive, reliable, resilient sensor for detecting and identifying specific nerve agents. This project continues efforts initiated in a Phase I project and will expand the understanding of the key recognition elements in various nerve agents, pesticides, and simulants to develop a sensor for accurately and selectively identifying a given agent. This type of detector could ultimately be used to identify a particular agent to which a warfighter or first-responder has been exposed, leading to the use of targeted measures for protection, decontamination, and treatment.

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

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Biomimetic Membranes for Direct Methanol Fuel Cells. Three Phase I STTR contracts were awarded to Giner, Inc., Lynntech, Inc., and Oceanit Laboratories, Inc. to develop new biomimetic membranes with chemical stability and reduced methanol crossover to enable micro direct methanol fuel cells (DMFCs). Current methanol-fueled polymer electrolyte based fuel cells suffer from methanol cross over, which reduces overall system efficiency and necessitates the use of diluted methanol solutions decreasing the system specific energy. Biomimetic membranes with ion channels either inspired by natural systems or membranes with channels from organisms offer several potential advantages, including improved conductivity and selective permeability. At the same time, bioderived systems represent several challenges including: chemical stability, dehydration, integration of bioderived materials into synthetic membranes, and the challenges of orienting and aligning pores to allow their use in thicker, mechanically robust membranes. The goal of these SBIR projects is to prepare and validate mechanically-robust biomimetic membranes that have conductivities on par with Nafion-based counterparts with reduced methanol crossover, and are chemically stable when exposed to high methanol concentrations. The membranes will be integrated into a fuel cell. If successful, this research may lead to new lightweight power sources with high energy density for powering electronic devices or recharging batteries.

2. Methanol Electrolyzer for Hydrogen Generation. A Phase I STTR contract was awarded to Lynntech, Inc. to develop an advanced direct methanol fuel cell (DMFC) that utilizes methanol electrolysis to produce hydrogen. A current method for generating hydrogen from methanol, called thermal reforming, requires operation at high temperatures, which increases the system complexity and thermal signature. Current DMFC methods suffer from reduced efficiency and yield over time. Methanol electrolysis offers a potential low-temperature approach to generate hydrogen efficiently from methanol, circumventing the high-temperature requirement of thermal reforming and the current limitations of DMFCs. The ultimate goal of this SBIR contract is to demonstrate methanol electrolysis using advanced electrocatalysts, characterizing the products, and demonstrating a method for integrating the electrolyzer into a fuel cell system. If successful, this research may lead to a new generation of methanol fuel cell systems that can directly convert methanol to electrical power, providing a low-weight system for powering electronic devices or recharging batteries.

3. Sensitive and Shape-Specific Molecular Identification. A Phase I STTR contract was awarded to Ryon Technologies, Inc., to develop a compact and portable instrument that couples mass spectrometry and Rydberg spectroscopy to provide a complete "fingerprint" of a molecule. Mass spectrometers (MS) are powerful and widely used tools for molecular analysis in chemical and pharmaceutical industries, for environmental analysis, in forensic labs, and in basic research. However, the standard instruments have two primary drawbacks for application in-the-field: their large size and their inability to rapidly identify isomers and conformers of molecules of interest. In recent years it has been shown that excited electronic (Rydberg) states could distinguish among molecular shapes (isomers) for several different atomic compositions. Laser-induced Rydberg spectra may provide "fingerprints" that, when joined with MS molecular mass spectra, would enable unambiguous identification of molecular structures (isomers) and further, different molecular shapes (conformers) of the same isomer. If successful, this research will enable a major advance in selectivity for threat identification in the field with minimal sample consumption, and at reduced instrument footprint and cost.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) – 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). The FY11 new starts within these programs are described here, while the missions of each of these programs were described *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. DoD REP Awards. As described in more detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, REP awards aim to enhance or increase the programs, capabilities, and graduates in scientific and engineering disciplines in universities serving underrepresented minorities. In FY11, the Chemical Sciences Division managed seven new REP projects, totaling $3.6 million. The equipment purchased with this award is promoting research in areas of interest to ARO, such as investigating methods for the adsorption and sensing of organophosphates, and exploring protein conformational dynamics and aggregation.

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

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. New Microstructures for Old Monomers: Syntheses of Gradient Pi-Conjugated Copolymers. The objective of this PECASE, led by Professor Anne McNeil at the University of Michigan, Ann Arbor, is to create novel organic materials with useful properties by developing a fundamental understanding of the relationship between material structure and bulk properties.

Organic pi-conjugated polymers are the active components in emerging military technologies, such as fluorescent sensors for chemical agents, solar cells for operation in the field, and artificial muscles. Unfortunately, the widespread exploitation and application of these polymers has not materialized due to the current lack of diversity in polymer structure and properties and the inability to control morphologies of polymer blends. The investigator aims to overcome these limitations by generating a new class of pi-conjugated copolymers that have gradient microstructures and unique properties. The ability to tailor properties by simply altering the monomer sequence will provide a powerful new design strategy for preparing the next generation of organic materials that can have unique and tunable optical, electronic and physical properties, including phase-compatibilization. This research, if successful, will have a significant impact on current and future applications utilizing pi-conjugated materials, such as controlled, nanostructured thin films for use as fluorescent sensors that warn the Soldier of chemical or biological threats, lightweight solar-to-electrical energy converters for light-weight power generation in the field, films for shielding from electromagnetic interference, and as a component of artificial muscles.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY11, the Chemical Sciences Division managed ten new DURIP projects, totaling $1.2 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of electrocatalysts, dynamic combinatorial chemistry and the gas-phase decomposition of energetic materials, and the interactions between metals, support materials, and chemisorbed gases within carbon silica materials.

I. 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) Light Weight, Multifunctional Nanostructured Fibers and Materials, (ii) Battle Suit Medicine, (iii) Blast and Ballistic Protection, (iv) Chemical and Biological 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 FY11, the ISN supported 50 faculty, 110 graduate students, and 40 postdoctoral fellows across 12 departments at MIT. The ISN program is unique in that it currently has 17 industrial partners positioned to receive promising technical results and work to bring new products and capabilities to the Soldier, as well as a mechanism for additional industry partners to join and leave the Institute, depending on needs and activities. A U.S. Army Technical Assessment Board and an Executive Steering Board annually review the ISN research portfolio, assessing the goals of the various projects and research results. The ISN and its industry partners are well-situated to perform basic and applied research in response to Soldier needs now and in the future. A total of $12.6 million of program funds was allocated to the ISN in FY11, which was the fourth year of a contract that was renewed in FY07 for a five-year period. Of these FY11 funds, $9.5 million was allocated for 6.1 basic research and $3.1 million was allocated for eight applied research projects, including two new projects.

J. Joint Science and Technology Office for Chemical and Biological Defense

Traditionally ARO has been a strong partner with the Chemical Biological Defense (CBD) Program. The Reactive Chemical Systems Program manages several basic and applied research efforts for the CBD program. The goal of this program is to develop technologies for protection of the warfighter from chemical and biological agents. Basic research efforts in the areas of biomimetic catalysts, bio/abio interfaces, and mass transport and diffusion are aligned with and enhance the Army basic research program. Research in this program includes fundamental surface chemistry, molecular recognition, and enzyme stabilization. ARO also manages the Decon Enabling Sciences program, which strives to accelerate the transition of fundamental research to the development of decontamination and chemical detection technologies.

K. DARPA Biofuels Alternative Feedstocks

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

L. DARPA Limits of Thermodynamic Storage of Energy

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

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

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

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. Electrostatic Control of Protein-Surface Interactions

Professor Lauren Webb, University of Texas-Austin, Single Investigator Award

The overall goal of the current project by the Webb laboratory is to create surfaces that mimic the biological electrostatic mechanisms of natural protein interfaces. Peptide functionalized gold surfaces are being investigated to control protein orientation at surfaces, and to ultimately reproduce protein function at a non-biological surface. An azide-terminated self-assembled monolayer and an α-helical peptide containing two nitrile groups a known distance apart are reacted via click chemistry to produce a peptide that is chemically tethered to the surface at two points (see FIGURE 1).

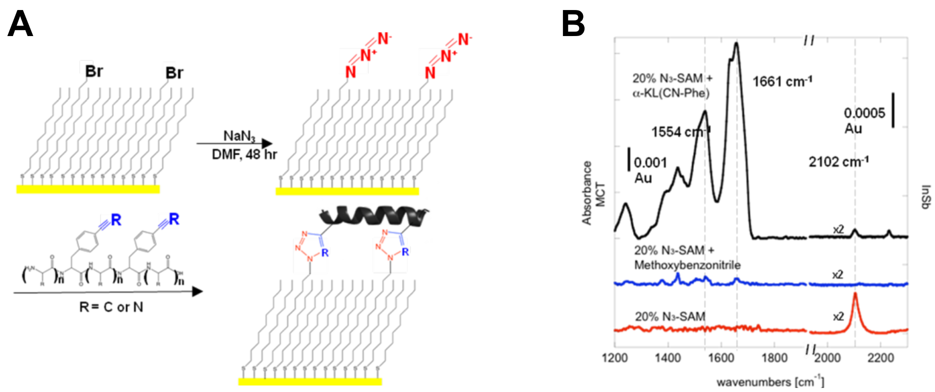

FIGURE 1

Surfaces mimicking biological electrostatic mechanisms of natural protein interfaces. (**A**) The schematic displays the surface functionalization route, while (**B**) FTIR spectra indicates N_3-terminated surface (red), N_3-terminated surface reacted with nitrile (blue), and N_3-terminated surface reacted with α-helical peptide (black).

Analytical techniques including X-ray photoelectron spectroscopy, ellipsometry, and grazing incidence angle reflection-absorption infrared spectroscopy (GRAS-IR) are used to determine the chemical composition of the resulting surface. GRAS-IR is also used to monitor the disappearance of the azide, quantifying the extent of reaction/functionalization; the relative intensity of the amide peaks is indicative of the relative orientation of the peptides. Data has shown that the peptides are randomly oriented and/or unstructured. In order to further address this preliminary finding, current research is focused on optimization of the surface-bound azides, modifying the distance between the reactive nitrile groups on the peptide, and overall reaction conditions. The ability to precisely control peptide orientation and conformation on abio surfaces is critical to many areas of DoD relevance including sensing, protective materials, coatings, drug delivery, and prosthetics.

B. Nanoscale Probing of Electrical Signals in Biological Systems Using Carbon Surfaces

Professor Ryan O'Hayre, Colorado School of Mines, PECASE Award

Professor Ryan O'Hayre and colleagues have been studying dopant/catalyst combinations to understand the fundamental electrochemical properties that may ultimately enhance the performance of direct-methanol fuel cells. A potential long-term application of this research is the development of a next-generation fuel cell catalyst system purposely "engineered" using dopant-mediated growth and stabilization. This "dopant engineering approach" is based on the observation that the activity and stability of a nanoparticulate catalyst supported on a high-surface area electrode material (such as a carbon nanotube support) can be enhanced by purposely doping, or chemically modifying, the support surface. In other words, the chemistry of a support surface influences the behavior of the overlying catalyst nanoparticles. Prior results revealed dramatic increases in catalytic activity for methanol-oxidation and oxygen-reduction reactions when Pt catalysts were supported on nitrogen-doped carbon materials instead of on pure carbon materials. Building on these prior results, the investigators have been quantifying dopant-induced catalytic effects to determine whether these effects can be extended to other dopant and catalyst systems. In comparison to a conventional approach using a non-modified carbon support, the dopant-engineering approach employs heterovalently-doped carbon support materials decorated by catalyst nanoparticles. The dopant atoms can influence the size, density, distribution, and perhaps even the activity of the overlying catalyst nanoparticles.

In FY11, the researchers examined nitrogen, argon, and fluorine doping of PtRu-alloy catalysts, and demonstrated significant durability enhancement effects from the nitrogen-doping approach. After cycling of potential PtRu/HOPG substrates, the investigators found that the coverage of the metal phase changes dramatically and that these changes vary greatly depending on the implantation dosage of dopant. Analysis of the results revealed that despite nearly constant initial coverage, all samples show a significant decrease in catalyst coverage after cycling (see FIGURE 2).

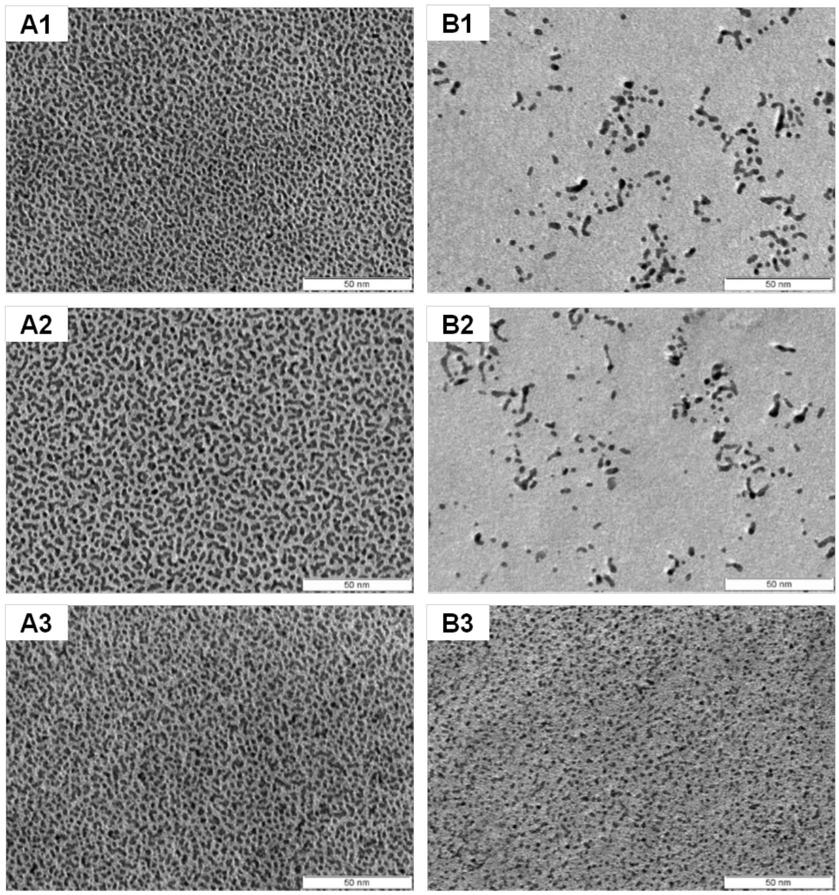

FIGURE 2

Metal phase coverage dependent on implantation dosage of dopant. Transmission electron micrographs representative of sputtered PtRu deposited on HOPG substrates (**A**) precycled, demonstrating coverage and range of nanoparticle sizes, and (**B**) postcycled, demonstrating changes in the coverage, particle size, and formation of agglomerations. The sputter deposition method was found to result in catalyst deposition without preference to nitrogen/defect sites; therefore, significant loss of the metal phase is expected for all the samples. Within each category (A-B), dosages of (1) 0.0×10^{16}, (2) 1.3×10^{16}, and (3) 4.7×10^{16} ions cm^{-2} (0, 15, and 45 s) were employed.

The loss in coverage area is particularly severe for the low-nitrogen dose sample (see FIGURE 2, dosage row 2). The low-nitrogen dose retained less than 10% of its initial catalyst coverage after cycling. Intriguingly, the high-dose sample (see FIGURE 2 dosage row 3), previously used as an optimum implantation condition in prior Pt/N-HOPG studies, also appeared to provide the optimum durability performance for this PtRu/N-HOPG study. This sample retained 40% of its original coverage after cycling. The difference in the loss for various implantation doses however can be directly related to the amount and speciation of the nitrogen introduced during implantation.

Professor O'Hayre has successfully utilized a model catalyst system to explore the effect of nitrogen doping on the durability of PtRu nanoparticle catalysts. Magnetron sputtering of the PtRu enabled deposition of the metal nanophase without preference to defect sites or nitrogen functionalities, in contrast to electrodepostion routes, which result in preferential deposition on defects/nitrogen sites. The sputtering conditions resulted in high metal coverages in the range of 3440% with particle sizes in the range of 2-3 nm. While all samples were somewhat ruthenium-rich, the behavior and morphology were consistent across the series of samples independent of the nitrogen implantation dose. After potential cycling, the coverage and morphology of the metal phase changed dramatically and were shown to be greatly dependent on the implantation dosage. The undoped (only carbon sites) and low-dosage samples (oxygen and nitrogen sites are present, nitrogen concentration is low) showed significant coverage loss and substantial morphological changes and had an overall negative effect on PtRu nanoparticle stability. Highly N-doped samples, on the other hand (oxygen and nitrogen sites are present, nitrogen concentration is high), showed less coverage loss and minimal morphological changes. The optimum stability of the PtRu nanoparticles was obtained with an implantation dosage of 4.7×10^{16} ions cm^{-2}. In summary, these observations may ultimately enable the development of catalysts for low-temperature direct-alcohol fuel cells, which are attractive because of the higher energy densities and improved logistics of alcohol fuels compared to primary batteries.

C. Embedded density functional theory methods for modeling of reactions in complex systems

Professor Thomas Miller, III, California Institute of Technology, STIR Award

Computational modeling of chemically reactive systems in the condensed phase faces extraordinary challenges from the perspective of electronic structure theory. Target applications include accurate prediction of organic crystal structure, metal dendrite formation at electrolyte/electrode interfaces, and the chemical decomposition of crystalline high energy density materials. These problems combine large system sizes with subtle but important intermolecular interactions, and in many cases, they involve multiple dynamic timescales and electronically non-adiabatic effects. The development of new methods to perform reliable, on-the-fly electronic structure calculations at a computational cost that makes feasible the simulation of long-timescale dynamics in large systems remains the central challenge in theoretical chemistry.

The goal of this research project is to develop a first-principles electronic structure approach that (i) avoids the computational cost of conventional density functional theory (DFT) and wavefunction methods, (ii) allows for the seamless molecular dynamics simulation of chemical reactions without introducing the parameterization demands and system specificity of reactive force fields, and (iii) allows for the multi-level partitioning of the electronic structure calculation, while providing a systematically improvable treatment of the interactions between the partitions and without introducing interfaces between spatial domains. The approach is to employ an exactly embedded DFT method. Embedded DFT (e-DFT) offers a multi-scale approach to electronic structure calculations in which the interactions between subsets of a system are evaluated in terms of the subset electronic densities. The major weakness of e-DFT has been a lack of a quantitative non-additive kinetic potential (NAKP), which arises from partitioning a system into subsystems. This term, which is typically largest for cases in which the subsystem densities are strongly overlapping, is a significant source of error in many e-DFT calculations, and it generally limits the method to applications in which the subsystem densities involve nonbonded or weakly interacting molecular groups.

A recent breakthrough by Professor Miller has resulted in the development of a formally exact protocol for calculating the NAKP contribution in e-DFT calculations. The result is that the new e-DFT method, which uses the exact NAKP, is equivalent to standard Khon-Sham DFT. This method is referred to as embedded density functional theory (exact embedding), or e-DFT-EE. Use of e-DFT-EE makes e-DFT much more useful for simulating molecular dynamics in large systems. For example, consider the dissociation of the water dimer, $(H_2O)_2$. The system consists of the dimer and the subsystems are the individual water molecules. The potential energy curve for dissociation was calculated via e-DFT using the new e-DFT-EE method and two popular approximate kinetic energy functionals: TF or LC94 (see FIGURE 3).

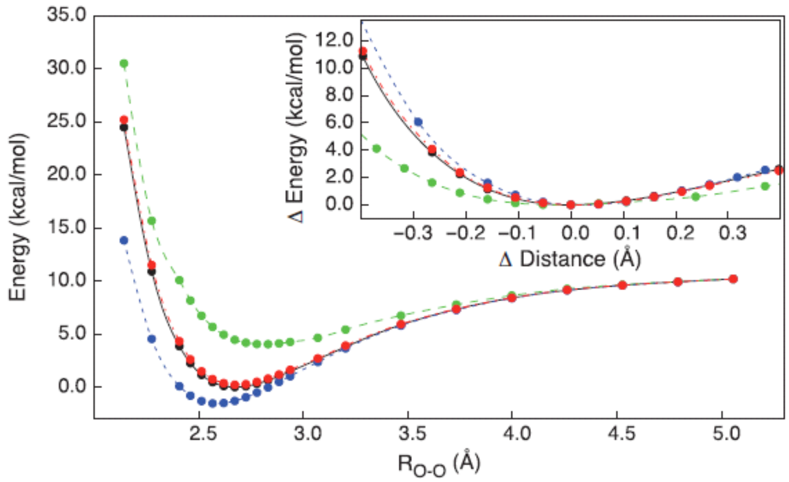

FIGURE 3

Potential energy curves for $(H_2O)_2$ dissociation. The water dimer dissociation curve was obtained using e-DFT-EE (red), e-DFT-TF (green), and e-DFT-LC (blue). Also shown is the reference KS-DFT result (black), which is graphically indistinguishable from the e-DFT-EE curve. Inset, the curves are shifted vertically to align the energy minima and horizontally to align the equilibrium distances.

The potential energy curves shown in FIGURE 3 reveal that e-DFT-EE and KS-DFT are in quantitative agreement, and that use of approximate NAKPs results in significant error even for small systems with non-covalent interactions. These results establish e-DFT-EE as a promising methodology for performing accurate, first-principles molecular dynamics calculations.

D. Stimuli Responsive Amphiphilic Colloidal Assemblies

Professor S. Thayumanavan, University of Massachusetts-Amherst, Single Investigator Award

Professor Thayumanavan's effort focuses on the design and synthesis of responsive amphiphilic assemblies. These supramolecular assemblies act in a "catch and release" mechanism such that the micellar assembly acts as a host for small guest molecules and releases the guests in response to an external stimulus (see FIGURE 4).

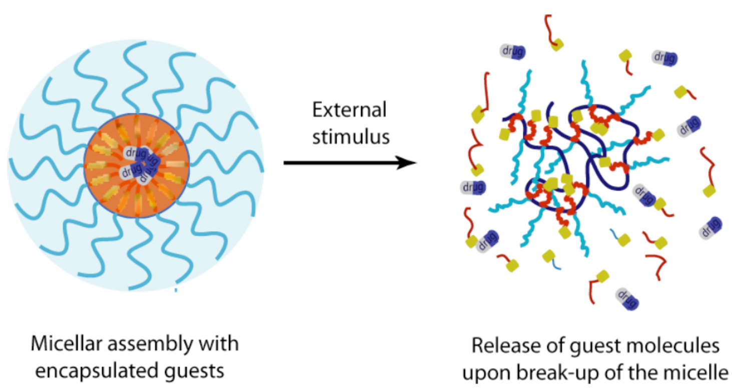

FIGURE 4

Micellar assembly response to stimulus. The schematic illustrates the release of guest molecules due to stimuli-responsive disassembly.

Because the hydrophilic-lipophilic balance (HLB) of the system dictates the formation of micellar assemblies, molecules are specifically designed in which a trigger (change in pH, redox, temperature) disrupts the HLB causing disassembly and guest release. To illustrate this concept, a self-assembling, micelle-forming amphiphilic dendron with cleavable hydrophobic moieties has been synthesized (see FIGURE 5). A hydrophobic guest molecule can be encapsulated within the micelle in aqueous conditions. Upon photochemical irradiation, the amphiphilic dendron is cleaved, the micelle disassembles, and the guest molecule is released. Stimuli-responsive systems have the potential to impact many areas of military and civilian importance such as drug delivery, self-healing materials, and self-cleaning systems.

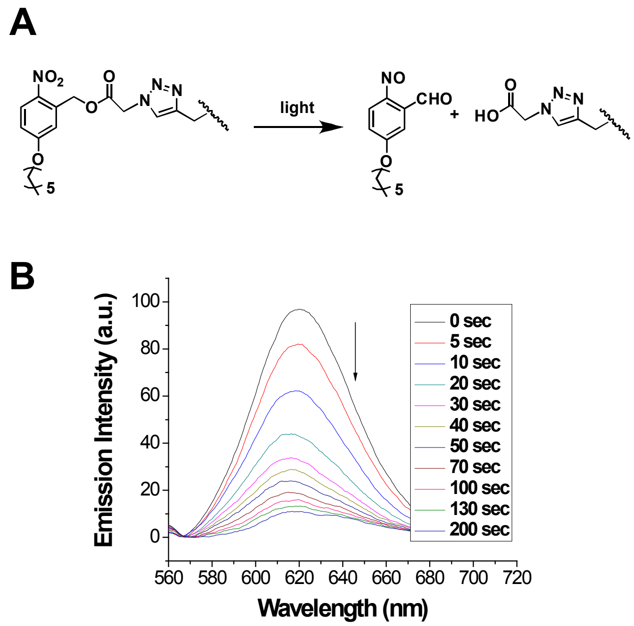

FIGURE 5

Self-assemblying, micelle-forming amphiphilic dendron. (A) the model reaction of photochemical cleavage and (B) spectroscopic evidence for release of non-covalently encapsulated dye molecule with increasing irradiation time.

E. Composition and Properties of Novel Polymers Containing Metal Ligands in Side Chain

Professor Greg Tew, University of Massachusetts – Amherst, Single Investigator Award

Professor Tew's laboratory previously discovered that metal-containing monomers that are polymerized into block copolymers form morphologies for which the metals segregate into nanostructured domains leading to ferromagnetic materials. Interestingly, when the same polymer composition was used to prepare a homopolymer with no structure, the film showed no magnetism. Professor Tew's current research builds on these discoveries, with the goal of understanding how the observed ferromagnetic behavior depends on nanostructured self-assembly and monomer chemistry.

In FY11, Professor Tew successfully prepared novel block copolymers that are pre-programmed with the necessary chemical information to micro-phase separate and deliver room temperature ferromagnetic properties. The importance of the nanostructured elements is demonstrated by comparison with the homopolymer, which yields only paramagnetic materials, despite the fact that it is chemically identical and has a higher loading of the magnetic precursor (see FIGURE 6). Exploring the phase morphology of the block copolymer confirms the role of the nanostructure and also provides insight into the role confinement plays in the magnitude of the magnetic response. The *in situ* generation densely functionalizes the surface of the magnetic elements, rendering them oxidatively stable. Nanostructured magnetic materials remain important for many advanced applications, thus new methods for their fabrication are critical. However until now, it has proven challenging to couple self-assembly to the generation of magnetic materials in a simple, straight-forward manner.

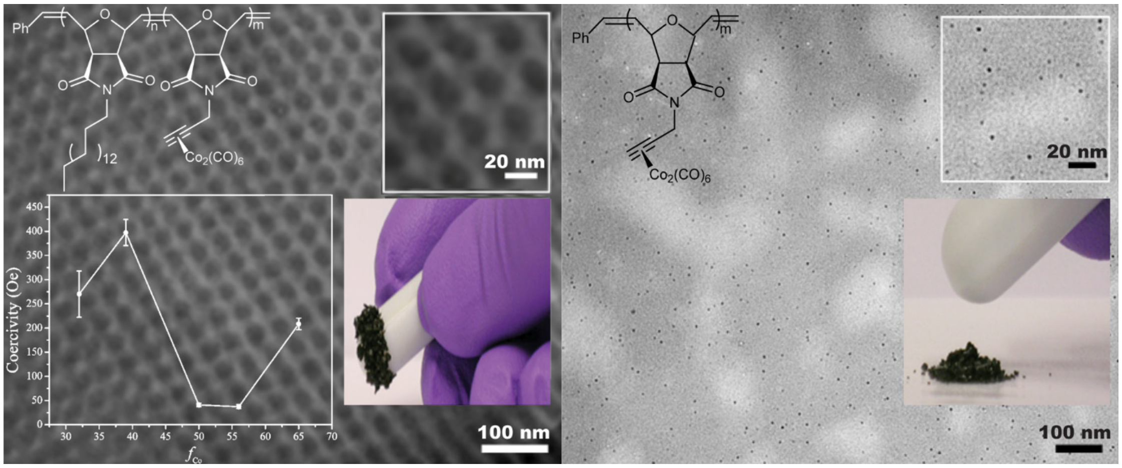

FIGURE 6

Chemical structure of the block copolymer and homopolymer. A larger-area TEM image (background) reveals the cylindrical block copolymer morphology with cobalt-rich cylinders and the homopolymer, which is unstructured but contains small (~4 nm) cobalt particles following heat treatment. Both images show a zoomed TEM inset as well as a photograph of the resulting magnetic powder. The block copolymer is clearly a room temperature ferromagnetic material while the homopolymer shows no room temperature attraction to the magnetic bar. This material is only paramagnetic at room temperature. The block copolymer's phase morphology is shown on the left image as a function of coercivity. The cylindrical phase has the highest coercivity followed by the inverted cylindrical phase and then the lamellar phase.

F. Mechanistic Studies of Li+ Catalysis of Radical Reactions

Professor Josef Michl, University of Colorado – Boulder, Single Investigator Award

The objective of this project is to understand structural and mechanistic effects on catalytic solutions of the lithium salt $LiCB_{11}Me_{12}$ in solvents with low polarity, such as benzene and 1,2-dichloroethane.

More specifically, Professor Michl and his colleagues have been studying the remarkable effect of a polar additive (sulfolane) on the $LiCB_{11}Me_{12}$ catalysis of radical polymerization of isobutylene in 1,2-dichloroethane initiated with azo-*t*-butane at 80℃. In FY11, the research team found that at concentrations that are effective (about 10%), solutions of $LiCB_{11}Me_{12}$ in 1,2-dichloroethane are colloidal, and dynamic light scattering suggests that the aggregates present are 100 - 200 nm. This size does not change perceptibly as sulfolane is added, but most other properties change dramatically. The conversion of the monomer to a polymer and the polymer molecular weight are essentially zero in the absence of sulfolane, rise to a sharp maximum when the molar ratio of sulfolane to $LiCB_{11}Me_{12}$ reaches about 0.15, and then drop precipitously at higher sulfolane concentrations. Although there is clear evidence that the catalysis is due to a complexation of the isobutylene monomer to Li^+, the exact nature of the Li^+ containing species involved in the complex is not known. Apparently, the concentration of this active species is maximized at a sulfolane molar ratio of 0.15. At present, it is not clear if this species is present in the inside or on the surface of the colloidal particles of $LiCB_{11}Me_{12}$, or if it is present outside of the particles.

A fundamental mechanistic understanding of Li+ catalysts may ultimately unable the design of novel polymer architectures and new kinds of polymer structures and compositions. In addition, these studies may lead to more efficient synthesis of commercial polymers by reducing the pressure and temperature required for preparing polymers, such as low-density polyethylene.

G. Exploring Photoluminescence (PL) Properties of Single-walled Carbon Nanotubes

Professor Michael Strano, Massachusetts Institute of Technology, ISN (UARC)

Professor Strano has been exploring the properties of single-walled carbon nanotubes (SWNT) to provide the basis for a trace-sensing platform. In FY10, the research team applied diameter confinement and the large aspect ratios of SWNT to detect single ions. In FY11, the investigators extended this approach to utilize the photoluminescence (PL) properties of SWNTs in the detection of nitroaromatic compounds. By wrapping nanotubes with the bombolitin-II peptide, conformational changes in the peptide can be elicited from the peptide upon binding of a nitroaromatic (see FIGURE 7). These conformational changes can be detected as a change in the fluorescence intensity and/or a spectral shift. In addition, different nanotube chiralities can demonstrate differences in their spectral responses to different analytes. It was found that the variances in chiral-specific intensity changes and wavelength shifts for different analytes generate distinct fingerprints among these analytes. Professor Strano has confirmed unique spectral signatures for the binding of six nitroaromatic analytes from eight chirally-distinct SWNT species via their segregation on a principal components analysis plot.

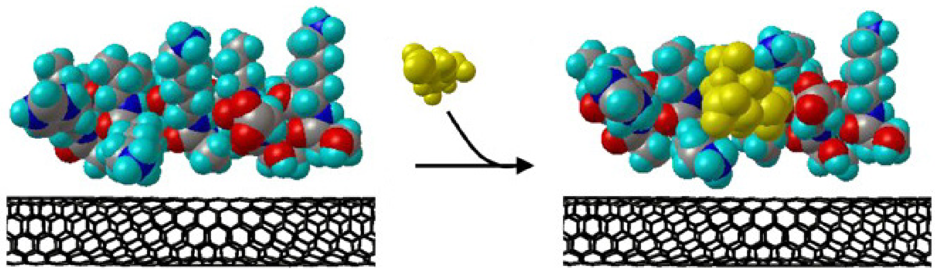

FIGURE 7

Energy-minimized structure of nanotube-wrapped bombolitin II. Conformational changes in the peptide were detected upon binding of a nitroaromatic. *[Heller D.A., et al., PNAS 2011; 108: 8544-8549]*

The bombolitin/SWNT-based platform was also used to monitor individual binding events of single analyte molecules. For this analysis, a dual-channel microscope was used to split immobilized SWNT PL images into distinct short- and long-wavelength channels. Addition of RDX to SWNT/bombolitin results in concomitant long-wavelength increases and short-wavelength decreases in intensity (see FIGURE 8). From this, discretized single-molecule adsorption and desorption events over time were observed; corresponding intensity traces of individual nanotubes demonstrated anti-correlated steps where intensity increases in long-wavelength emissions are coupled to intensity decreases in short-wavelength emissions and vice versa. These findings can provide the basis for a sensing platform with high specificity and sensitivity toward the detection of explosive compounds.

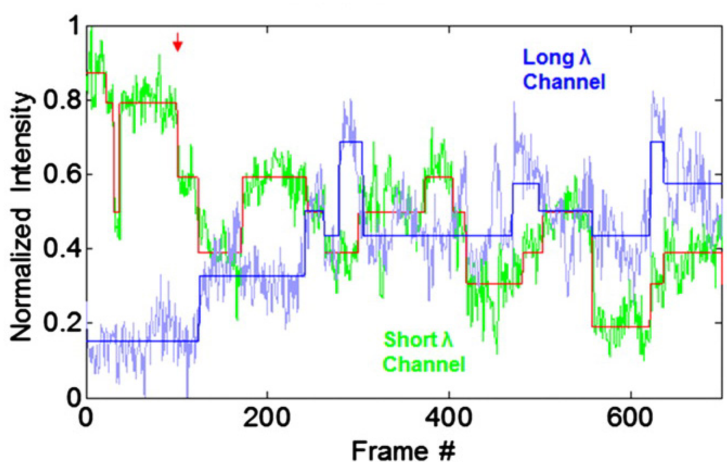

FIGURE 8

Long-wavelength increases and short-wavelength decreases in intensity result from addition of RDX to SWNT/bombolitin. The plot is a time trace of the intensity of a single (7,5) SWNT/bombolitin II PL fit by an iterative error minimization. The addition of 9 mM RDX occurred at time 100 s (red arrow). *[Heller D.A., et al., PNAS 2011; 108: 8544-8549]*

F. Radical Reactions in the Decomposition of Energetic Materials
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 detonation process. The chemical mechanism by which an energetic material releases energy begins with an initial chemical reaction which may or may not be exothermic, followed by a complicated sequence of elementary reactions that sum to the net exothermic reaction. The objective of this project is to reveal the key elementary reactions of the radical intermediates, formed when energetic molecules undergo decomposition. Professor Butler has been measuring product branching fractions and internal energies of chemical radicals formed in these reactions via a crossed laser-molecular beam apparatus coupled to a time-of-flight mass spectrometer. The work is currently focused on the study of unimolecular decomposition reactions relevant to the energetic molecule 1,3,3-trinitroazetidine (TNAZ). Previous work by the Nobel laureate Y. T. Lee[1] involving the infrared multiphoton dissociation of TNAZ within the ground electronic manifold led to a postulated reaction mechanism (see FIGURE 9).

Professor Butler's experiments are aimed in part at testing and validating this postulated mechanism. To develop a predictive description for the thermal decomposition of TNAZ, experiments were initiated that allow direct access to two intermediates relevant to the dissociation pathways of TNAZ. An intermediate with a C-C•(NO_2)-C moiety results from initial C-NO_2 fission in TNAZ. When the initial step in TNAZ dissociation is C-NO_2 bond fission, a radical species is created with the unpaired electron density formally on the C atom, but delocalized over the NO_2 moiety. In order to generate a locally analogous radical under collision-free conditions, C-Br photofission of 2-nitro-2-bromopropane was used. This results in the H_3C-C•(NO_2)-CH_3 radical, which is available to cleanly test predictions in the next step of the decomposition mechanism. Another probable initial decomposition step involving HONO elimination, which results in a radical with a C-C(NO_2)=C moiety, was considered. HBr elimination from 2-nitro-2-bromopropane generates 2-nitropropene, with a C-C(NO_2)=C moiety similar to that formed upon HONO elimination from TNAZ.

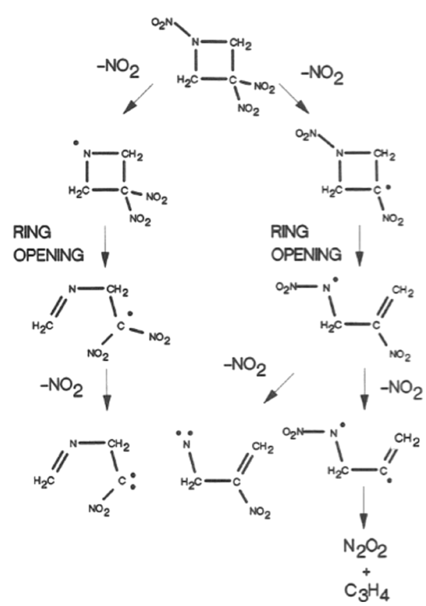

FIGURE 9

Proposed mechanism for thermal decomposition of TNAZ. Previous work by Y. T. Lee led to this postulated reaction mechanism.

Photodissociation of the carbon-bromine bond in 2-nitro-bromopropane produces H_3C-C•(NO_2)-CH_3 radical. In order to guide experiments, G4 composite calculations for several different product channels were conducted and

[1] Studies of Initial Dissociation Processes in 1,3,3-Trinitroazetidine by Photofragmentation Translational Spectroscopy, D. S. Anex, J. C. Allman, and Y. T. Lee, in *Chemistry of Energetic Materials*, Ed. by G. A. Olah and D. R. Squire (Acad Press, New York, 1991), pp. 27-54.

a potential energy diagram was produced (see FIGURE 10). RRKM calculations predict that the HONO elimination channel should dominate when one takes into account the vibrational energy distritubtion of H_3C-C•(NO_2)-CH_3. The momentum matched co-fragment to HONO elimination, H_3C-C=CH_2 was detected in the imaging apparatus using 10.5 eV photoinoization. The resulting *m/z* 41 image, corresponding to this radical, was fit with a two-step dissociation mechanism based on observed translational energy distributions of the initially formed $CH_3C(NO_2)CH_3$ or $CH_3C(NO_2)CH_2$. The portion of *m/z* 41 data due to HONO dissociation was identified by requiring the velocities to the two secondary products to be momentum matched (see FIGURE 11).

These results revealed that branching into the HONO elimination channel is comparable to the C-N fission channel forming CH_3C•CH_3 and NO_2. The investigator is continuing to more fully map out branching channels and energy thresholds for this TNAZ model system.

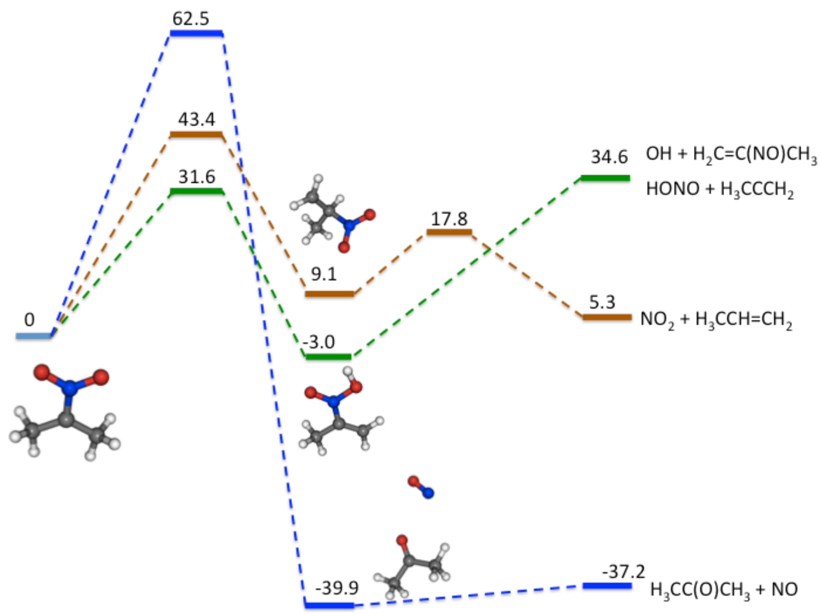

FIGURE 10

Possible dissociation channels of the H3C-C•(NO2)-CH3 radical intermediate. Photodissociation of the carbon-bromine bond in 2-nitro-bromopropane produces H_3C-C•(NO_2)-CH_3 radical. The potential energy diagram was produced using G4 composite calculations for several different product channels.

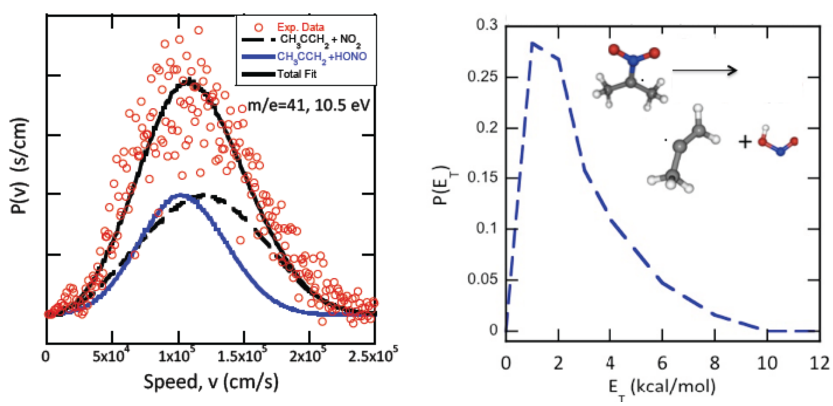

FIGURE 11

Velocity map imaging signal at m/z 41. The contribution assigned to the dissociation of the CH3-C•(NO2)-CH3 radical to HONO + H3C-C=CH2 is shown in the blue solid line, based on the distribution of energies partitioned into recoil energy in the right frame.

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. Adsorption Effects on Photoluminescence of Metal Oxide Nanoparticles

Investigator: Professor James Whitten, University of Massachusetts-Lowell, Single Investigator Award
Recipient: ECBC

The objective of this research is to investigate the use of photoluminescent metal oxides to chemisorb molecules of interest towards their application as residual life indicators. XPS and UPS are used to confirm adsorption of gases, and photoluminescence experiments determine changes in fluorescence upon adsorption of gases. It has been successfully demonstrated that photoluminescence changes occur in nanoparticulate ZnO, CeO2, and $Zr(OH)_4$ upon exposure to hydrogen chloride, sulfur dioxde, and nitrogen dioxide gases. Exposure of only 35 ppm of sulfur dioxde to ZnO resulted in distinct changes in the photoluminescence spectra (see FIGURE 12).

Most recently, metal oxide nanoparticles mixed with the currently used filtration media are being tested for PL measurements, and algorithms are being developed to correlate PL changes to residual capacity. This novel approach to measuring residual life of filters is being transitioned to the ECBC Filtration team for further studies.

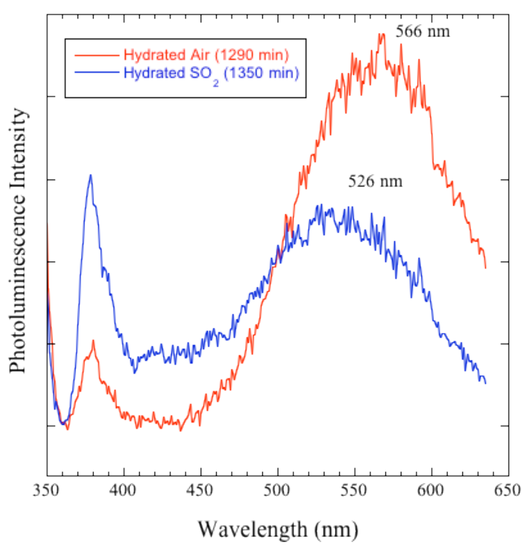

FIGURE 12

PL changes due to exposure of nano-ZnO to 35 ppm wet SO_2. Exposure of only 35 ppm of sulfur dioxde to ZnO resulted in distinct changes in the photoluminescence spectra

B. Electrochemical Models Reveal Unexpected Atomic Interactions in Proton Transfer

Investigator: Professor Stephen Paddison, University of Tennessee - Knoxville, Single Investigator Award
Recipient: 3M Corporation, Fuel Cell Components Group

The objectives of this single investigator project were to develop a multi-scale modeling approach for studying polymer electrolyte membranes (PEMs), to elucidate microscopic proton transport mechanisms, and to design a modeling protocol capable of predicting actual rates of proton diffusion.

Professor Paddison successfully developed a new multi-scale modeling approach that has already provided innovative design guidelines for the next generation of fuel cells. Fuel cells that convert liquid fuels to electricity could provide cleaner, quieter power to military bases than today's diesel generators. Alternatively, when configured as portable power systems, fuel cells such as the one shown in FIGURE 13 could reduce the weight of the batteries that are carried by soldiers by 60% compared with current solutions, or by more than 80% when used to power equipment directly. Today's fuel cell technology requires components that are more robust, work in a wider range of ambient conditions, and can be manufactured at lower cost. A major limitation in meeting these needs is the performance of PEMs. To address this need, Professor Paddison's research focused on characterizing the properties of PEMs, in part through developing new multi-scale modeling approaches.

FIGURE 13

Electrochemical modeling may improve future battery systems. This portable power system was developed from a previous ARO-funded project. The electrochemical models developed through this research may enable improved PEMs for fuel cells, ultimately enhancing the performance of portable battery-charging systems.

PEMs allow protons to permeate from one side of the cell to the other, thereby generating current. To understand this process, researchers must characterize the atomic-scale interactions between the protons and the polymer, as well as identify the mechanisms affecting the macroscale morphology of the polymer. The investigator has been approaching this problem using carbon nanotube (CNT) scaffolds to mimic the molecular environment of a PEM (see FIGURE 14). In this case the CNTs were functionalized with perfluorosulfonic acid (-CF_2SO_3H) groups, which are typical for PEMs, and hydrated with water molecules. Unexpectedly, the results of this model revealed that under certain conditions, hydrogen bonding occurred between the protons and CNT-bound fluorine atoms. This previously-undiscovered interaction influences the way that protons move through the membrane, and thus contributes to the effectiveness of the PEM.

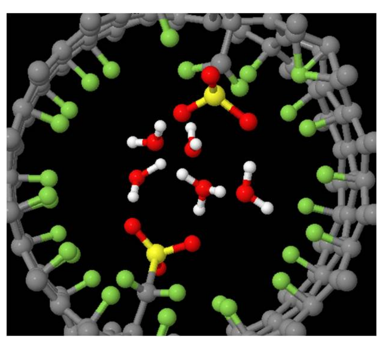

FIGURE 14

CNT scaffolds used to mimic and model PEM environment. The researchers used large-scale molecular dynamics simulations to successfully predicted changes in morphology for different PEM chemistries. More specifically, model systems comprising carbon nanotubes decorated with PEM functional groups were used to study the effects of hydration, confinement, and hydrophobicity on proton interaction and transport.

While the newly-discovered atomic-scale interactions are interesting, the immediate value of this effort was the application of these results to a larger-scale molecular dynamics model that can predict changes in polymer morphology and the distribution of water molecules under different hydration conditions. The atomic-scale modeling results were used to improve the accuracy of the input properties for this larger scale model, and thus improve the accuracy of the results. Using this model, the researchers successfully predicted the morphological properties and water distribution in three common PEM types (see FIGURE 15). After these results were verified experimentally, this new model transitioned to a commercial PEM developer (3M Corp.) to potentially improve the next generation of fuel cells.

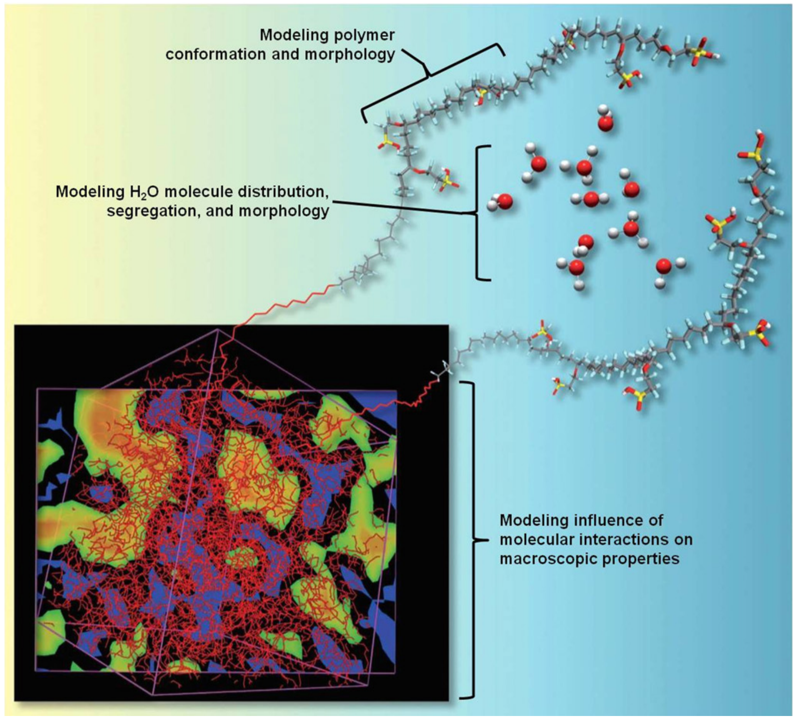

FIGURE 15

Predicting morphological properties and water distribution in PEMs. Based on the newly-developed CNT-based molecular model, scientists were able to use large-scale molecular dynamics simulations such as the one illustrated here to successfully predict the phase segregation, morphology, and distribution of water molecules for different PEM chemistries. Understanding these properties are critical in understanding how molecular interactions influence the performance of the PEM.

C. Understanding Morphology-property Relationships in Novel Metallopolymers

Investigator: Professor Stuart Rowan, Case Western Reserve University (CWRU), Single Investigator Award
Recipient: ARL-WMRD

Professor Rowan's laboratory previously discovered a new class of supramolecular metallo polymers that exhibit photo-induced healing. The goal of Professor Rowan's current research project is to fully understand the mechanism for healing and how it depends on factors such as polymer composition, polymer entanglements, and the metal salts and ligands that are responsible for the supramolecular assembly of the ditopic macromonomers.

A series of metallo-polymers previously synthesized in Professor Rowan's laboratory have transitioned to ARL-WMRD for further study. Professor Stuart Rowan (CWRU) and Dr. Rick Beyer (ARL-WMRD) are conducting collaborative research to understand the relationship between morphology and properties in a series of these novel metallo-polymers. These materials have properties expected to have a significant impact on technologies needed by the Warfighter.

This collaborative research led to the recent discovery of a relationship between long-range order and self-healing efficiency. A transmission electron microscopy (TEM) image of a sample containing Zn^{2+}, revealed that at 80% of the equimolar amount, the metal can form the metal-ligand bonds needed for supramolecular assembly (see FIGURE 16). Interestingly, using only 80% of the equimolar amount resulted in a morphology where grains of well-ordered lamellae are surrounded by sizable regions in which the material appears microphase separated but disordered. The materials exhibiting these partially-ordered morphologies exhibited substantially better self-healing characteristics than those with much better long-range order, counter to our expectations. This behavior is not yet well-understood, will continue to be explored through this collaborative research. The results were recently published in *Nature*[2], with a second manuscript accepted for publication in *Macromolecules*[3].

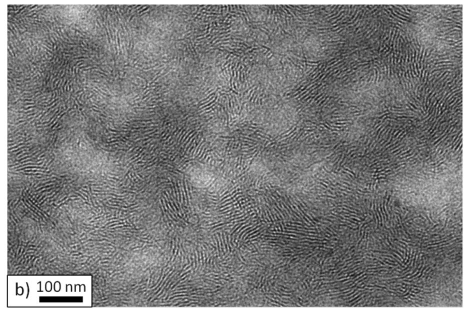

FIGURE 16

TEM micrograph of 3•$[Zn(NTf_2)_2]_{0.8}$ reveals the lamellar morphology, with regions of microphase separated but the material disordered. *[Burnworth, et al., Nature 2011, 472, 334-338]*

D. Air Purification: Nanostructured Media for Individual Protection

Investigator: Professor Krista Walton, Georgia Tech University, PECASE Award
Recipient: ECBC

This effort focuses on the synthesis, characterization, and modeling of metal-organic frameworks (MOFs) with molecule-specific adsorption properties. Previous water stability experiments confirmed the importance of metal-oxygen or metal-nitrogen coordination. Recently, Professor Walton has investigated how ligand functionality affects the MOF stability. A variety of ligand functionalized MOFs were synthesized using BDC isostructures (see FIGURE 17).

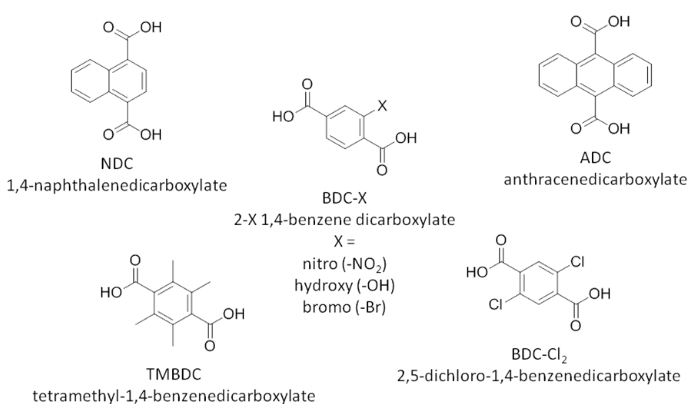

FIGURE 17

Ligand-functionalized MOFs. These ligand-functionalized MOFs were synthesized using BDC isostructures.

The investigator characterized each of the materials using powder X-Ray diffraction (PXRD), pore volume, BET surface area, and thermal stability. Water vapor isotherm data indicate that the Zn-TMBDC-DABCO and Zn-ADC-DABCO isostructures are the most stable (see FIGURE 18). These data revealed that linker

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[2] M. Burnworth, L. Tang, J. R. Kumpfer, A. J. Duncan, F. L. Beyer, G. L. Fiore, S. J. Rowan, & C. Weder. "Optically Healable Supramolecular Polymers." *Nature* **2011**, *472*, 334-337. DOI: 10.1038/nature09963.

[3] J. R. Kumpfer, J. J. Wie, J. P. Swanson, F. L. Beyer, M. E. Mackay, & S. J. Rowan. "Influence of Metal Ion and Polymer Core on the Melt Rheology of Metallo-Supramolecular Films." Submitted to *Macromolecules*.

functionalization can also impact water vapor adsorption and overall MOF stability. Stable, down-selected structures will be further investigated by the ECBC Filtration group towards development of nanostructured media for the use in air purification devices.

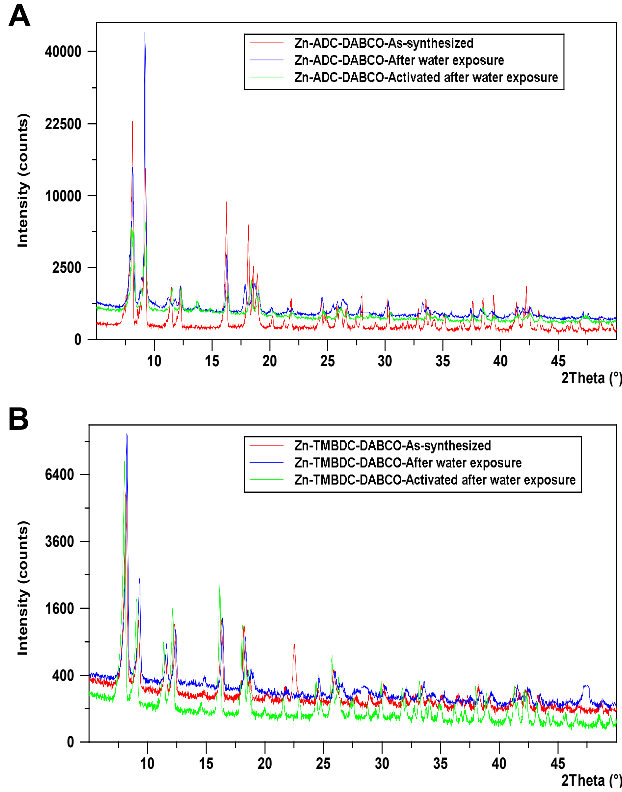

FIGURE 18

Characterization of ligand-functionalized MOFs. Water vapor isotherm results revealed that (**A**) Zn-ADC-DABCO and (**B**) Zn-TMBDC-DABCO isostructures are the most stable.

E. Exactly Embedded Density Functional Theory

Investigator: Professor Thomas Miller, III, California Institute of Technology, Single Investigator Award Recipient: ARL-WMRD, University College Cardiff Consultants Ltd., and research laboratories worldwide

The objective of the research project leading to this transition is to identify and validate a fundamentally new way to accurately calculate the properties of chemically reacting systems. More specifically, the investigator is pursuing a new method, based on embedded density functional theory (e-DFT), that avoids the computational cost of DFT, and allows for seamless molecular dynamics simulation of chemical reactions.

e-DFT offers a multi-scale approach to electronic structure calculations in which the interactions between subsets of a system are evaluated in terms of the subset electronic densities. A recent breakthrough by Professor Miller has overcome a severe weakness of e-DFT: the lack of a quantitative non-additive kinetic potential (NAKP), which arises from partitioning a system into subsystems. This term, which is typically largest for cases in which the subsystem densities are strongly overlapping, was a significant source of error in many e-DFT calculations. The new method, which incorporates an exact NAKP, is termed e-DFT-EE and will pave the way for the seamless molecular dynamics simulation of chemical reactions without introducing artificial parameterization. Also, e-DFT-EE allows for the multi-level partitioning of the electronic structure calculation, while providing a systematically improvable treatment of the interactions between the partitions without introducing interfaces between spatial domains. In addition, e-DFT-EE has been implemented in the commercially-available MolPro quantum chemistry package (licensed via University College Cardiff Consultants, Ltd.), enabling DFT methods to model reactive systems containing thousands of atoms and making the new methodology available in over 500 research laboratories worldwide.

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. Biologically Patterned Amyloid Scaffolds for Multifunctional and Multi-scale Materials

Professor Timothy Lu, Massachusetts Institute of Technology, Young Investigator Program (YIP) Award

Professor Lu is designing and making multi-functional biological nanowire scaffolds with intricate patterning capabilities (see FIGURE 19). Utilizing curli fibers (amyloid fibers produced from *E. coli*), nanoscale patterning will be carried out in synthetic gene circuits, ultimately leading to fiber scaffolds that can be used to direct the organized patterning of multiple biomaterials, inorganic materials, and enzymes. The functionalizable sites on the curli fibers will be mapped, with a focus on maintaining fiber formation. Nanoscale patterning of these functionalized fibers will then be done in synthetic gene circuits. Several proof-of-concept patterns will be developed. Once patterning of single scaffolds have been obtained, multifunctional nanowires will be created by direct fusion of heterologous domains to curli subunits; co-secretion of heterologous domains and curli subunits followed by attachment using protein-protein interactions; and synthesis and release of curli scaffolds followed by heterologous domain attachment. These novel, multi-functional scaffolds and materials are critical towards the development of self-healing materials, drug delivery, energy storage, and biosensors.

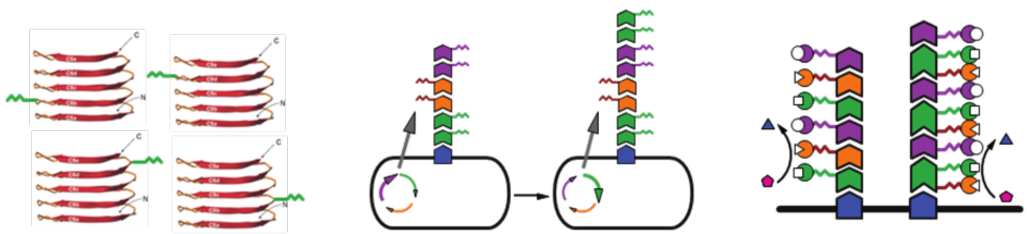

FIGURE 19

Bacterial amyloid scaffolds. The schematics illustrate the overall approach used for the development of bacterial amyloid nanowires as multifunctional scaffolds for nanomaterials.

B. Preparation of Polarized Molecular Targets by IR Stimulated Raman Adiabatic Passage

Professor Richard Zare, Stanford University, Single Investigator Award

In almost all experiments to date, polarized molecules are prepared in specific vibrational, v, rotational, J, and magnetic sublevel, M, states so the final-state is a superposition of unequally populated M sublevels. Professor Zare and his colleagues are engaged in a radically different approach for preparing oriented and aligned molecules. The investigators approach is not based on preparing different populations of M sublevels, but instead on locking together in a coherent manner the phase relations between the different M sublevels, causing the ensemble of vibrationally-excited molecules to be synchronized so that in the vector model the angular momentum vectors J all precess in the same way about the quantization axis. It is anticipated that in FY12, the investigators will construct specialized equipment from infrared laser sources (quantum cascade lasers), that will allow for transfer of nearly all the population in the ground rovibrational level, (v=0, J-2) to the final vibrational level (v=2,J) by causing the molecule to climb in a coherent manner the v=0→v=1→v=2 vibrational ladder in a process that is called infrared stimulated Raman adiabatic passage (IR STIRAP). These polarized molecules will provide a unique potential for new experiments from collision processes to quantum computing.

C. Understanding Ion Transport under Alkaline Conditions in Polymeric Materials

Professor Andrew Herring, Colorado School of Mines (MURI)

Professor Herring and colleagues are 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 exploring 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.

The MURI team has successfully synthesized polystyrene-block-poly (vinylbenzyltrimethylammonium tetrafluoroborate) (PS-b-[PVBTMA][BF4]) via sequential atom transfer radical polymerization (ATRP) of styrene and vinyl-3/4-benzyl trimethyl ammonium tetrafluoroborate. Polystyrene-b-poly (vinylbenzyltrimethylammonium hydroxide) (PS-b-[PVBTMA][OH]) was subsequently prepared by ion exchange with hydroxide. The MURI team has also synthesized tris(2,4,6-trimethoxyphenyl)polysulfone-methylene quaternary-phosphonium-hydroxide (TPQPOH), a phosphonium-based hydroxide exchange membrane (HEM) which will be characterized in the following year (see FIGURE 20). TPQPOH shows high conductivity (45 mS/cm and is tough, flexible, and stable in alkaline solution. The ability of TPQPOH to self-crosslink provides added control over its mechanical properties and water uptake.

It is anticipated that in FY12, the MURI team will characterize TPQPOH using small angle X-ray scattering, NMR, and IR to determine the chemical and physical properties. In addition, new functional block copolymers will be synthesized through combinations of anionic polymerization and nitroxide mediated radical polymerization. Anionically-polymerized polybutadiene is produced with high 1,4-content and then converted to a nitroxide functional chain end by substitution with 2,2,6,6-tetramethyl-1-(2-bromo-1-phenylethoxy) piperidine. The nitroxide functional macroinitiator is used to polymerize a mixture of isomers of vinylbenzyl chloride to produce a block of poly(vinylbenzyl chloride). The block copolymer is solution cast into films and then reacted with trimethylamine to convert the benzyl chloride pendent groups into benzyltrimethylammonium groups, making polybutadiene-blockpoly(vinylbenzyltrimethylammonium chloride) (PB-b-PVBTMA [Cl]).

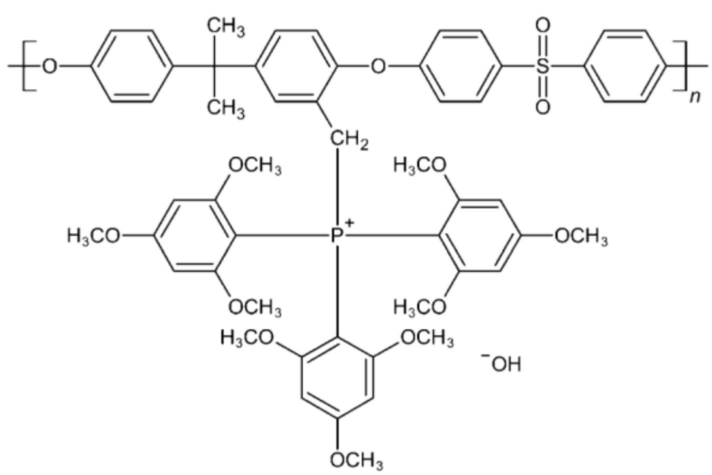

FIGURE 20

Structure of TPQPOH. TPQPOH was synthesized by the MURI team in FY11. In FY12, new functional block copolymers will be synthesized. The new compounds, along with TPQPOH, will be extensively characterized in FY12 using Small Angle X-Ray scattering, liquid and solid state NMR, and IR to determine their chemical and physical properties. In addition, the chemical stability and conductivity at varying relative humidity will be determined. These results will then be applied to the theory and modeling of anion transport at multiple length scales.

D. Molecularly-defined Porous Thin Film From Cyclic Peptide-Polymer Conjugates

Professor Ting Xu, University of California - Berkeley, Single Investigator Award

The objective of this project is to synthesize peptide-polymer conjugates and prepare films with precise pore sizes, shapes, and surface chemistry. The ultimate goal is to develop an understanding of the effects of polymer composition and peptide-polymer assembly on film properties.

In FY12, it is anticipated that the research team take advantage of newly designed cyclic peptide nanotubes by investigating their co-assembly with a commercially available triblock copolymer, Kraton, (polystyrene-block-polyethylene/butylene-block-polystyrene; SEBS). SEBS can be readily processed into thin films, and preliminary results revealed that cylindrical microdomains can be oriented normal to the surface (see FIGURE 21). The investigator will synthesize peptide-polymer conjugates using PS or alkyl-based polymers, and the co-assembly of cyclic peptide-polymer conjugates and SEBS in thin films will be investigated. Initial studies on the co-assembly will be carried out on flat Si substrate, and assemblies of cyclic peptide-polymer conjugates/SEBS blends on commercial membranes will be prepared. If successful, these studies may provide a versatile approach to modify existing commercial membranes to control transport for a variety of applications of interest to Army.

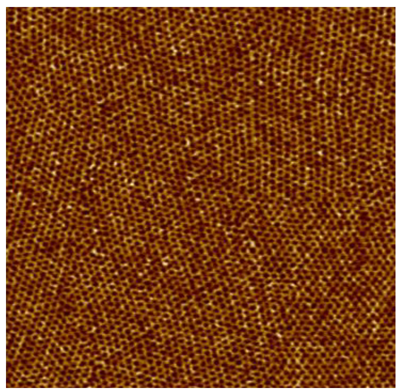

FIGURE 21

SEBS can be processed into thin films. This atomic force microscopy image of a 100 nm SEBS thin film reveals hexagonally packed cylinders oriented normal to the surface. Image size: 1.5 x 1.5 μm^2

E. Thin Film Morphology of Block Copolymers with Strong Surface Associations

Professor Michael Hickner, Pennsylvania State University, Single Investigator Award

The objective of this research is to determine how the phase behavior and surface interactions of ion-containing block copolymer thin films coated on solid substrates are influenced by the ion type, the functional groups, and the properties of the polymer chain, thin film processing, and the solid surface chemistry.

In FY12, it is anticipated that Professor Hickner and his research team will synthesize new block copolymers with high ion conductivities and order them on surfaces. Previous research has shown that ion-containing block copolymers tend to have a significant number of grain boundary defects (see FIGURE 22), likely due to kinetic trapping during solvent casting of dense films. The strong attraction of ion-containing polymers to surfaces will facilitate ordering of the phases over longer length scales than can be achieved in the bulk. The structure and transport properties of these highly ordered materials will be characterized to probe the limits of fast transport in these systems. Understanding how surface ordering and orientation controls the transport of water and other small molecules and ions may enable the design of new polymer membranes for energy storage, water treatment, and chemical protection applications.

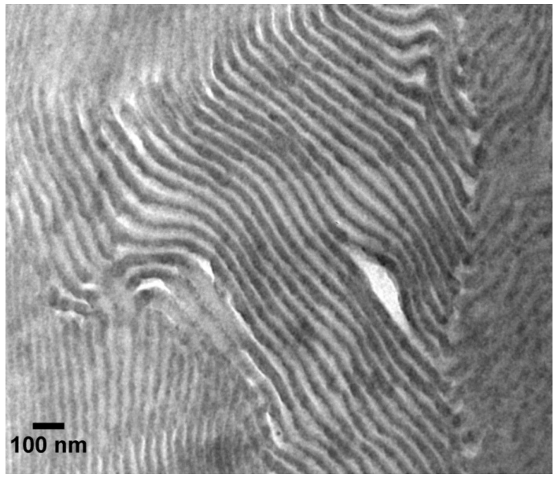

FIGURE 22

Ion-containing block copolymer showing grain boundaries in a bulk sample. Dark features highlight the ionic channels in these materials. Surface-ordering of these structures will be used to create defect-free structures over large length scales, which may lead to greatly increased ion transport.

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

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

Professor Abbott's research focuses on the fundamental understanding of the interfacial phenomena between liquid crystalline phases and amphiphiles or nanoparticles. Experiments will be carried out to determine and control the dynamic and equilibrium phase behaviors of amphiphiles at liquid crystalline/aqueous interfaces and nanoparticle/liquid crystalline interfaces. Manipulation of the phase behavior will be attempted by varying the liquid crystal (LC) composition, including the chemical composition, size of LC chain length, and LC phase (see FIGURE 23). The ordering of silica nanoparticles will be controlled by varying the LC composition. The fundamental knowledge gained through the proposed experiments will lead to a comprehensive understanding on how to control interfacial properties and dynamics. This research has broad potential impact in the development of hybrid materials for use in stimuli responsive materials, tunable plasmonic metamaterials, sensors, and protective materials.

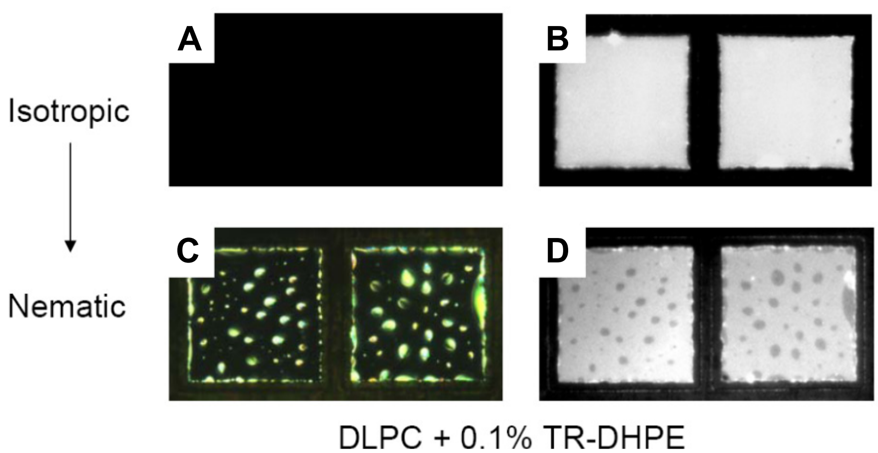

FIGURE 23

Phase separation of monolayer of phospholipid. (**A,C**) polarized light micrographs and (**B,D**) fluorescent micrographs of the labeled phospholipid reveal the phase separation of a monolayer of phospholipid at the interface between a LC and aqueous phase. In the isotropic phase (A-B), the fluorescence image shows a uniform distribution of lipid; upon inducing LC order (C-D), the lipid phase separates (D), which also leads to patterned orientations of the LC (C).

VI. DIVISION STAFF

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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 2011* is to provide information on the programs and basic research efforts supported by ARO in FY11, 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 FY11.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of the ARO Computing Sciences Division is to provide increased performance and capability for processing signals and data, extract critical information and actionable intelligence to enhance the warfighters' situation awareness, improve decision making, and improve weapon systems performance. The Division supports basic research efforts to advance the Army and nation's knowledge and understanding of the fundamental principles and techniques governing intelligent and trusted computing systems. More specifically, the goal of the Division is to promote basic research to establish new computing architectures and models for intelligent computing, to create novel data fusion and extraction techniques for efficient information processing, and to build resilient computing systems for mission assurance. The results of these research efforts will stimulate future studies and help to 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. The transformation of the Army to the Future Force will require investment in science and technology, especially computing and information science. 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 the increased complexity of future battlefield information systems, dependence on them will only increase, therefore they must be extremely reliable and secure. For this reason, computing science is a key technology underpinning the Future Force. The research topics described here are needed to provide the Future Force the information processing, computing, security, and reliability needed to achieve the vision of future Army operations. Research in this program has application to a wide variety of developmental efforts and contributes to the solution of technology-related problems throughout the Army's Future Force operational goals.

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

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

B. Program Areas

To meet the long-term program goals described in the previous section, the Computing Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY11, the Division managed research efforts within these three Program Areas: (i) Information Processing and Fusion, (ii) Computational Architectures and Visualization, and (iii) Information and Software Assurance. 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 five Thrusts for this Program Area: (i) Mathematical Image Processing, (ii) Image Understanding, (iii) Data and Information Fusion, (iv) Target Acquisition and Tracking, and (v) Brain-computer Interfaces. With the pervasive availability of unmanned systems in future military operations, advanced sensing will be of critical importance to the future force. This program emphasizes mathematical methodologies underlying automated sensing and scene understanding. Research efforts support the development of novel algorithms for robust video-based tracking under challenging urban environments. Also supported is research on area monitoring using a network of cameras and other sensing modalities. Potential applications include detection of improvised explosive devices and persistent surveillance. There is also a new research initiative on brain signal understanding for brain-computer interfaces using both minimally invasive and non-invasive imaging modalities.

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

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

The V Thrust addresses the issue by investigating innovative algorithms to render massive data sets and/or massive geometric models and to perform large scale simulations of importance to the Army.

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

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

Within these research areas, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. Research in the Resilient and Robust Information Infrastructure Thrust is focused on exploring and establishing resilient computing and survivability principles, and understanding system trade-off among performance, resiliency, and, survivability. The Highly Assured Tactical Information Thrust may lead to the development of novel situation awareness theories and techniques to obtain an accurate view of the available cyber-assets, to automatically assess the damage of attacks, possible next moves, and impact on cyber missions, and also model the behavior of adversaries to predict the threat of future attacks on the success of a mission. Information assurance for the individual Soldier and for the systems that the Army must employ in the next few years is of paramount importance to the defense of this nation. The Objective Force must have unprecedented situational awareness (including enemy and friendly awareness) at all times. It follows then, from the Army perspective, that 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. As the Army places more reliance on winning the information war and providing the Soldier with highly automated and sophisticated tools, there must be an increased and improved awareness of the vulnerabilities that these systems possess. Ubiquitous, mobile, wireless, scalable, high-speed, and highly-assured information processing systems will be placed in areas of usage never imagined in the past. Attacks on these systems will occur from hostile forces in times of war and times of peace.

C. Research Investment

The total funds managed by the ARO Computing Sciences Division for FY11 were $22.6 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY11 ARO Core (BH57) program funding allotment for this Division was $3.1 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $9.4 million to projects managed by the Division. The Small Business Innovation Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided $2.7 million for awards in FY11. Finally, $7.4 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

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

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). 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. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. ARO Workshop on Hardware Security (11-12 April 2011, Arlington, VA). The aim of this workshop was to provide a deeper understanding of the hardware-oriented security and trust problem. Currently, many researchers in academia and industry are investigating various aspects of the problem such as IC authentication, hardware trust, IP security and trust, physically un-clonable functions, watermarking, IC metering, un-trusted foundry, and hardware cryptography. The workshop provided a forum to discuss the above challenging issues and current solutions, in addition to helping provide a detailed roadmap for researchers as well as ARO.

2. Workshop on Frontiers in Computer Vision (Cambridge, MA; August 20-24, 2011). Computer vision began with the goal of building machines that can see like humans and perform perception for robots, but the idea has broadened since inception. Applications such as image database searches via the internet, computational photography, security, assistive systems, medical image processing, biological imaging, vision for graphics, biometrics, document analysis, vision for nanotechnology, and analysis of videos, were completely unanticipated, and other applications arise as computer vision technology continues to develop. The objective of this ARO/NSF workshop was to explore frontiers of computer vision, articulate a national computer vision agenda, and provide a roadmap for computer vision research. Specifically, the workshop (i) identified the future impact of computer vision on the nation's economic, social, and security needs, (ii) outlined scientific and technological challenges to address, and (iii) drafted a roadmap to address those challenges.

3. Triangle Computer Science Distinguished Lecture Series (Research Triangle Park, NC; throughout FY11). The Triangle Computer Science Distinguished Lecture Series is jointly administered by the Computer Science departments at Duke University, North Carolina State University, and the University of North Carolina - Chapel Hill. Nine distinguished lecturers are invited to the Research Triangle Park (RTP) area each year. The lecturer presents a talk at one of the three universities and the talk is transmitted over NC-REN, a statewide microwave video and digital network that links eleven research and educational institutions. NC-REN sites are located in Research Triangle Park and at each host department thus encouraging participation by not only faculty and students but local computer professionals from industry as well. The broadcasts are also electronically recorded and stored for later viewing. The lecturer spends at least two days in RTP and visits all three universities. This lecture series has been extremely successful in attracting leading researchers in computer science to the RTP area. The series has promoted and continues to promote collaboration between the three sponsoring universities, interaction with local industry, and to publicize Army interests to a wide audience.

C. Multidisciplinary University Research Initiative (MURI)

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

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

The emphasis of these studies is on network science, 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. Brain-to-muscle Communication. This MURI began in FY08 and is led by Professor Gerwin Schalk at Albany Medical College. The objective of this MURIs 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 project led by Professor Michael D'Zmura (see CHAPTER 7: LIFE SCIENCES DIVISION).

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

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

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

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

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

4. Cyber Situation Awareness. Two MURIs in this topic area began in FY09, with one research team led by Professor Richard Kemmerer at the University of California, Santa Barbara, and the second team led by Professor Peng Liu at the Pennsylvania State University. The goal of these projects is to explore cyber situation awareness theories and frameworks that may support effective defense against cyber attacks, and to develop 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 will focus their 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) establish 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 will be investigated to obtain an accurate view of the available cyber-assets and to automatically determine the assets required to carry out each mission task. A proposed situation awareness framework that ties together cyber assets, cyber configuration, attack impact, threat analysis and situation visualization under cyber mission is illustrated in FIGURE 1.

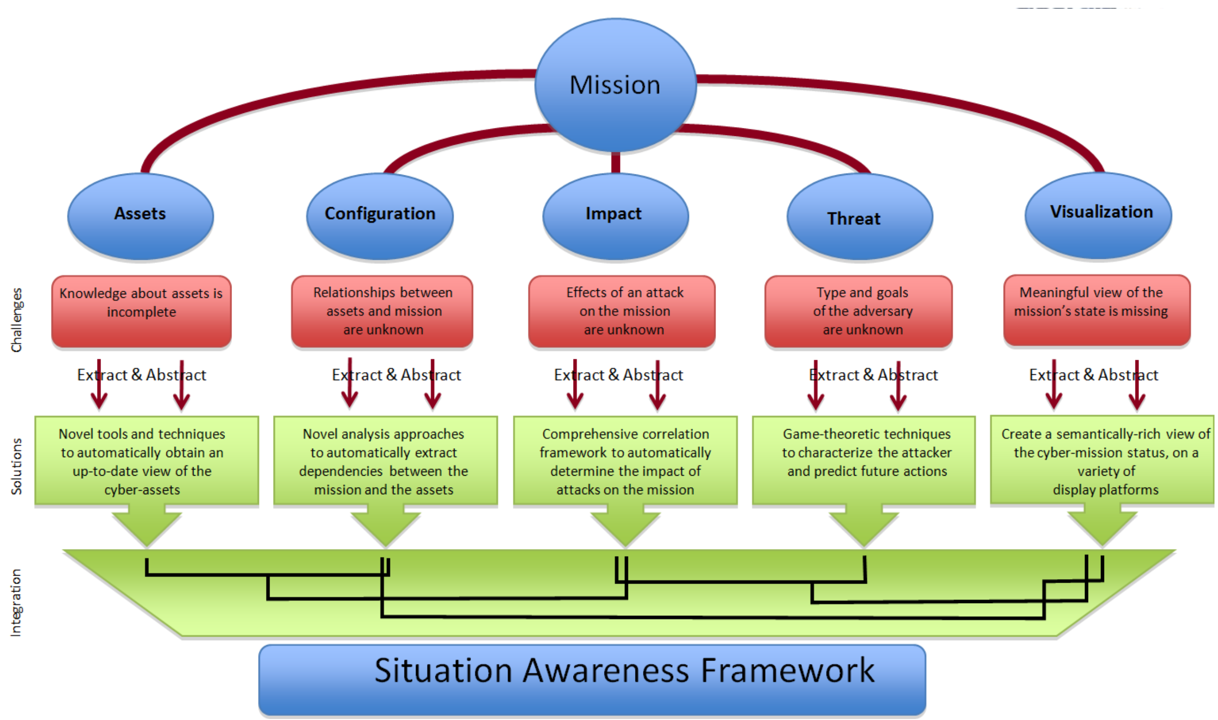

FIGURE 1

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

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

There are four focus areas in this research focusing on 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 for Adaptive Learning, Inference, Tracking, and Exploitation. This MURI began in FY11 and was awarded to a team lead by Professor Alfred Hero III at the University of Michigan. The objective of this MURI effort 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 result in improving our understanding of the fundamental limits of performance and create better algorithms for extracting and exploiting information in distributed sensor systems.

In this effort, research will focus 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 approach comprises of 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.

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

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as was discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. LureID: A Scalable, Highly Accurate Anti-Phishing Filter. A Phase I SBIR contract was awarded to Odyssey Research Associates, Inc. to develop and commercialize LureID: an automated tool for real-time detection and elimination of phishing attacks. Phishing is an increasing danger to the military and other organizations that must prevent information leakage. Targeted phishing (spear-phishing) and even regular phishing attempts evade regular spam detectors because phishing attacks are designed to look like legitimate e-mail. Furthermore, spam detectors expect high false positive rates and force users to periodically analyze rejected messages. The SBIR project will develop high-accuracy, low-latency automatic identification and mitigation techniques to detect and stop phishing attacks. A successful R&D outcome will lead to new capabilities to be able to rapidly identify and stop suspicious emails with a high confidence.

2. Robust and Efficient Anti-Phishing Techniques. Two Phase I SBIR contracts were awarded to Altusys Corporation and Wombat Security Technologies to establish robust and efficient anti-phishing techniques. Phishing emails have become a significant threat to mission success, civilian infrastructure, and civilian enterprise success. The SBIR project will develop high-accuracy, low-latency automatic identification and mitigation techniques to detect and stop phishing attacks. A successful R&D outcome will lead to new capabilities to be able to rapidly identify and stop suspicious emails with a high confidence.

3. Angler: Phishing Prevention and Defense Framework. A Phase I SBIR contract was awarded to Pikewerks Corporation to research and develop automated system for preventing and protecting against phishing and spear phishing attacks across a broad spectrum of user and email interaction. The SBIR project will develop high-accuracy, low-latency automatic identification and mitigation techniques to detect and stop phishing attacks. A successful R&D outcome will lead to new capabilities to be able to rapidly identify and stop suspicious emails with a high confidence.

4. Preventing Sensitive Information and Malicious Traffic from Leaving Computers. Two Phase I SBIR contracts were awarded to Siege Technologies, LLC and RAM Laboratories, Inc. to develop a system to prevent sensitive information and malicious traffic from leaving computers. The ability to mitigate information leakage from enterprise networks is a critical capability for both the military and commercial sectors. Without such capabilities, a single compromised host has the ability to transfer large amounts of sensitive information out of the network. This project will research and develop real-time, automatic identification and mitigation techniques to detect and stop unauthorized information leakage as well as unwanted and malicious traffic emanating from a computer at all time and locations. New techniques and implementations will be developed to monitor applications and user activities on a computer in order to detect and stop outgoing data and traffic that is not intended or authorized by the user or security policies.

5. Enforcing Hardware-Assisted Integrity for Secure Transactions from Commodity Operating Systems. A Phase I SBIR contract was awarded to Secure Command, LLC to develop a secure hardware-assisted switching system as a form of a Tailored Trustworthy Space (TTS) that will allow users to switch between an untrusted operating system and a trusted operating system on the same machine, on demand, with a very short switching time. With the increased reliance on personal computers for everyday activities, operating systems and applications have increased in both size and complexity. There is a need to ensure the integrity and trust for the entire software stack, including the underlying operating system. This project will research and develop real-time, automatic identification and mitigation techniques to detect and stop unauthorized information leakage as well as unwanted and malicious traffic emanating from a computer at all time and locations. New techniques and implementations will be developed to monitor applications and user activities on a computer in order to detect and stop outgoing data and traffic that is not intended or authorized by the user or security policies.

6. Gyrus: Preventing Sensitive Information and Malicious Traffic from Leaving Computers. A Phase I SBIR contract was awarded to Security Axioms, Inc. to develop a system, Gyrus, which will stop malware from communicating with another host, thus preventing the malware from fulfilling its malicious goals such as information theft and sending out attack traffic. This project will research and develop real-time, automatic identification and mitigation techniques to detect and stop unauthorized information leakage as well as unwanted and malicious traffic emanating from a computer at all time and locations. New techniques and implementations will be developed to monitor applications and user activities on a computer in order to detect and stop outgoing data and traffic that is not intended or authorized by the user or security policies.

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

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Analysis of Target Surface Characterization. A Phase II STTR contract was awarded to Spectral Sciences, Inc., in partnership with Professor Alexei Maradud at the University of California, Irvine, to develop an extended Laser Radar (LADAR) capability for characterizing and classifying surface material and texture by exploiting multispectral polarimetric LADAR signatures utilizing the Bidirectional Reflectance Distribution Function (BRDF). This innovation will unify waveband spectra, polarization, tomographic reconstruction, and material science with LADAR-based remote target classification. The key features of the capabilities to be developed in this project include BRDF modeling, a database of target and ground materials, range profile simulation, and material inversion algorithms.

2. A System to Analyze Facial Features to Enable Operator Condition Tracking (AFFECT). A Phase II STTR award was made to Charles River Analytics in partnership with Professor Mark Frank, University of Buffalo to design and demonstrate a system, the Analyze Facial Features to Enable Operator Condition Tracking (AFFECT) system, for non-contact classification of Stress, Anxiety, Uncertainty, and Fatigue (SAUF) in interface applications. The AFFECT system combines classification techniques with a multi-dimensional, temporal data model of novel visible and thermal features to enable automatic, non-invasive detection of SAUF conditions in a subject. The development of this technology will in turn enhance training, workflow, and overall effectiveness of the Soldier and analysts.

3. Dynamically Programmable and Adaptive Multi-band Compressive Imaging System. A Phase I STTR award was made to Bridger Photonics Inc. in partnership with Dr. Amit Ashok, University of Arizona, to develop a passive multi-band compressive sensor for imaging and object recognition applications. Multi-band systems offer enhanced discrimination capability and the ability to perform in adverse conditions (*e.g.*, night, smoke, fog). Compressive sensing is ideally suited to multi-band imaging systems as it offers improved performance while reducing size, weight and power, as well as hardware and data bandwidth requirements. Compressive sensing is particularly beneficial when some of the desired spectral bands lie outside of the visible spectrum as focal plane arrays, especially in the mid-wave and long-wave IR bands, have poor performance and high costs. This project aims to develop an advanced compressive sensing algorithm for operating any compressive, multi-band imager, and ultimately to design a prototype system and determine its feasibility.

4. Interactive Acoustic Simulation in Urban and Complex Environments. Two Phase I STTR contracts were awarded to Impulsonic, Inc. (in partnership with Professor Dinesh Manocha at the University of North Carolina, Chapel Hill), and to EE Boost, Inc. (in partnership with Professor Tian Xiao at North Carolina State University), to develop efficient acoustic simulation technologies that can model large urban and complex environments. These projects will address deficiencies in current state-of-the-art outdoor acoustics prediction methods that are restricted, slow, or limited to simple environments. No existing method can simultaneously model atmospheric acoustical phenomena, surface interactions with terrain and obstacles, and moving sound sources; therefore, these projects aim to develop novel hybrid acoustics prediction techniques to model complex urban and outdoor environments.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) – 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). The FY11 new starts within these programs are described here, while the missions of each of these programs were described *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. DoD REP Awards. As described in more detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, REP awards aim to enhance or increase the programs, capabilities, and graduates in scientific and engineering disciplines in universities serving underrepresented minorities. In FY11, the Computing Sciences Division managed six new REP projects, totaling $2.8 million. The equipment purchased with these awards is promoting research in areas of interest to ARO, including efforts to investigate compressive sensing and ultra-wideband radar technology for detection and imaging, to investigate virtual interfaces and characteristics with respect to human responses with these interfaces, and to explore the use of mobile sensing platform to enhance security of wireless sensor networks.

2. DoD TCU Instrumentation Awards. As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the TCU program aims to enhance science, mathematics, and/or engineering education programs and/or research capabilities through the acquisition of equipment and/or instrumentation that will augment existing facilities, enhance curricula, or help develop new laboratories, programs, and capabilities in these areas. In FY11, the Computing Sciences Division managed one new TCU project. The equipment purchased with these awards is promoting education and research in areas of interest to ARO, including equipment for training faculty in multimedia techniques.

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

No new starts were initiated in FY11.

H. Defense University Research Instrumentation Program (DURIP)

As detailed 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 FY11, the Computing Sciences Division managed seven new DURIP projects totaling $1.4 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including resilient wireless communication systems, large scale modeling, simulation, and visualization of complex dynamics and phenomena, multi-robot collaboration, opportunistic sensing, and new techniques for providing cyber-security to both data networks and telecommunication infrastructure.

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 and H. John Heinz III School of Public Policy and the 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.

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.

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, 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.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. Sparse Representation of Multimodality Sensing Databases for Data Mining and Retrieval

Professor Alfred Hero, University of Michigan, Single Investigator Award

Professor Hero has utilized spatiotemporal analysis using information theory to investigate two new information theoretic methods for image and video representation: Fisher Information Non-linear Embedding of Video (FINE-V) manifolds and Shrinkage Optimized Directed information Assessment of Video (SODA-V) for human-interaction-based indexing and retrieval. These information theoretic representations capture video features by exploiting intrinsic geometric structure of the associated joint probability distributions. Unlike classical model-free discriminant models these information representations are sensitive to non-linear and time varying structure that exists in the full feature probability distributions. Furthermore, unlike model based approaches a minimum of model assumptions are required: the joint distributions are estimated directly from the data and parsimony is achieved by dimensionality reduction (FINE-V) or shrinkage (SODA-V). As a result, the new information theoretic representations naturally handle high dimensionality features without brittle models, reduce the effect of nuisance parameters, have as good or better performance than competing methods, and simplify theoretical analysis of accuracy. The significance of a simplified accuracy analysis is that the analysis is used to both predict performance for benchmarking and also to specify automated procedures for selecting optimum tuning parameters, thereby eliminating the need for human intervention in implementation.

FINE-V has been tested to indexing and retrieval of videos in a database. By performing the FINE-V embedding of similarities between the embedded trajectories of two or more videos, the videos can be compared using curve distance measures such as geodesic Haussdorf. In this embedded space one can quickly and accurately identify frames in a pair of videos that contain common information: these will correspond to points of intersection or near intersection of the two curves. It has been demonstrated that this novel approach outperforms traditional approaches to video indexing and retrieval with real world data. The new SODA-V framework was validated for human-interaction-based indexing and retrieval of videos with impressive results. SODA is an information measure that is specifically designed to extract "causal" relations between objects over time. As physical phenomena unfold over time in a video they generate events whose mutual dependency is directed and asymmetric: past events influence future events but not conversely (see FIGURE 2).

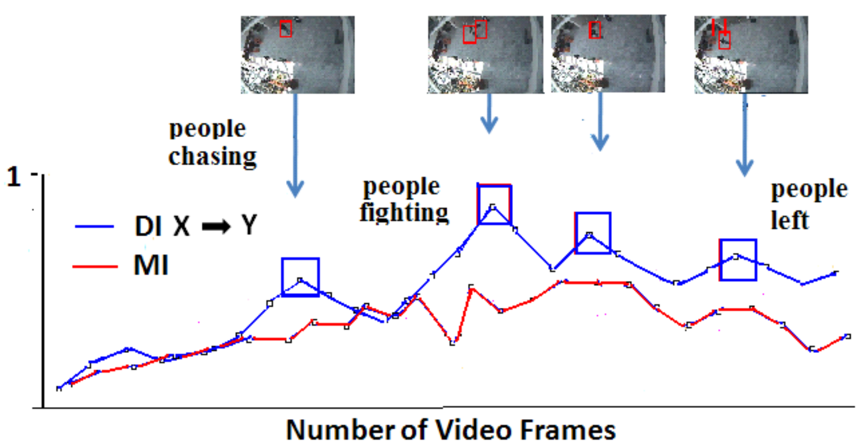

FIGURE 2

Utilizing SODA-V to extract "causal" relations between objects over time. SODA-V (DI) is an information measure specifically designed to extract relations between objects over time, as illustrated by purposeful human behavior that generates highly complex non-linear patterns of directed dependency.

Among all such phenomena, purposeful human behavior generates some of the most highly complex non-linear patterns of directed dependency. Model-free information theoretic approaches have been previously proposed to discriminate complex human activity patterns but have only had limited success. SODA-V is a very different measure of information that is more sensitive to strongly directed non-linear dependencies in observable behavioral events. The SODA-V approach is conceptually simple, is of low implementation complexity, and selects tuning parameters automatically and in an optimal manner. It has been demonstrated that SODA-V performance on indexing/retrieval tasks and activity clustering tasks is superior to the state of the art for videos containing human interactions (see FIGURE 3).

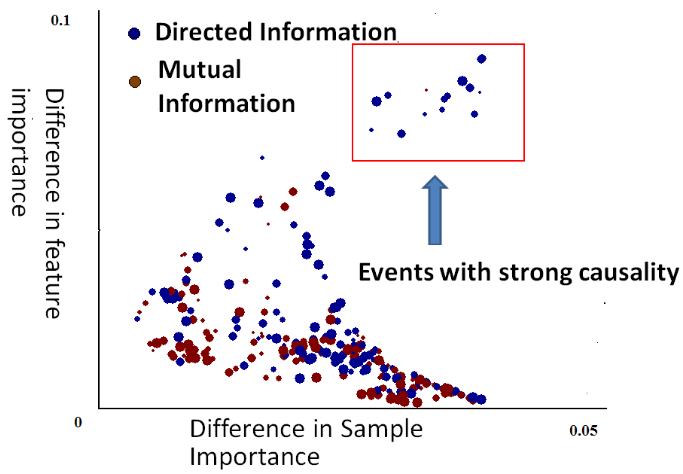

FIGURE 3

SODA-V captures strongly causal events. SODA-V is more sensitive to strongly directed non-linear dependencies in observable behavioral events. SODA-V performance on indexing/retrieval tasks and activity clustering tasks is superior to the state of the art for videos containing human interactions.

B. Physics-based Approaches to Visual Scene Analysis

Professor Todd Zickler, Harvard University, Single Investigator Award

Most cameras capture three spectral measurements (red, green, blue) to match human trichromacy, but there is additional information in the visible spectrum that can be exploited by vision systems. Hyper-spectral images provide a dense spectral sampling at each pixel and have proven useful in many domains, including remote sensing, medical diagnosis, and biometrics. These images may also be able to simplify the analysis of everyday scenes. When developing vision systems that acquire and exploit hyper-spectral imagery, investigators aim to exploit knowledge of the underlying statistical structure. By modeling the inter-dependencies that exist in the joint spatio-spectral domain, it should be possible to build, for example, more efficient systems for capturing hyper-spectral images and videos, and better tools for visual tasks such as segmentation and recognition. Unlike previous analyses that have separately considered the spectral statistics of point samples, Professor Zickler has analyzed the statistics of large number of real images. The spatial and hyper-spectral dimensions are jointly used to uncover additional structure. Different choices of spatio-spectral bases for representing hyper-spectral image patches have been evaluated. The researchers discovered that a separable basis for image representation is appropriate, and characteristics of the statistical properties of the coefficients in this basis have been established. The basis was found to be sparse and inter-dependent, which establishes the physical foundation of the compressive sensing research for hyper-spectral image representation and analysis.

C. Interactive Computational Algorithms for Acoustic Simulation in Complex Environments

Professors D. Manocha and M. Lin, University of North Carolina - Chapel Hill, Single Investigator Awards

The objectives of these projects are to develop new interactive algorithms for acoustic simulation for analyzing wave propagation in complex environments. This research could offer fundamental scientific capabilities for solving wave/sound propagation problems in highly complex, vast domains for seismology, geophysics, meteorology, geomagnetism, urban planning, and immersive training. The research efforts include the 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. They will also develop parallel algorithms that can exploit the parallel capabilities of current multi-core CPUs and many-core GPUs for fast computations.

In FY11 these researchers developed efficient and accurate simulations of sound propagation in 3D. An order of magnitude performance gain was achieved compared to standard Finite Difference implementations by exploiting the known analytical solution of the Wave Equation in rectangular domains combined with ray tracing techniques from computer graphics. In addition, a high performance supercomputer facility is not required. The researchers were able to efficiently implement their techniques on a desktop computer which has not been previously accomplished for sound propagation in large complex urban scenes (see FIGURE 4). Acoustic scientists at the U.S. Army Corps of Engineers (USACE) have also collaborated in this research. The USACE researchers are interested in developing 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.

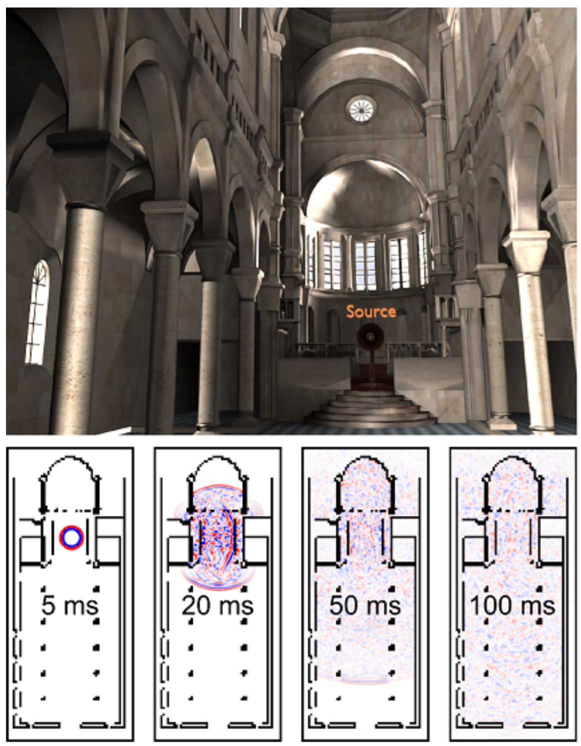

FIGURE 4

Sound simulation in a cathedral. The dimensions of this scene are 35m x 15m x 26m and it contains 11.9 million simulation cells. Numerical sound simulation for a 2 second long impulse response on this complex scene was performed on a desktop computer in 15 hours, taking 1.5GB of memory. A commonly used approach, Finite-Difference Time-Domain (FDTD) method, would take 2 weeks of computation and 25GB of memory for this scene.

D. Realistic Simulation of Environments of Unlimited Size in Immersive Virtual Environments

Professor Eric Bachmann, Miami University, Single Investigator Award

Immersive virtual environments (VE) hold great promise for training, education, research, and entertainment. Unlike "desktop VEs" or "CAVEs," immersive VEs treat the user's body as an input device, and thus fully incorporate body-based sources of information. The incorporation of body-based information provides an intuitive and natural interface and has been shown to be critical for allowing users to maintain their orientation in the environment. To date, however, immersive VEs have had difficulty simulating large-scale environments because they typically have a limited tracking area. A popular method of overcoming the physical space constraints of current immersive VEs is by developing and implementing a computer algorithm known as redirected walking (RDW). RDW works by imperceptibly rotating the virtual scene around the user's viewpoint so that the user's real body is continually directed away from the tracking space boundaries (see FIGURE 5).

FIGURE 5

A virtual environment utilizing RDW. Test subject in RDW comparison study performed at Miami University's Huge Immersive Virtual Environment (HIVE) VE facility.

In FY11, Professor Bachmann and his collaborator, Professor David Waller, have implemented and analyzed these algorithms with the purpose of determining their relative benefits. Several generalized candidate RDW algorithms have been proposed in the literature, including by these researchers. Perhaps more significant than any specific numbers related to the performance of various algorithms, the comparison study has lead to the understanding that determining the minimum area required in order to successfully perform RDW is more complex than previously thought. Prior to this work, experimenters have focused on the ability of users to detect RDW rotations while engaged in no other tasks. Commonly, the threshold values have been combined with a typical speed of movement in order to determine a minimum curve radius onto which a redirected user could be steered. This has been inferred to be the minimum area required for RDW. The results of the algorithm study indicate the area required to successfully accommodate users performing unconstrained navigation tasks is also highly dependent on the steering algorithm and the behavior of the individual user. Given that users performing unconstrained navigation may change their direction and speed of movement at any moment, it is not possible to steer them precisely in some pre-established pattern. Rather, the steering instructions can only be thought of as guidance which must be continuously updated based on the ever changing movement goals of the user.

E. Situation Knowledge Reference Model

Professor Pen Liu, Penn State University, MURI Award

In both military operations and the commercial world, cyber situation awareness (SA) is a key element of mission assurance. The critical cyber SA needs to perform attack damage and impact assessment and to identify asset and task prioritization go beyond the initial stage of intrusion detection and attack graph analysis. The MURI team led by Professor Liu has proposed an interconnected cross-layer situation knowledge reference model (SKRM) to address the unique cyber SA needs of real-world missions. SKRM provides a new insight into how to break the "stovepipes" created by isolated situation knowledge collectors and how to gain "stitched-together" big-picture awareness. The cross-layer situation knowledge reference model (SKRM) enables an important set of cyber SA analytics. For instance, top-down cross-layer analysis helps identify mission assets (see FIGURE 6). Bottom-up cross-layer analysis can be carried out to evaluate mission impact. A comprehensive damage assessment can be performed through U-shape analysis. In addition cross-layer Bayesian networks could be constructed to reason about uncertainty. SKRM can be used to classify mission assets and generate "asset maps," enable the exploration of different mitigation plans, provide insights into how to recover from network intrusions, and help gain essential knowledge representation for cognitive engineering.

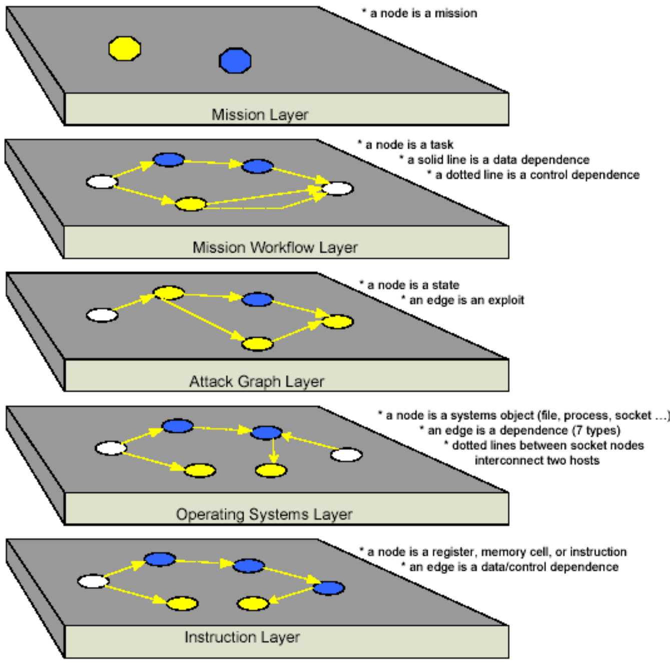

FIGURE 6

Interconnected cross-layer situation knowledge reference model (SKRM) for cyber-SA research. The cross-layer situation knowledge reference model (SKRM) enables an important set of cyber SA analytics, and can be used to classify mission assets and generate "asset maps," enable the exploration of different mitigation plans, provide insights into how to recover from network intrusions, and help gain essential knowledge representation for cognitive engineering.

In FY11, the team demonstrated that SKRM is the key enabler for mission asset identification and mission impact analysis, two SA capabilities beyond intrusion detection and attack graph analysis. In particular, the team has developed novel methods that use SKRM to perform cross-layer top-down mission asset identification and bottom-up mission impact assessment. Compared to the existing methods, the new methods are more systematic, less error-prone, and can be executed in a more automated way.

F. Proximity-based secure system Using Ambient Wireless Signals

Professor Wade Trappe, Rutgers University, Single Investigator Award

Professor Trappe, in collaboration with the *AT&T Security Research Center, has made an important discovery regarding how to use* information surrounding a wireless channel to solve the traditional key establishment problem. Instead of transmitter and receiver probing the channel to each other, he examines the problem of whether a third party can assist two devices in close proximity to establish keys with each other. An example of where such a problem might arise is in forming secure associations between mobile wireless devices that meet for the first time and lack a prior trust relationship. A new system called Clique allows wireless devices in proximity to securely and autonomously pair, by generating a common cryptographic key contingent upon their being in spatial proximity. Clique works by allowing devices in proximity to tap into a surprisingly abundant and cheap source of shared randomness – namely, fading channels relative to a public RF source, such as FM or TV broadcast transmitters. The shared key can be used by devices to communicate confidentially and/or to authenticate each others' physical proximity. Clique is information-theoretically secure, and does not require the adversary to be computationally bounded.

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. Nonparametric Bayesian Statistics for Adaptive Sensing

Investigator: Professor Lawrence Carin, Duke University, Single Investigator Award
Recipient: U. S. Army Aviation and Missile Research Development and Engineering Center (AMRDEC)

Professor Lawrence Carin at Duke University has created a novel approach to integrate compression and sensing for measurement of general hyperspectral data, integrating existing camera technology with new mathematics. The research team has realized massive reductions in the quantity of data that need be measured, while retaining sensing performance comparable to that of existing systems. The quantity of data measured by the Army continues to increase, manifesting problems for storage, communication and analysis. A new mathematical construction exploits the fact that most natural scenes produce data that live on a low-dimensional manifold or union of subspaces, despite the fact that the data itself may be very high-dimensional. In this computational imaging framework, one randomly samples voxels that would be measured by a conventional camera, and by exploiting the inherent low-dimensional latent structure of the data, the missing data may be inferred very accurately. By contrast, in typical sensing systems one measures the entire datacube, and then compresses afterward using techniques like JPEG. Since the quantity of data constituted after compression is typically much smaller than that measured, conventional direct measurement of the entire datacube is wasteful of resources (time, energy, bandwidth, etc.). In the new sensing construct developed in this project, a much smaller fraction of data is measured in the first place, thereby unifying sensing and compression. An important aspect of this new construction is that existing cameras may be utilized, but the way the data is pulled off of the camera is changed via random sampling. In tests with real hyperspectral data, the quantity of data measured is as small as 2% of that measured conventionally, with no degradation in sensing quality. This approach has transitioned to AMRDEC, and Professor Carin's laboratory is working with AMRDEC to build in-house capabilities.

B. Real-Time LINUX for Multi-core Platforms

Investigator: Professor James Anderson, UNC - Chapel Hill, Single Investigator Award
Recipient: AT&T Research

Multi-core platforms provide significant processing power that could potentially be harnessed to support complex, resource-demanding real-time applications (with less energy consumption). However, for this to happen, appropriate real-time scheduling and synchronization algorithms must be devised, analyzed, and implemented within a working operating system (OS). That is precisely the objective of this project. Industry is also interested in the potential of multi-core platforms for real-time applications. This has lead to collaboration between these researchers and Dr. Theodore Johnson at AT&T Research. Together they are devising real-time scheduling and synchronization algorithms for performing real-time queries in multi-core based systems used by AT&T to process queries (in real time) on streamed network data. In FY11, multiprocessor real-time scheduling algorithms developed by Professor Anderson and his collaborator Professor Sanjoy Baruah, at UNC - Chapel Hill, have been incorporated into a data-stream processing system called DataDepot developed by AT&T to house and process streamed network data. Technology transfer to AT&T is expected to continue as a result of summer internships by UNC - Chapel Hill graduate students.

C. New Joint Performance and Vulnerability Metrics for MANET

Investigator: Professor Radha Poovendran, University of Washington, MURI and PECASE Awards
Recipient: ARL Computational and Information Sciences Directorate (ARL-CISD)

To protect user information and provide robust network operation, a network designer must know what types of attacks to protect against and what threats the network must be robust against. Hence, a necessary prerequisite to robust protocol design is to model network vulnerabilities and the impact of malicious attacks on the network. Protecting the information exchange between users is a problem that is well studied in cryptography, but the introduction of an entire network of users into the scenario introduces additional vulnerabilities when the information security is jointly considered with network protocols such as routing and multiple access. Furthermore, the propagation of information throughout a large network allows a locally-constrained adversary to have a more significant impact on information and network security, as the effects of the adversary's attack can quickly spread beyond the local.

Professor Poovendran and ARL-CISD scientists have been jointly pursuing metrics of performance and vulnerabilities for MANET routing. The new metrics quantify the cost of a link based on both performance and vulnerability characteristics, so that shortest paths chosen using this metric will be both efficient and resilient to attack. Based on the new metrics definition, they have successfully introduced a new class of resilience-enhanced routing protocols, which make route decisions based on a combination of security and performance metrics. The researchers have carried out extensive experimentation with this new approach. A piece of software that implements the new resilient-enhanced routing protocol for MANET has been written and incorporated into ARL-CISD research efforts. In addition, a PhD student from of Professor Poovendran's laboratory conducted experiments at ARL during FY11. The transition of this software and related research has also led to three joint publications from Professor Poovendran’s laboratory and ARL-CISD.

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. Theory and Methods for Automatic Image and Video Annotation

Professor Rong Jin, Michigan State University, Single Investigator Award

The objective of this research project, to be pursued in collaboration with Professor Anil Jain at Michigan State University, is to establish mathematical foundations and computational methods for large-scale image annotation based on the efficient method for key point quantization. It is anticipated that in FY12, methods will be developed for an image annotation that can handle millions of images, which is the key step in extending the image annotation system to automatic video annotation. In addition, methods will be developed for image retrieval that are able to take in to consideration the noise in auto-annotations when measuring the similarity between textual queries and auto-annotations. The first step will be to establish a theoretic framework for noisy auto-annotation retrieval based on the idea of information ranking. Then algorithms will be designed for automatic image annotation to automatic video annotation with the focus on exploring the unique features of videos such as motion features and audio features. Specific anticipated accomplishments include the design of (i) a large-scale automatic image annotation system based on the efficient method for key point quantization, (ii) robust retrieval models for noisy auto-annotations based on information ranking, and (iii) algorithms for automatic video annotation that explicitly explore video-specific features.

B. Compositional Framework for Complex Real-Time Systems on Multicore Platforms

Professor Insup Lee, University of Pennsylvania, Single Investigator Award

The goal of this research project, led by Professor Lee and in collaboration with Professors Linh Phan and Oleg Sokolsky, is to develop a novel component framework for real-time embedded systems (RTS) implemented on multi-core architectures. Such a framework will allow compositional modeling and analysis of open systems with tight resource constraints and complex dependencies between components, which exhibit dynamic changes in resource use patterns. Composition of such components needs to be certifiably correct and robust to uncertainty in the component parameters and their environment. An important objective of the project is to build a robust and stable research prototype of the development environment for RTS components on multi-core architectures.

It is anticipated that in FY12, the researchers will develop and test new component interfaces for other resources besides processor capacity (*e.g.*, memory, networking), as well as analyze communication and synchronization dependencies between components. The interfaces for multi-core platforms need to capture sufficient information about the application needs and their assumptions to achieve good tradeoffs between accuracy (*i.e.*, how close they are to the actual resource needed by a component) and computability (*i.e.*, how efficiently they are computed and represented). This research outcome will lead to a significant increase in computational efficiency for important Army RTS applications on multi-core platforms by decreasing communication delays between components while enhancing application performance.

C. Analysis and Application of Physical Unclonable Functions (PUF)

Professor Farinaz Koushanfar, Rice University,Young Investigator Program Award

Providing security for the current and pending generation of pervasive computing devices is a challenging task. Over the last decade, a set of new security and protection mechanisms, tools, protocols, and devices based on physical unclonability and disorder has gained increasing attention. Harnessing the inherent, inerasable, unclonable mesoscopic disorders of the physical processes and phenomena could lead to new security mechanisms that offer multiple advantages: (i) new key generation capability that provides an alternative to digital storage of the secret keys in vulnerable memory, (ii) Exact control of the complex physical fabric fluctuations is extremely difficult and even if possible, prohibitively expensive, making hardware based security primitives inerasable and hard-to-forge (clone), (iii) the physical disorder-based security leads to an alternative security foundation that does not rely on number theory based approaches that depends on the complexity of computation. It is anticipated that in FY12, Professor Koushanfar will establish a formal foundation for physical disorder-based security primitives, consisting of a set of new concepts, classification, analysis, tools, and protocols, along with proof-of-concept implementations on current and pending technologies. This research may ultimately enable a paradigm shift in the theory and practice of physical disorder-based security.

VI. DIVISION STAFF

Dr. Cliff Wang
Division Chief
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Dr. Mike Coyle
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Dr. Liyi Dai
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Dr. John Lavery
Program Manager, Social Informatics (new program established at the end of FY 11)

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 2011* is to provide information on the programs and basic research efforts supported by ARO in FY11, 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 FY11.

A. Scientific Objectives

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

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

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

B. Program Areas

To meet the long-term program goals described in the previous section, the Electronics Division engages in the identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY11, the Division managed research efforts within four Program Areas: (i) Solid State and High Frequency Electronics, (ii) Electromagnetics, Microwaves, and Power, (iii) Optoelectronics, and (iv) Electronic Sensing. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have long-term objectives that collectively support the Division's overall objectives.

1. Solid State and High Frequency Electronics. The goal of this Program Area is to conduct research into quantum phenomena, internally and externally induced perturbations, and novel transport and optical interaction effects in nano-scale electronic structures. This Program Area is divided into two research Thrusts: (i) Nanoelectronic Engineering Sciences, and (ii) Teraherz-frequency and Ultra-fast Electronics. These Thrust areas guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. This Program Area includes research efforts in quantum-confined structures, nonequilibrium and dissipative electron processes in low-dimensional device structures, novel contact and interconnects to nanoscale devices, physics and modeling of nanoscale devices and advanced synthetic materials, novel materials and heterostructures, device based upon mixed-mode principles, mixed technology (*e.g.*, photonics, acoustics and magnetics) systems, and heterogeneous (*i.e.*, different materials and device principles) systems. This research program will have a particular emphasis towards ultra-fast and terahertz frequency electronics and will include a strong component for sensing science at very high frequencies.

This Program Area's research efforts involving nano-devices and molecular-level electronics will address issues related to the design, modeling, fabrication, testing and characterization of novel electrically and magnetically-controlled electronic structures. This research will enable the development of novel materials, advance processing and fabrication science, enable advanced physical modeling and simulation capabilities, and identify advanced electronic device concepts. These investigations will ultimately lead to improvements in the current limits on the functionality, power, speed (frequency) and power consumption of electronic components. This research is a key enabler for many future electronic goals of the Army, as it supports an array of capabilities in densely-integrated nanoscale architectures for ultra-sensitive and high-discrimination sensing, high-speed, high-data-rate communications and signal processing, and enhanced high-frequency power.

2. Electromagnetics, Microwaves, and Power. The goal of this Program Area is carry out basic research leading to the creation of a transmit/receive system that will receive and demodulate any electromagnetic signal from any direction, modulate and transmit any electromagnetic signal in any direction, reconfigure to implement a variety of radio and sensor functions, adapt to the ambient environment, and respond to changing requirements. This Program Area is divided into three research Thrusts: (i) Electromagnetics and Antennas, (ii) RF Circuit Integration, and (iii) Power Efficiency and Control. These Thrust areas guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. Research efforts within these Thrusts include studies of the generation, transmission, and reception of high frequency microwave and millimeter wave radiation, as well as specific technical problems at high frequency (HF), very high frequency (VHF), and ultra-high frequencies (UHF). Research efforts within these Thrusts include studies of the coupling of electromagnetic (EM) radiation into and out of complex structures, active and passive antennas, transmission lines and feed networks, power combining techniques, EM wave analyses of electrical components, and EM modeling techniques that advance mixed-signal design to the state of current digital design.

The research efforts within this Program Area may lead to the discovery of novel active and passive devices and components with improved dynamic range, linearity, bandwidth, and loss performance. This includes improvements which have the greatest system leverage in reducing radio and radar power requirements, battery size, and system size. Physical constraints imposed by 2D mixed-signal circuit integration and parasitic power loss in passive components are being addressed and novel approaches to circuit integration, such as use of 3D, plug and play circuit integration are being explored. Army applications of this technology include communications (both tactical and strategic), command and control, reconnaissance, surveillance, target acquisition, and weapons guidance and control.

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

4. **Electronic Sensing.** The goal of this Program Area is to extend the underlying science behind action-reaction relationships in electronic materials and structures as well as understand target signatures. This Program Area is divided into two research Thrusts: (i) Infrared Detectors and (ii) Non-imaging Sensing. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. The scientific objective of the Infrared Detector Thrust area is to understand and control the stimulus and response of infrared materials and devices. This includes the design and fabrication of novel detector structures, such as superlattice or barrier structures, as well as devices made of amorphous materials. 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. Research in this Thrust area includes both high performance detector materials and structures and uncooled, low cost, detector materials and structures. The Non-Imaging Sensing Thrust strives to uncover the underlying relationships behind signature phenomenology and use it to guide sensor development and decision techniques. Non-Imaging sensing modalities include acoustic, magnetic, infrasound, and "passive" environmental signals such as radio or TV broadcasts. Efforts in the this Program Area seek to give the Soldier 100% situational awareness of vehicles, personnel, weapon platforms, projectiles, explosives, landmines, and improvised explosive devices (IEDs), in day/night, all weather, and cluttered environments through natural and man-made obstructions.

C. Research Investment

The total funds managed by the ARO Electronics Division for FY11 were $37.6 million. These funds were provided by multiple sources and applied to a variety of Program Areas, as described here.

The FY11 ARO core (BH57) program funding allotment for this Division was $5.7 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $3.5 million to projects managed by the Division. The Division managed $13.8 million provided by the Defense Advanced Research projects Agency (DARPA), and $2.5 million provided by other agencies. The Small Business Innovative Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided $6.9 million for awards in FY11. Finally, $5.2 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

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

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). 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. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. **Optical Fiber Technology Workshop (Cocoa Beach, FL; October 17-19 2010).** This workshop originated through discussions between ARO (Dr. Gerhold) and Professor Martin Richardson of the University of Central Florida to bring together international experts on optical fiber technology for the advancement and dissemination of the progress being made around the globe. Leading groups from the U.K., Germany, and the U.S. presented results on state-of-the-art fabrication techniques and potential for future optical fiber research. Group sessions were held on the potential for polymer fiber research such as that being pursued at the MIT Institute for Soldier Nanotechnologies by Professor Yoel Fink. Other groups presented research performed in the U.S. in industry (AT&T, NuFern, IMRA America, and others) and academia (Arizona, Clemson, MIT, and Central Florida).

2. **Workshop on Physics and Chemistry of II-VI Materials (New Orleans, LA; 26-28 October 2010).** This workshop provided a platform for the exchange of information on state-of-the-art research and development in II-VI materials and their applications. The technical program covered a wide range of topics of interest to the materials community including wide and narrow gap materials, matched and mismatched substrates, dopants, defects, and unique characterization techniques. Dr. William Clark served on the planning committee and was session chair of the special session on Advanced III-V Detector Architectures.

3. **National Radio Science Meeting (Boulder, CO; 5-8 January 2011).** This open scientific meeting was sponsored by the U.S. National Committee of the International Union of Radio Science (USNC-URSI). The USNC-URSI is appointed by the National Research Council of The National Academies and represents U.S. radio scientists and engineers in the international community. Papers on any topic in radio communications; electromagnetic phenomena, remote sensing, and other radio science areas of interest were presented. The meeting provided an excellent snapshot of the state of radio science and a common ground for discussion of future basic research topics.

4. **IEEE Radio and Wireless Symposium (Phoenix, AZ; 16-20 January 2011).** This symposium focused on the intersection between radio systems and wireless technology, which created a unique forum for engineers to discuss hardware design and system performance of the state-of-the-art wireless systems. The symposium attracted engineers from academia, government, and industry from the U.S. and around the world. The 2011 meeting featured a technical track on Advanced Techniques in Software Defined and Cognitive Radio, an emerging technology with the potential to revolutionize Army ground mobile wireless communication.

5. Eighth Conference on the Foundations of Nanoscience, FNANO 2011 (Snowbird, Utah, 11-15 April, 2011) The Foundations of Nanoscience (FNANO) meeting was established by the International Society for Nanoscale Science, Computation, and Engineering in 2004 as a venue for the wide range of researchers interested in various aspects of self-assembly as it relates to nanoscience and nanotechnology. Nanoscience is an important cross-disciplinary area that incorporates research and development from all branches of engineering as well as from chemistry, physics, biology, computer science, and even mathematics. This conference is organized to facilitate the impact of evolving self-assembly techniques on new and novel types of devices and architectures. The unifying theme of the FNANO meeting is self-assembly, and this area has enormous potential for revolutionalizing nanofabrication. This conference has very important relevance to the U.S. Army and DoD because it offers insights into the future development of novel devices and system architectures at the nanoscale and molecular levels. More specifically, it is a facilitator for the discovery of new types of biological and/or organic structures that could offer more advanced capabilities for sensing, data processing, computation and communication.

6. Workshop on Advanced Technologies for Audio Collection and Transmission (Adelphi, MD; 2-3 June 2011). The goal of this workshop was to discuss fundamental concepts and new ideas in acoustic transduction and audio processing. The workshop was co-hosted by the ARL Sensors and Electron Devices Directorate (ARL-SEDD) Acoustic and EM Sensing Branch, and brought experts from the academic community together with scientists from the DoD and the intelligence community (IC) to review groundbreaking research in audio-related technologies, identify needs within DoD and the IC, and form recommendations for possible future basic research in acoustics and related fields. Dr. Dev Palmer of the ARO Electronics Division served as co-chair of the workshop.

7. 2011 Nanoelectronic Devices for Defense and Security Conference (Brooklyn, NY; 28 August – 1 September) The goal of this bi-annual meeting is to review the evolving research and development (R&D) activities in the arena of nanoelectronic devices that have direct relevance to critical capability needs for national defense and security in the future. This conference has a well-established tradition of being organizing around an applications-oriented framework that will allow for capturing the important science and technology (S&T) challenges to realizing the next generation in nanoelectronic devices, while being strongly inclusive to a host of innovative solutions that are continually evolving from the highly multidisciplinary areas of nanoscience, nanomaterials, nanofabrication, nanoengineering and nanomedicine. The 2011 meeting was built around the theme of "Present & Future Roles of Nanotechnology in the Forensic Sciences," and was coordinated with the U.S. Army Criminal Investigation Laboratory (ACIL), the U.S. Defense Threat Reduction Agency (DTRA), ARL, and many other Army & DoD agencies. Dr. Dwight Woolard of the ARO Electronics Division was the lead technical organizer of the conference, which included several presentations by ARO-funded investigators.

8. Antenna Applications Symposium at Allerton (Monticello, IL; 20-22 September 2011). The Antenna Applications Symposium and its predecessor, the Air Force Antenna Symposium, have for more than fifty years provided a unique forum for exchange of ideas and information about antenna design and development. The symposium brought together key researchers from all three military services, law enforcement, companies from the U.S. and abroad, and universities from across the country and around the world. Technology reviewed at the Allerton Symposium demonstrates the breadth of antenna applications, ranging from arrays for radar, communication, navigation and remote sensing, to innovative, multidisciplinary basic research concepts for antenna reconfigurability and multi-functionality, to numerical modeling techniques, all of which are highly relevant to Army missions in electromagnetic sensing and communications. Dr. Dev Palmer of the ARO Electronics Division presented the keynote address "Antenna Research for Army Electromagnetic Systems."

C. Multidisciplinary University Research Initiative (MURI)

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

1. Standoff Inverse Analysis and Manipulation of Electronic Systems (SIAMES). Two efforts under this MURI topic began in FY05, with one effort led by Professor Michael Steer at North Carolina State University, and the second led by Professor Lawrence Carin at Duke University. These research teams are studying the interaction between electromagnetic fields and electronic circuits, with the ultimate goal of enabling rapid and accurate extraction of system, functional, and device information from external stimulus and monitoring of electronic systems.

At the most basic level, the interaction between electromagnetic fields and electronic circuits is visualized as a radio signal being received through an antenna by a radio circuit. Most analytical models and system-level simulations are limited to this level of complexity, which gives accurate results only within the designed operating bandwidth of the system. In reality, electromagnetic fields can couple in and out of electronic circuits in a variety of ways and through a variety of components, reducing performance and causing interference to other circuits. The MURI team is using sophisticated laboratory equipment to illuminate electronic circuits with EM signals over a wide range of frequencies using a variety of waveforms, and measure the signals re-radiated from the circuits. This approach has already revealed previously unknown phenomenology that has the potential for significantly improving the capability to identify, locate, and disrupt electronic devices at a distance.

Discoveries made by the SIAMES MURI team have transitioned into important fielded applications and follow-on research programs. The scientific merit and technical relevance of the research was recognized by the international research community through the award of the 2010 IEEE Microwave Prize. Professors Cangellaris, Chappell, and Delp each received the ARL Director's Coin for Excellence in recognition of their contributions to Army science and technology. Professor Steer received the Commander's Award for Public Service medal from the Commanding General of the Army Research, Development, and Engineering Command (RDECOM), cited for leading innovative theoretical and experimental research programs, developing and sustaining strong working relationships with Army scientists and engineers, and aggressively transitioning research breakthroughs into important electronic warfare applications in support of the Warfighter.

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

The main focus of this research is on vanadium oxide (VO_x) and amorphous silicon germanium (***a***-$Si_{1-x}Ge_x$:H) but other novel materials are also being explored, such as the spinel family and zinc oxide (ZnO). A combination of theory, microanalysis, optical measurements, and feedback to growers is employed to unravel the mysteries of the structure, absorption mechanism, and transport properties in these largely disordered materials. During the course of this MURI the microstructure of production-quality VOx was well characterized and it was shown that the films exhibit composite-like behavior. In FY11, the researchers developed an atomistic picture of Boron doping in ***a***-Si. The researchers also grew nickel manganite with low noise and reasonable temperature coefficient of resistance using spin spray techniques at 90°C. It is hoped that the knowledge gained from this MURI can be used to make improvements in materials to fully exploit their capability for uncooled infrared-detector applications. Understanding the dynamics of the materials at the molecular level will provide a quantitative fundamental base toward achieving the goal of an infrared camera for every Soldier.

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

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

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

This research effort includes an in-depth study of the origins and structural, electrical and optical properties of defects, in-situ & 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. In addition, use of the III-V materials family will leverage the vast infrastructure already in place to further reduce the cost.

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

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as was discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Short-Range Detection of Radio Transceivers for Physical Security. A SBIR Phase II Enhancement contract was awarded to Vadum, Inc. for further development and technology transfer of a signature-based active RF transceiver detection sensor system. The Vadum signature-based active RF transceiver detection sensor can detect the presence of radio transceivers (*e.g.*, mobile phones) whether they are powered on or powered off, even if the battery has been removed. The sensor detects the unique RF signature of the transceiver, similar in concept to radar detecting the signature of an airplane. Vadum uses an active RF method; a waveform is broadcast and a reflection of that waveform is analyzed. If a transceiver is present, a distinct transceiver signature is detected. Two versions of the technology were developed in earlier stages of the project. The narrowband version has been successfully tested against nearly 100 unique models of mobile phone, and operates best at short range, for example in a walk-through portal form factor. The broadband version uses new interrogation waveforms and is significantly more sensitive. It has been tested in a low-clutter outdoor environment. Using the Phase II Enhancement funding, this project will test the broadband signature-based active RF transceiver detection in an indoor form factor, integrate the broadband and narrowband sensors into a single system, and advance the current system technology readiness level (TRL) from TRL 5/6 to TRL 7/8. The technology has many potential military and commercial applications: wall-mounted sensors for physical security at sensitive military facilities, robot-mounted systems for explosive ordnance detection (EOD) and route-clearance missions, non-invasive package inspection for Homeland Security, and for mobile phone detection at State, Federal, and privately operated correctional institutions.

2. Narrowband Perfect Absorber using Metamaterials. Two Phase I Chemical and Biological Defense (CBD) SBIR contracts were awarded to Lumilant, Inc. and Phoebus Optoelectronics, LLC to establish the foundation for the future development and demonstration of metamaterial technology for developing a narrowband perfect absorber that functions in the LWIR region for the purpose of realizing highly sensitive uncooled hyperspectral imagers. A metamaterial is a substance that acquires its electromagnetic properties from imbedded physical structures instead of from its chemical composition, and can bend light in ways not possible with any natural material. In order for the embedded structures to strongly affect electromagnetic waves, a metamaterial must possess features with sizes comparable to the wavelength of the electromagnetic radiation with which it interacts. Since the electric permittivity and magnetic permeability of metamaterials can be manipulated to create a very strong absorber their application offers the potential for realizing narrow-band perfect absorbers and completely new and novel types of optical devices. In particular, perfect absorbers have the potential to significantly improve the function of microbolometer focal-plane arrays. Such microbolometer arrays would offer enhanced and/or expanded capabilities for chemical and biological sensing, especially in regards to standoff detection and monitoring. These two efforts aim to investigate various types of metamaterial structures for their effectiveness in realizing microbolometers that offer very high absorption over a very narrow bandwidth (~ 10 wavenumbers) that can be dynamically tuned over 8-12 micron region.

3. UV-enhanced Raman Spectroscopy. Two Phase I SBIR contracts were awarded to Spectral Platforms, Inc. and TIAX, LLC to study how UV LEDs can be used to enhance the sensitivity and spectral resolution of Raman spectroscopy systems for biomolecule sensing.

Spectral Platforms will develop a highly specific bioterror threat agent detection system using ultraviolet light emitting diodes (UV LED) in a Raman spectrometer, combined with a 2D correlation analytic technique. Validation of proposed methods with experimental results collected using a breadboard instrument on an accepted anthrax simulant. Methods will be demonstrated to improve the detection sensitivity by 100,000-fold compared to the current approach for point detection. The research will aid in making improved chemical or biomolecule sensors which is responsive to Army needs for high sensitivity and selectivity sensors for warfare agent threats. Specifically, anthrax will be the focus in phase I to improve upon existing point sensors which use Raman based sensing (or other methods) to improve upon false alarm probability and sensitivity of detection. Miniaturized sensors which can accurately detect the presence of such threats could be used in both military and civilian environments and reduce the need for bulky PCR (Polymerase Chain Reaction) systems which have had problems even though they are much bulkier and elaborate. UV LEDs have recently been improved in terms of their efficiency and output power because of two other ARO SBIR phase II programs. UV lasers on the other hand are not currently available in miniaturized form and also can destroy the analyte molecules making their viability as a threat agent no longer detectable.

The TIAX phase I SBIR aims to utilize UV light to enhance Raman spectroscopy by up to 5 orders of magnitude and spectral resolution by up to 2 orders of magnitude compared to spectroscopy methods without UV light. Their approach is to study representatives of important analyte classes (toxics, chemical/biological agent simulants, and air pollutants) using a two-light-source Raman technique involving a UV LED and an ordinary visible/near infrared laser. Raman spectroscopy holds great potential for the Army in both chemical and biomolecule detection but has been hindered by sensitivity issues and by background noise from autofluorescence. Another approach is to use a UV laser with wavelengths below 250 nm, because (a) Raman sensitivity goes as the inverse of wavelength to the fourth power; and (b) wavelengths below 250 nm tend not to induce autofluorescence. Drawbacks to this approach include potential damage to the analytes by high energy photons; and the current cost of deep-UV lasers (diode lasers below 250 nm will not be available for some time). Deep-UV LEDs are thus being studied for ways that they can improve sensor performance since they have been developed in arrays with milliwatt level output powers in the past few years.

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

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. MEMS Based Thermopile Infrared Detector Array for Chemical and Biological Sensing. A Phase II STTR contract was awarded to Black Forest Engineering (BFE), in collaboration with Case Western Reserve University, with the goal of fabricating silicon compatible thermopile arrays for spectroscopic sensing of chemical and biological molecules. Thermopile arrays which respond in the mid-wave and long-wave regimes will be fabricated, as well as broad band IR arrays. Both poly-Si and poly-SiGe based thermopiles will be fabricated. The poly-Si material is standard CMOS gate material and should be a low risk approach; however the poly-SiGe material is less straight forward but should be higher performance. Linear arrays of both materials will be fabricated on 100 or 150 mm diameter silicon wafers. The poly-Si array will be interconnected with BFE's readout integrated circuit at the wafer level. The poly-SiGe array will use a wire bond approach with each thermopile having two separate bond pads. The potential advantages of monolithic thermopile sensor arrays include low cost, very small power consumption, small size, and high sensitivity. The ability to fabricate thermopiles arrays from silicon compatible materials using standard integrated circuit processes holds the potential to improve infrared sensing capabilities within DoD. The thermoelectric coefficients and resistivity of silicon and polycrystalline silicon make them very attractive materials for rugged, inexpensive infrared spectrometers.

2. Integration of 360°-Retrodirective Noise Correlating Radar with Panoramic Imager. A Phase II STTR contract was awarded to Physical Domains Inc. to leverage recent breakthroughs in retrodirective noise-correlating (RNC) radar and to develop and demonstrate a new technological capability for imaging sniper bullet trajectories and the local terrain. Radar-based tracking and imaging tools for the real-time detection and geo-locating of high-velocity threats, such as rocket-propelled grenades and large-caliber bullets, represents a unique and extremely important new technology for Force Protection and Homeland Security. Because the response time for these types of threat scenarios must be tens of milliseconds or less, it is a requirement that the envisioned radar system possesses extremely short detection and acquisition times and should thus be "auto-cued". This system must also provide real-time imaging of the projectile assaults overlaid onto the surrounding 3-D terrain and environment. This Phase II effort will address these requirements by developing the components and algorithms needed for a 360° field-of-view retrodirective radar system operation and projectile tracking and various components for hardware-software interfacing. This technology may ultimately offer a unique capability to the military and law enforcement for countering (and documenting) threats presented by sniper attacks.

3. Electrophoretic Nanofluidic Biochip Sensor Platform for THz Spectroscopic Fingerprinting of Biological Species. A Phase II STTR contract was awarded to Redondo Optics, Inc. to develop and demonstrate an integrated electrophoretic nanofluidic biochip sensor platform for the accurate, reliable, and fast-throughput "label-less" THz spectroscopy finger printing of biological species and agents. This project aims to develop and demonstrate a nanofluidic chip technology and the associated manufacturing methodology that will provide a cost-effect capability for the accurate label-less THz spectroscopy detection and identification of biological species such as DNA, RNA, proteins, and enzymes to enable the detection and identification of biological species. The proposed technology and manufacturing development is very strong and therefore has a high probability of leading to effective approach for controlling biological species in solution for the purpose of achieving high repeatable THz spectroscopic characterization of the biological targets. This capability is expected to make impacts to the bio-defense applications.

This new research and development will build upon extremely noteworthy Phase I achievements which include, but are not limited to: the demonstrations of two types of INTRay-Nanochip™ prototypes including one-dimensional, single layer, and two dimensional, two-layers of parallel-weaved and cross-weaved, nanofluidic channels; the development of an innovative soft-nanolithography technique that enables the wafer scale production of disposable nano-imprinted PMMA INTRay-Nanochip™ prototypes; development of a capability to observed the separation of long and small DNA fragments using electrophoretic techniques within the nanoporous structure of the INTRay-Nanochip™ using fluorescence detection techniques; design and development of a methodology for the integration of micro-fluidic pumps to the INTRay-Nanochip for the repeatable and reliable sample fluid delivery to the active nanofluidic channels of the chip; integration of electro-kinetic fluid diffusion and control elements to enable the manipulation of biological samples within the nanofluidic channels of the chip; and, a full performance demonstration of the integrated INTRay-Nanochip™ prototype using a coherent frequency domain THz spectroscopy instrument that included detection, analysis, and identification of the high resolution THz spectral signatures associated with certain biological samples. These are very outstanding demonstrations that attest to the merits and the potential of this Phase II project, and suggest a very high probably for realizing an integrated electrophoretic nanofluidic biochip (i.e., INTRay-NanochipTM) sensor platform that will be capable of accurate, reliable, and fast-throughput "label-less" THz spectroscopy finger printing of biological species and agents, and as such, may define a revolutionary new detection and identification technology for field applications.

4. Burst mode lasers for trace molecule detection from LIBS (Laser Induced Breakdown Spectroscopy). Two Phase I STTR contracts were awarded to Performance Lasers and Q Peak, Inc. to study the potential of making lower cost, compact, high peak power lasers at multiple wavelengths. The goal of these two Phase I

STTR programs is to develop a compact, rugged, and low-cost wavelength-versatile burst laser for a variety of potential military applications. Performance Lasers will focus on the development of a wavelength-versatile burst laser that is very compact (<33% of current size), lightweight (<25% of current weight), and inexpensive (<33% of current cost; develop a proof-of-concept 'breadboard' demonstrator; and then produce a conceptual prototype. The required academic collaboration will be with Prof. Dryver Houston in the School of Engineering at the University of Vermont. The research focus of the contract with Q-Peak is to design a novel diode-pumped, scalable, and high-efficiency master-oscillator-power-amplifier (MOPA) laser for near-IR pulse generation that is compact, rugged, and low-cost. The required academic collaboration will be with Professor Paul Dagdigian in the School of Arts and Sciences at John Hopkins University. Both of these efforts will contribute technologies to facilitate the development of a new approach to landmine detection for humanitarian and military post-operational demining.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) – 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). The FY11 new starts within these programs are described here, while the missions of each of these programs were described *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. PIRT: Bayesian Imaging and Advanced Signal Processing for Landmine and IED Detection Using GPR. This five-year PIRT project was awarded in FY11 to a team led by Professor John Anderson at Howard University. The goal of this project is to develop and apply innovative signal processing and computational electromagnetic methods to ground penetrating radar (GPR) based landmine and improvised explosive device (IED) detection systems in order to drastically improve their performance, and evaluate the methods using synthetic and real GPR data.

Professor Anderson will also work closely with the ARL-SEDD SIRE radar team and will collaborate with the Center for Advanced Algorithms at Delaware State University. His research will focus on developing improved techniques for pre-processing the data to suppress noise due to radio frequency interference, self-interference, and sampling jitter, and developing image formation methods that are adaptive and incorporate a priori information about scatterers due to landmines and IEDs. These image formation methods will be implements using parallel MATLAB and computing architectures based on graphical processing units (GPUs). The use of parallel computing is necessary because of the extremely large computational expense of the proposed image formation methods. In conjunction with the image processing, Professor Anderson will develop inverse scattering methods in order to reduce false alarms from man-made object that are not landmines and IEDs. This reduction in false alarms is enabled by the estimation of certain parameters that are directly related to the material of the landmines and IEDs. Finally, the algorithms will be tested against government simulation data and real data from the SIRE GPR system.

2. PIRT: Center for Advanced Algorithms. This five-year PIRT project was awarded in FY11 to a team led by Professor Fengshan Liu at Delaware State University. The goal of this project is to create a new Center for Advanced Algorithms, a partnership between Delaware State University, the University of Delaware, and the Pennsylvania State University, which will develop and transition fully-tested algorithms and software for the detection and discrimination of landmines and improvised explosive devices (IEDs) for wideband ground penetrating radar (GPR) applications.

Researchers at the Center for Advanced Algorithms will collaborate closely with the team at ARL-SEDD engaged in the development of the SIRE ground penetrating radar system. This collaboration will allow the newly developed signal processing techniques to be tested against ground truth with experimental data, and will accelerate transition of the research into the SIRE system. The research will focus on five primary tasks: mitigation of multiplicative noise, ultra wide-band (UWB) spectral shaping with reduced compression artifacts, change detection for improved sub-clutter visibility, inverse scattering methods, and automated detection of anomalous motion. This research has a very high potential positive contribution to the Army counter-IED mission through significant performance improvements in Army forward-looking ground penetrating radar systems.

3. DoD REP Awards. As described in more detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, REP awards aim to enhance or increase the programs, capabilities, and graduates in scientific and engineering disciplines in universities serving underrepresented minorities. In FY11, the Electronics Division managed seven new REP projects, totaling $3.7 million. The equipment purchased with this award is promoting research and education in areas of interest to ARO, such as the characterization of piezoelectric and magnetic materials for Micro-Electro-Mechanical-Systems (MEMS), and studies of the physics of irregularities and turbulence in space plasmas.

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

1. Single-Nanoparticle Transducer. A PECASE award was granted to Professor Lan Yang at the University of Washington to develop a nanoparticle transducer with single particle resolution and exploit it to achieve ultra-sensitive, nano-scale sensors with unprecedented performance and explore interesting physical phenomena for innovative photonic devices. The research will study the fundamental physics associated with mode-splitting effects induced by light scatters, such as particles/molecules, and it will also utilize such phenomena to achieve novel nanosensors which will overcome technological barriers faced by existing resonator based sensors and traditional bulky/expensive single molecular analytical tools. The work will also consider methods for introducing more functionalities to the photonic devices by prior work on wet-chemical synthesis of high-quality photonic materials to mix different materials system and tailor the materials composition at molecular level, with the goal of achieving a larger optical gain in the resonator so as to enhance the quality factor to resolve small amounts of mode splitting which otherwise would not be detected in a passive resonator (*i.e.*, a resonator without optical gain). The proposed research will investigate completely new and novel mode-splitting sensing technique which could lead to novel types of photonic devices and sensors. These devices and sensors have potential for impacting such applications areas as environmental monitoring, medical diagnostics and chemical/biological/radiological/nuclear/explosive detection and identification.

2. Precision Controlled Carbon Materials for Next-generation Optoelectronic and Photonic Devices. A PECASE award was granted to Professor Michael Arnold at the University of Wisconsin (Madison) to develop and integrate new non-metallic, high-efficiency photonic carbon nanotubes and graphene quantum dots into optoelectronic devices particularly for application to high speed, high efficiency and brightness light emitters. Other photonic devices such as photodetectors and solar cells would be sub-thrusts that fall under this work since their active region would use similar materials. Synthesis and sorting on carbon nanotubes (CNTs) will be studied to achieve high luminescence efficiency. Once that is achieved work on the electrical generation and control of excitons and device fabrication will be pursued. CNTs with both polymer blend and inorganic heterostructures will be pursued for appropriate control of excitons and the injection of charge into and extracted out from CNTs for photonics applications. Nanosphere lithography will be pursued on graphene for nanoscale patterning of dots. Optical characterization of the quantum dots will be made in relation to their size, shape and orientation and potential use in infrared LEDs. IR photodetectors with type-II heterostructures and optimized dark current and detectivity levels will be studied. Carbon based materials have a significant potential to impact the photonics world due to their high carrier mobility and recent discovery of high luminescence efficiency.

H. Defense University Research Instrumentation Program (DURIP)

As detailed 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 FY11, the Electronics Division managed six new DURIP projects, totaling $0.87 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including efforts to explore high energy laser optical coatings, advanced piezoelectric devices, and DNA-based superstructures.

I. DARPA Parametric Optical Processes and Systems (POPS) Program

The goal of the DARPA POPS program is to advance four-wave mixing (FWM) to Si-based photonic structures that will lead to optical processing at data rates beyond 1 Tb/s. ARO is currently managing a project at Cornell

University that is focused on using silicon to enhance optical processing. Other projects within this program are focused on using highly non-linear glass optical fibers to achieve the same goals. The high optical confinement of the Si structures enables FWM devices that can operate not only at relatively low powers, but also with short lengths, which will greatly enhance the phase-matching bandwidth. Losses from free carrier absorption (FCA) were mitigated using a reversed-biased diode structure integrated into the FWM waveguide architecture. The DARPA POPS program manager encouraged the ARO Electronics Division to take a lead role in the program by leading multiple teleconferences with the ARL Computational and Information Sciences Directorate (ARL-CISD) to establish an optical networking workshop. This workshop will enable the Army and DoD to gather input and find direction for putting together test-bed architectures proving the advanced capabilities provided by this FWM technology.

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

The DARPA NACHOS program has been managed by ARO since its inception, and began Phase III in FY11. The goal of the program is to demonstrate a sub-wavelength electrically injected semiconductor laser in all 3 dimensions. Although such lasers far exceed the state-of-the-art in terms of size, much work needs to be done to understand the ways in which they could be used in future Army or non-military systems. Further consideration of nanolasers and their potential uses was made this year through a number of avenues including an international topical meeting Dr. Gerhold organized for the IEEE and a special session of the Nano-DDS focused on the potential use of nanolasers for biosensing. Both meetings brought together several NACHOS PIs and experts internationally to highlight the advances being made and discuss where the lasers may make their first impact. As part of ARO interest in high-speed lasers and interconnects, a potential MURI program was proposed to further the research of modulating and interfacing with nanolasers to make them useful for next generation photonic networks such as those used in electronic-photonic integration schemes being pursued at Luxtera. The programs that moved to phase III were led by professors at Berkeley, Caltech, and UCSD with the goal of making room temperature electrically injected sub-wavelength lasers still not achieved. Progress has been made though at both Arizona State (Berkeley group) and UCSD both in terms of laser size and electrical injection operating temperature that approach the end goals. The NACHOS program has been coordinated with ARL-SEDD through Dr. Wayne Chang.

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

ARO currently manages six MRI programs for the High Energy Laser Joint Technology Office in Albuquerque (managed by OSD). Three of those are new MRIs which were kicked off this fiscal year and awarded through ARO's Electronics Division. The previous ongoing programs focused on fiber laser research including use of new gain media, new waveguide designs, and one program on gas lasers. The new MRIs are led by professors at U. New Mexico, Central Florida (CREOL – Center for Research in Electro-Optics and Lasers), and Clemson. Their respective foci are on three different subjects: fundamental physics of creating a high power handling optical coatings, material loss improvement and beam combining techniques with volume Bragg gratings, and solid core photonic crystal fiber laser development for larger core sizes and suppressed acoustic mode interference. ARO continues to play a significant role in leading the MRI programs by organizing a number of ARO workshops, particularly on the fiber laser efforts, to review progress and aid in technology transition and the development of new research programs (see Optical Fiber Technology workshop under conferences). Other ARL Directorates have been made aware of the programs through their participation in HEL-JTO programs including several reviews annually, and ARL-CISD and ARL-SEDD have participated in various ways.

L. DARPA HiPER (High Power Efficient and Reliable Lasers) 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 funded to Science Research Laboratory (SRL), 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 where SRL will complete four additional tasks in twenty four months. The start of this effort is to begin after month 3 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 2.5kW/cm2, thermal resistance of < 0.25K/W and optical power extraction of 170mW/µm. The second add-on Task will focus on the attachment of 3.6mm, kW LD bars on an impingement cooler with the goal of demonstrating a high-brightness, 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 following related efforts are tied into ARO and DoD goals of developing higher power, more efficient laser diodes and is being coordinated with SEDD and another ARO single investigator program for potential transition and impact to future programs.

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

The objective of this work is to develop compact, efficient and bright laser-diode (LD) sources that will result in extremely light-weight and inexpensive high-energy lasers (HELs) for the U.S. military. The SRL technologies developed in the HiPER I program will increase the power-to-weight ratio of LD pumps for HELs by 20-fold, to 20W/g from the present state-of-the-art (SOA) of 1W/g. This program follows on previous DARPA/ARO funded program (HiPER I). HiPER II takes the thermal modeling efforts of HiPER and pushes the whole pump module forward to create an array of 5 x 5 sq. cm modules in a 10 x 10 array that will be used in the DARPA Adaptive Photonic Phased Locked Elements (APPLE) program together with RIFL (Revolution in Fiber Lasers) to make a steerable HEL weapon with upwards of 300 kW of coherent power in a small package that could fit into a fighter jet or larger plane depending on the form factors. ARO is involved in this program by providing assistance in leveraging technical knowledge of many related JTO-HEL programs and DARPA's APPLE program to make this a success. 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. Great progress was made on the program this year with several results presented at Photonics West 2011. A joint ARO/DARPA workshop was held in 2011 to help disseminate these accomplishments and discuss additional issues such as beam combining and power scaling at other wavelengths.

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

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

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

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

P. DARPA Microscale Plasma Device (MPD) Program

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

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

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

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

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

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

The DARPA CMUVT program was initiated due to advances from Sensor Electronic Technology and Nitek funded by ARO SBIR phase IIs using sapphire substrates coupled with advances at Hexatech (Morrisville, NC) and Crystal IS (Troy, NY) on AlN substrates to push LED and laser diode technology in the 225-275 nm region toward usable levels for water purification and biosensing. Program goals include 20% wall-plug efficiency LEDs in the 250-275 nm regime and laser diodes with wavelengths less than 250 nm. Both goals far exceed the state of the art for LEDs which only perform around 1-3% currently and laser diodes which don't exist commercially below 340 nm. Photon Systems, Inc. was awarded an ARO grant from this two-year program for $4 million to study ways to pump AlGaN heterostructure lasers with electron beams. The performers on the award include Boston University (epitaxy) and JPL (field emitters). The performers on the award include Boston University (epitaxy) and JPL (field emitters). Coordination with ARL-SEDD (Michael Wraback's team) occur through their co-management of the CMUVT program with DARPA, ARO, and others, and the SEDD team has been active in collaborating within the CMUVT effort.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. Infrared Properties of Carbon Nanotubes

Professor Judy Wu, University of Kansas, Single Investigator Award

The goal of this project is to achieve a thorough understanding of the basic physics that governs the infrared properties of both individual carbon nanotubes (CNTs) and thin films of CNTs. A particular emphasis is being placed on understanding the electron and phonon transport within multi-walled CNTs as well as the transport between CNTs in thin films. A second objective is to use this knowledge to guide development of high-performance uncooled CNT nanobolometers for infrared detection.

CNTs in either film or individual form have shown outstanding absorption and photoresponse in the infrared regime although a key figure of merit, the detectivity (D*), has remained orders of magnitude below that of conventional uncooled detectors. In the past year Professor Judy Wu of the University of Kansas has investigated the infrared properties of individual multiwalled CNTs (MWCNT) and obtained a high detectivity (D^* up to 6.2×10^9 cm.Hz$^{1/2}$/W) from individual MWCNTs with asymmetric Schottky contacts (see FIGURE 1). This is an order of magnitude *above* conventional uncooled detectors consisting of vadium oxide or amorphous silicon. Further tests are being carried out to establish the mechanism of the response, which is thought to be due to increased photocurrent due to contact to all the MWCNT shells coupled with reduced thermal conductance due to the nature of the Schottky contact resulting in thermally assisted photogeneration. This research may ultimately reduce costs and increase performance for various IR systems, with potential applications in target acquisition, navigation, unmanned vehicle sensors, and unattended sensors.

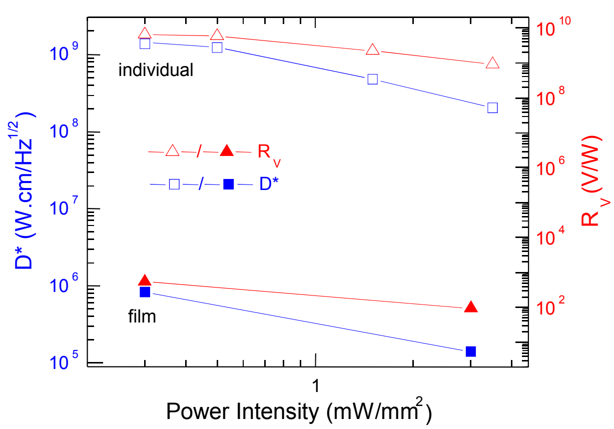

FIGURE 1

Photoresponse vs. power intensity for individual MWCNT and MWCNT film. Detectivity (boxes) on left axis and responsivity (triangles) on right axis.

B. High-speed Transistor Lasers

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

The goal of this research project is to develop high-modulation speed vertical cavity surface emitting transistor lasers (VC-SETL) based on heterojunction bipolar transistors. This work builds on previous research by Professor Nick Holonyak. Since the invention of the transistor laser (TL) in 2004 by Professors Feng and Holonyak, this type of laser has demonstrated the revolutionary performance of picosecond spontaneous recombination lifetime, high differential gain, unique 3-terminal electrical-optical characteristics permitting both current and voltage modulation, and electrical "read-out" of optical parameters. The TL with picosecond lifetime is capable of enhancing modulation optical bandwidth toward 100 GHz, achieving resonance-free frequency response, reducing relative intensity noise (RIN), and improving high quality transmitted eye diagrams (see FIGURE 2).

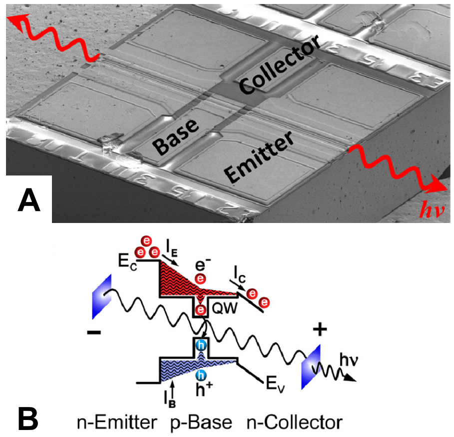

FIGURE 2

Fabricated transistor laser (TL). (A) SEM of a fabricated TL; (B) energy band diagram of TL.

Due to the zero-charge-density boundary condition at the reverse-biased collector junction, carriers with slow recombination lifetimes are removed at the collector, thus, achieving picosecond lifetime. A record recombination lifetime of ~ 29 ps , a reduced photon-carrier resonance amplitude, a 20 GHz small signal modulation bandwidth, and a 10 Gb/s "clean open-eye" signal have been demonstrated. The research team has also demonstrated that a "single quantum well" TL (cavity length L = 300μm) can be modulated simultaneous with both electrical and optical "open-eye" signal operation at 20 and 40 Gb/s data rate, a three-port operation device (see FIGURE 3). The researchers found that the TL exhibits simultaneous electrical and optical "open-eye" operation at 20 Gb/s for both 15°C and 0°C, and 40 Gb/s for 0°C. Hence, the TL modulation bandwidth is limited by the extrinsic parameters rather than the intrinsic optical modulation bandwidth.

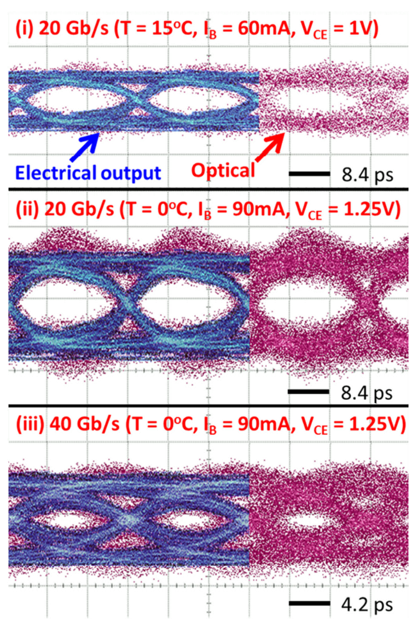

FIGURE 3

Schematic energy band diagram and charge population distribution of an n-p-n TL. Simultaneous unfiltered electrical (blue) and optical (red) eye diagram comparison of TL operation at 20 Gb/s (i, ii) and 40 Gb/s (iii) data rate. The operating conditions are (i) I_B = 60 mA, V_{CE} = 1 V, T = 15°C; (ii) I_B = 60 mA, V_{CE} = 1.25 V, T = 0°C; and (iii) I_B = 90 mA, V_{CE} = 1.25 V, T = 0°C. The electrical RF signal was generated by an Agilent 81250 43.2 Gb/s ParBERT signal generator and applied to the BE junction of the TL; laser output and the collector electrical output were sent to different ports of an Agilent 86100C DCA-J oscilloscope to record eye diagrams. The optical channel (red) eye diagrams are shifted to overlap with the reference collector electrical channel output (blue).

Transistor lasers hold potential for enabling faster integrated circuits and previously unimagined interfacing between electronics and photonics components due to their combined physics in the transistor operation. By improving the TL device design, the lasers may be capable of achieving higher modulation bandwidth and transmission data rates with the "OOK" format. The capability of simultaneous high speed electrical and optical output clearly indicates that the TL has essential electrical and optical feedback advantages for future high speed photonic integration and computation. In addition, they plan to apply the advanced modulation formats to fully characterize and understand the TL capability in energy efficient modulation at 100 Gb/s.

C. High-Resolution Direction of Arrival Determination with Electrically Small Antenna Arrays

Professor Jennifer Bernhard, University of Illinois - Urbana-Champaign, Single Investigator Award

The quality factor, Q, is often assumed to be a limiting factor in direction of arrival (DOA) estimation using electrically-small antenna elements. This stems from the assumption of fixed receive noise power. This assumption holds for internally noise limited systems, but for typical UHF brightness temperatures, the system will be externally noise limited. In an externally noise-limited system, Q has little effect on received SNR unless the signal level is near the minimum discernible signal of the receiver. Other non-ideal antenna properties, which significantly affect DOA performance, such as efficiency and mutual coupling, are often neglected in modeling electrically small receive arrays. This research assumes a vector-sensor geometry consisting of orthogonal loops and dipoles. Based on this assumption, typical values for antenna parameters (*e.g.*, efficiency, impedance, Q) can be used to determine bounds on direction finding parameters (*e.g.*, CRB, bandwidth) of the receiving system. This is accomplished through robust modeling of signal and noise including antenna effects such as mutual coupling and cross polarization reception.

Several vector-sensor arrays have been built and measured in the University of Illinois Electromagnetics Lab (see FIGURE 4). The array shown in FIGURE 4A consists of a straight dipole and two four-turn loops. The loops were made with multiple turns to lower their reactance and reduce the common mode contribution to the received signal. The set of antennas are capable of direction of arrival estimation of vertically polarized signals within a few degrees in high SNR environments. The array is designed to receive signals centered at 420 MHz. It has been tested against source signals from a vertically polarized half-wavelength dipole antenna. The received signal is down-converted to 10.7 MHz using a double-conversion superheterodyne receiver, then sampled using the National Instruments PCI-5105 digitizer. The array is measured with a test signal in a calibration step to store the array manifold. At this point, the system is capable of real-time direction finding at 420 MHz +/- 6°.

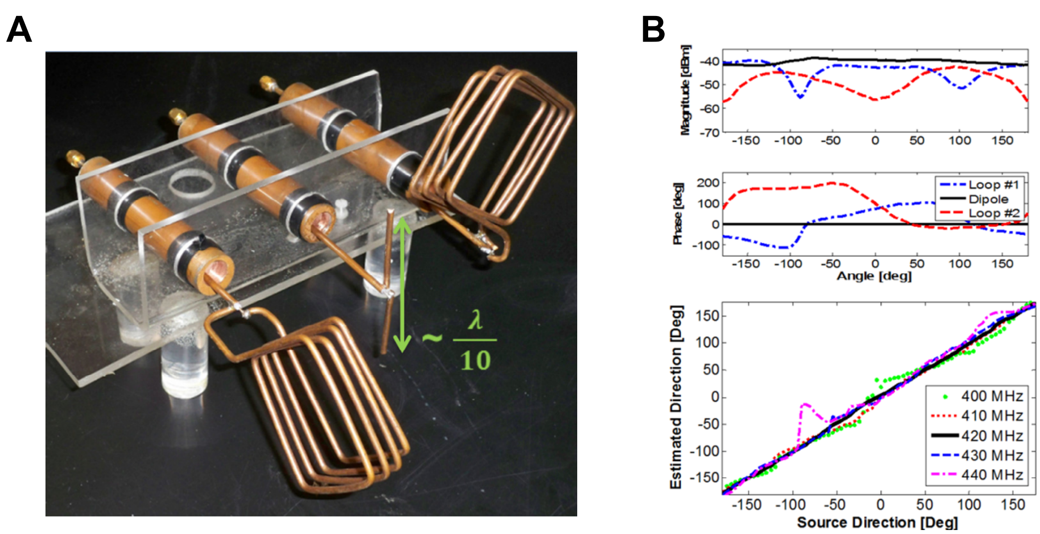

FIGURE 4

Vector sensor direction finding array of electrically small antennas. (A) A vector sensor array of electrically small antennas consists of orthogonal loop antennas with a co-located dipole one-tenth of a wavelength long at the design frequency of 420 MHz. (B) This set of antennas is capable of direction of arrival estimation of vertically polarized signals within six degrees over a bandwidth of 40 MHz around the design frequency.

This array can be extended to include estimation of three dimensional arbitrarily polarized signals. To accomplish this, the array will be expanded from three elements to six elements. The six element array will consist of three mutually orthogonal dipoles and three mutually orthogonal loops. Additionally, further co-location of the antenna elements presents new challenges in mutual impedance suppression. This is especially true of low-reactance arrays, which are in simpler to measure practice. Research and development in this area will contribute to the fundamental understanding of electrically small antennas. The knowledge gained from this research may significantly advance Army capabilities in intelligence, surveillance, and reconnaissance by reducing the form factor and increasing the performance of radio direction-finding systems.

D. Scale Effect in Flexoelectricity

Professor Xiaoning Jiang, North Carolina State University, Single Investigator Award

The goal of this project is to investigate flexoelectricity at the nanometer scale and determine the potential of flexoelectric nanostructures for multimodal sensing. The flexoelectric effect is due to coupling between the mechanical strain gradient and the electric polarization. This effect contributes to piezoelectric properties of a material with an inverse size dependence. Thus, in principle, the effective piezoelectric properties of flexoelectric structures can be significantly enhanced as the structures are scaled down. However, the contribution at small sizes was controversial due to an order of magnitude difference between the experimentally identified and theoretically calculated flexoelectric constants. Professor Jiang has demonstrated that the transverse flexoelectric coefficients μ_{12} of barium strontium titanate (BST) microcantilevers were found to keep the same value of 8.5 μC/m for microcantilevers for thickness ranging from 30 μm to 1.4 mm (see FIGURE 5). This result suggests that flexoelectricity induced polarization can be significantly increased as structures are scaled down, holding promise for flexoelectric micro/nano cantilever sensing applications.

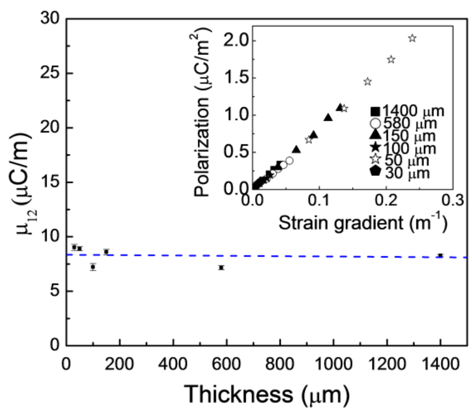

FIGURE 5

Transverse flexoelectric coefficient of BST. The plot displays the transverse flexoelectric coefficient μ_{12} and the measured relationship between flexoelectric polarization and strain gradient (inset) in the BST microcantilever with different thicknesses.

E. Integrated Sensing Using DNA Nanoarchitectures

Professor Michael Norton, Marshall University, Single Investigator Award

The goal of this project is to establish completely new and novel types of DNA-based nanoarchitectures that allow for the man-engineering of the dielectric properties and for the specification of electro/optical functionality at the molecular-level. The long-term goal is the development of novel functionalized materials that allow for the electro-photonic transduction of information regarding the microscopic mechanisms occurring within hybridized DNA-based nanoscaffolds. The realization of nanostructured biological and/or organic elements with molecular conformations that respond rapidly to light excitation (*e.g.*, within the terahertz and/or far infrared) will enable one to utilize detectable changes in the associated dielectric properties as spectroscopic-based probe and interrogation tool. Hence, this research has relevance to spectral-based sensing applications such as for: characterizing microscopic bio-chemical systems; medical diagnostics of biotics and tissue; and, sensors development for detecting biological, chemical and explosive threat agents. Some of the major challenges of this research project include: the development of large 2D (and 3D) DNA-based nanoscaffolds (*i.e.*, novel motif and/or origami-based scaffolds) with predefined regions for incorporating molecular functionality; the identification, synthesis, study and implementation molecular capture and reporting systems; and, the structural, optical and spectral characterization of molecular components and the superstructures. This research effort has produced a significant number of first-time accomplishments. For example, a novel new "J1" DNA motif (designed by Professor Nadrian Seeman of NYU under a companion ARO-funded project) has led to the successful fabrication of the world's largest (500 microns) high-quality DNA crystals (see FIGURE 6).

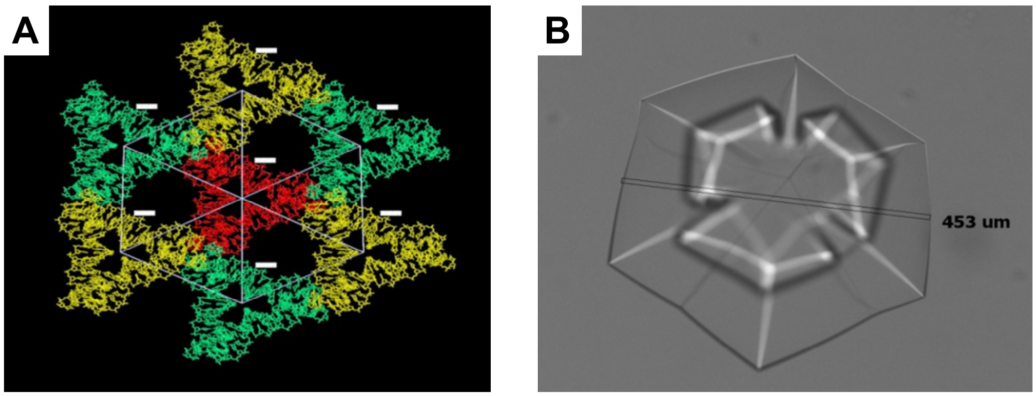

FIGURE 6

J1 DNA motif and resulting crystal structures. (A) The J1 DNA Motif was implemented to fabricate (B) the world's largest high-quality DNA crystal structures. Note that the white boxes on the left indicate planned locations for incorporation of functionalized molecules.

This accomplishment is important because these samples present an aperture size large enough for long-wavelength spectroscopic characterization. Even more recently, the researchers were able to implement hybrid fabrication technique that allowed for creating regular arrays of origami structures as a methodology for increasing the characterization (*e.g.*, optical, Raman, THz) aperture. This work also extended the technique to a functionalized example where the protein Streptavidin was used as a linker for locating Biotin in a controlled manner (see FIGURE 7). The generation of these structures establishes the foundation for binding additional designer structures, such as nanorods and carbon nanotubes, if the ends can be modified without negatively altering the properties of the nanoparticle.

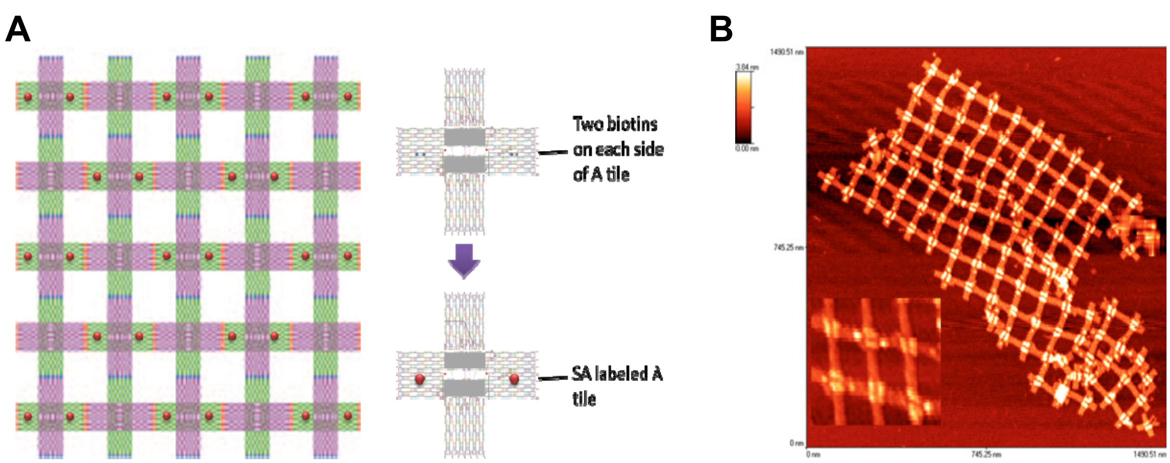

FIGURE 7

DNA nanoarchitectures for Streptavidin-Biotin binding. (A) The array structure was designed to consist of two cross-shaped tiles One origami tile binds two Strepatvidin binding locations and one tile is deisgned to be incompatible for binding Streptavidin. The binding locations are ~50 nm apart. (B) The AFM image of the nanoarchitechture array reveals two Streptavidin locations on alternating tiles.

F. Investigating III-V Nanowire Heterostructures for High-Frequency, Low-Power Circuitry

Professor Joerg Appenzeller, Purdue University, Single Investigator Award

This research is investigating the very important question of how to reduce power consumption in future integrated electronic circuitry. While nano-materials are discussed frequently in the context of high-density electronic applications, a much more fundamental opportunity exists in regards to their unique electronic properties and how these properties may be utilized to achieving enhanced performance. In particular, the goals of this project are the exploration and development of III-V nanowire heterostructure (NWH) transistors with special gate-controlled configurations for the purpose of substantially reducing the power consumption of field-effect based transistors and associated RF circuits while maintaining high cut-off frequencies. This effort is considering novel material combinations (*e.g.*, InAs/GaSb) for the purposes of creating both prototype n-type and p-type tunneling (T) NWH-FETs. The initial studies will employ simple n/i and p/i structures that will be side gated. Here, the injection of electrons (holes) from the source occurs from an n-doped InAs wire segment (p-doped GaSb wire segment) respectively. The nanowire portion next to the drain contact is assumed to be gated. Applying positive gate and drain voltages in case of the n-type NW-HFET and negative gate and drain voltages in the case of the p-type NWH-FET results in current flow as in any conventional MOSFET device. This research will utilize a unique structural approach for gating the T-NWH-FETs that only affects the intrinsic nanowire portion of the device and preserves the advantages in regards to the tunneling (*i.e.*, does not deplete the majority carriers in the source) and the parasitic capacitance (see FIGURE 8).

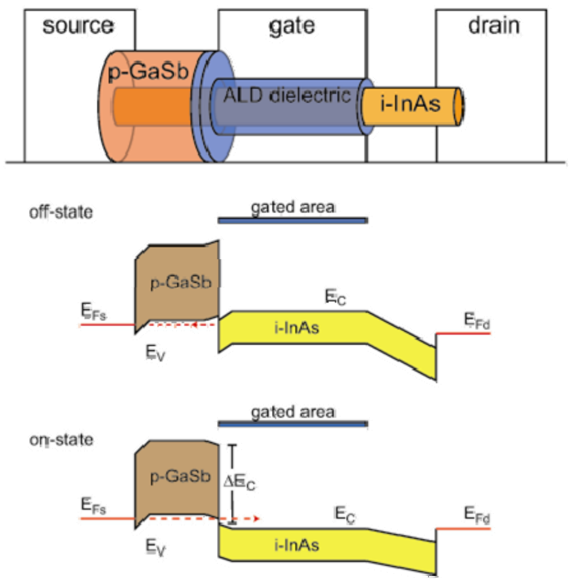

FIGURE 8

Proposed device structure and associated band bending profile of the n-type T-NWH-FET. A self-aligned gate structure becomes feasible due to the use of an InAs/GaSB core-shell structure. Note, that a portion of the InAs wire next to the drain is left un-gated to suppress leakage currents through the InAs valence band.

The initial phases of this project have been very successful including, including a demonstration of (i) InAs nanowire growth with crystalline quality and associated transistor device fabrication and characterization, (ii) demonstration of GaSb nanowires growth and GaSb nanowire transistors, and (iii) TEM images of successful growth of InAs/GaSb core-shell structures. The results for InAs nanowire grown on In and Si substrates demonstrated the capability for controlling planar and out-of-plane by adjusting the growth conditions and the growth substrate orientation (see FIGURE 9).

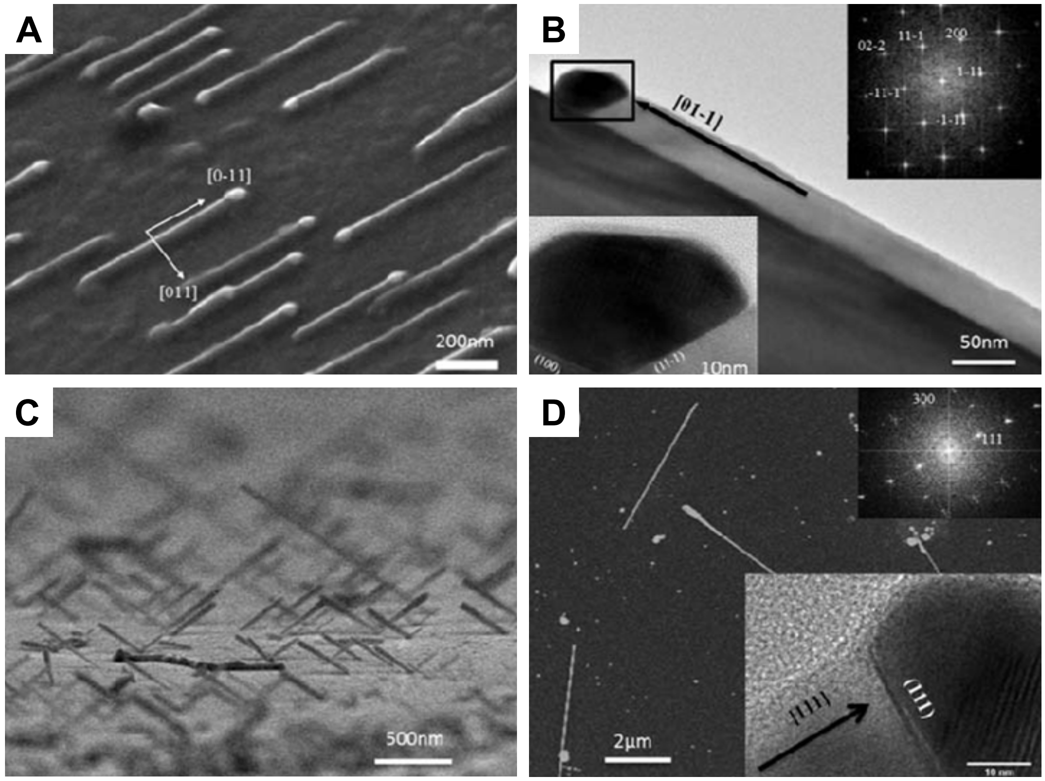

FIGURE 9

Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) images of InAs nanowires. (A) 45° tilted view of planar nanowires; (B) TEM image of planar nanowire showing growth directions and interface indices (inset) electron diffraction and HRTEM of Au and InAs nanowire interface; (C) out-of-plane nanowires grown on Si substrate (inset) electron diffraction and TEM showing growth direction and interface indices; (D) out-of-plane epitaxial nanowires growth.

Once the required growth conditions for InAs nanowires were established, efforts were then used to extend the growth to core-shell nanowire heterostructures, which is the key material for realizing the proposed T-NWH-FET devices. The GaSb shell layer was enabled through a dual precursor exchanging unit where GaSb powder (Alfa Aesar) was used in the second step as the source for shell growth. Transmission electron microscopy (TEM) Energy Dispersive X-ray (EDX) spectroscopy was used to confirm the first successful growth of InAs/GaSb core-shell nanowires (*i.e.*, with ~ 70 nm InAs core diameter and ~ 2 nm GaSb shell thickness). To date, the investigators have produced a variety of nanowire transistors (InAs, GaSb & InAs/GaSb core/shell) with alternative gating (*i.e.*, back and top gate) and executed preliminary characterizations. These results show excellent progress towards a novel III-V tunneling for with potential for future use in low-power RF applications.

G. Dilute-Nitride Antimonide Mid-infrared Semiconductors For Diode Lasers

Professor S. R. Bank, University of Texas - Austin, Single Investigator Award

The objective of this research is to explore the growth of dilute-nitride alloys and ascertain the feasibility for extending the emission wavelength of GaSb-based diode lasers to cover the 3-5 micron wavelength portion of the mid-infrared spectrum. Pseudomorphic diode lasers offer the potential for simple growth, as well as high output powers, wallplug efficiencies, and reliability. However, extending the emission wavelength of diodes lasers beyond ~3 microns is challenging and performance degrades rapidly. Dilute-nitride alloys offer significant advantages for extending the emission wavelength as they do not perturb the favorable valence band structure, potentially mitigating hole leakage and Auger recombination. Unfortunately, nitrogen incorporation into GaSb-based materials tends to degrade material quality and, in turn, laser performance.

Professor Bank has made significant progress in this area, resulting in the first room-temperature photoluminescence (RT-PL) spectra from dilute-nitrides grown on GaSb (see FIGURE 10).

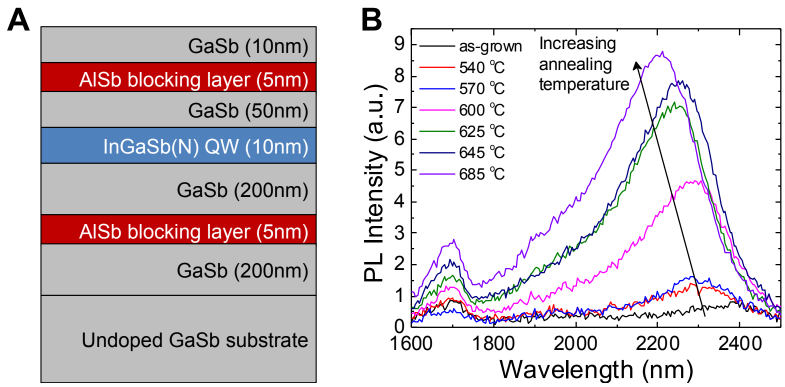

FIGURE 10

RT-PL spectra from dilute-nitrides grown on GaSb. (A) PL test structure for investigating GaSb-based dilute-nitrides and (B) RT-PL spectra for samples annealed at various temperatures for 30 minutes.

The most formidable challenge to high-quality dilute-nitrides on GaSb is to minimize the incorporation of interstitial nitrogen. Consistent with literature, and confirmed by the researchers' high-resolution X-ray diffraction (HR-XRD) and secondary ion mass spectrometry (SIMS) studies, the team determined that a major fraction of the non-substitutional nitrogen incorporates as Sb-N split interstitials, if the growth conditions are not optimized. The Sb-N split interstitials dilate the lattice, while substitutional nitrogen shrinks the lattice. Hence, the formation of Sb-N nitrogen is energetically favorable at the growth front to minimize strain. The importance of this growth regime was recently confirmed with nuclear reaction analysis Rutherford backscattering (NRA-RBS) measurements performed by Dr. Yu at Lawrence Berkeley National Laboratory (LBNL). The total and interstitial nitrogen contents were measured in a set of 100 nm GaNSb films, grown at different substrate temperatures. The LBNL studies revealed that the total nitrogen concentration remained constant with increasing growth temperature, while the substitutional nitrogen concentration decreased monotonically (see FIGURE 11). This indicates that the incorporation of nitrogen atoms into non-substitutional sites increases substantially at elevated temperatures, but the total nitrogen concentration remained unchanged with growth temperature. Therefore, interstitial nitrogen favorably incorporates into GaNSb at elevated growth temperatures, but becomes unfavorable at low temperatures, enabling RT-PL. Mid-infrared semiconductor lasers are important for a number of military applications. Quantum cascade lasers are performing very well at wavelengths greater than four microns but have limitations near three microns due to carrier escape from the conduction band. Type I quantum well lasers are advantageous due to simplified structure and potential for integration with other devices.

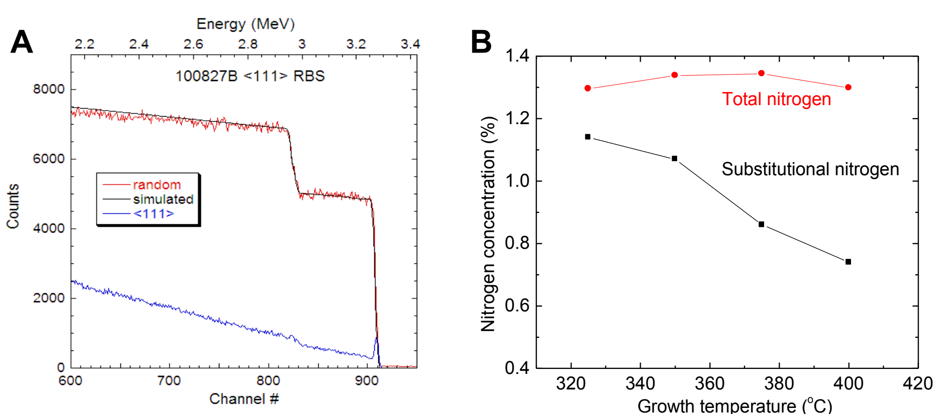

FIGURE 11

RBS measurements of GaNSB film. (A) Representative RBS measurements and simulations of a 100 nm GaNSb film, performed by Dr. Kin Man Yu at Lawrence Berkeley National Laboratory, under both <111> channeling and random sample orientations. (B) Results of NRA-RBS measurements on 100 nm GaNSb layers, grown at differing substrate temperatures.

IV. TECHNOLOGY TRANSFER

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

A. Advanced Microstructure Characterization of HgCdTe

Investigator: Professor David Smith, Arizona State University, Single Investigator Award
Recipients: ARL-SEDD, CERDEC-NVESD, BAE Systems

Professor David Smith is using advanced electron microscopy methods, including high-resolution imaging, nanoprobe spectroscopy, and nanoscale elemental mapping, to study infrared mercury cadmium telluride (HgCdTe) material growth and processing. This project involves a collaboration between Arizona State University, ARL-SEDD, and CERDEC-NVESD wherein the Army researchers are supplying special samples for microanalysis and Professor Smith's characterization results transition to the Army laboratories to refine the growth process. There are two main thrusts in this work, one is the reduction of defects in HdCdTe films grown on silicon based substrates and GaAs substrates. The other involves the evaluation of an alternate detector material, HgCdSe, grown on silicon and GaSb substrates. Results from the collaborative investigation of CdTe/ ZnTe / Si, as an alternative composite substrate for HgCdTe growth from researchers at NVESD, are shown in FIGURE 12.

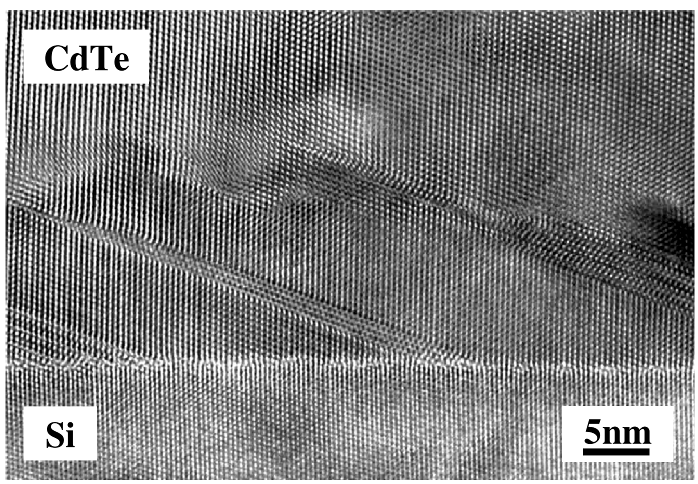

FIGURE 12

Cross-sectional electron micrograph of CdTe(211) / ZnTe / Si(211) heterostructure showing short {111}-type stacking faults that terminate close to substrate surface.

B. Higher-Order Finite-Difference Time-Domain Schemes and Corresponding Boundary Conditions

Investigator: Professor Constantine Balanis, Arizona State University, Single Investigator Award
Recipients: AMRDEC; Naval Air Warfare Center

Professor Balanis is developing advanced methods for finite-difference time-domain computational electromagnetics (EM). The research team has transitioned results to the Army AMRDEC Aviation Applied Technology Directorate at Ft. Eustis, VA and at the Naval Air Warfare Center at Patuxent River, MD, and with researchers from commercial helicopter manufacturers as part of the Advanced Helicopter Electromagnetics Consortium. The goal of this research is to improve the science behind software tools for design and computational modeling of antennas on helicopter platforms. The academic researchers have designed an L-band broadband stacked patch antenna array with hemispherical coverage, and used advanced tools to model the antenna performance on a UH-60 Blackhawk helicopter. The effect of rotor modulation on the communication signal was assessed by performing multiple full-wave simulations with the helicopter rotor blades at a series of static positions (see FIGURE 13). The excellent results from the simulations led to NAWC Pax River testing the antenna performance for potential use with an L-band satellite communications (SATCOM) system.

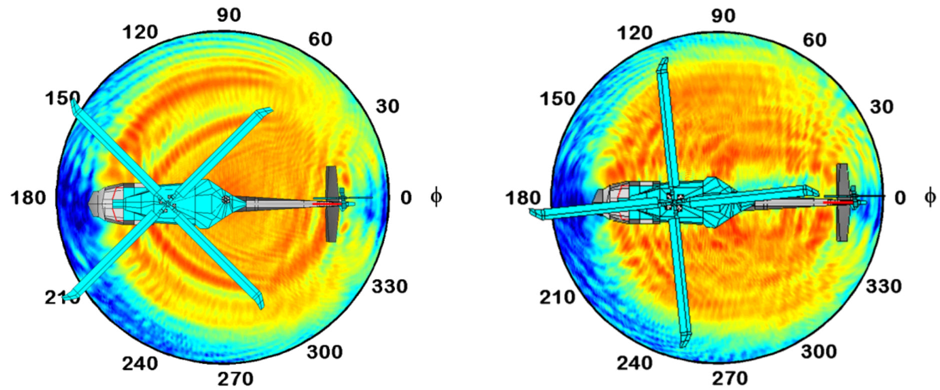

FIGURE 13

Simulated performance of an L-band SATCOM antenna on a UH-60 Blackhawk helicopter. The effect of rotor modulation on the communication signal was assessed by performing multiple full-wave simulations with the helicopter rotor blades at a series of static positions.

C. High-throughput Processing for Hyperspectral Imaging Sensors

Investigator: Physical Sciences, Inc, Phase II SBIR
Recipients: JPEO-CBD; ECBC; U.S. Army NVESD; Smiths Detection, Inc.

Under a Phase II SBIR project, Physical Sciences Inc. (PSI) has developed innovative algorithms, coupled to a high speed signal processor, that enabled the transition of Adaptive Infrared Imaging Spectroradiometer - Wide Area Detector (AIRIS-WAD) hyperspectral standoff chemical agent detection technology to the Joint Program Executive Office for Chemical Biological Defense's (JPEO-CBD) Next Generation Chemical Standoff Detection Program (NGCSD). The algorithms and processor enable the real-time registration of imagery which would otherwise be blurred by vehicle motion. Under this effort, approaches used for the registration of airborne imagery were adapted for use on ground platforms and implemented in post-processing. Evaluation of registration algorithms were performed by mounting the sensor on an SUV and acquiring on-the move-data in field tests against chemical agent simulants for ranges up to 5 km at Dugway Proving Grounds. Algorithms reducing false alarm rates to required levels were also developed and validated. Proof of detection capability has been demonstrated and final algorithms are being implemented in a GP-GPU processor in preparation for real-time testing in the summer of 2011 at Dugway.

PSI has also signed a Joint Development Agreement with Smiths Detection, Inc. (current manufacturer of the Joint Chemical Agent Detector) under which PSI and Smiths will jointly produce and service the sensors under the Smiths name at their Edgewood, MD facility. Under the agreement Smiths has already invested $1.3M in PSI product improvement activities, facilitated by a CRADA between PSI and the U.S. Army Edgewood Chemical Biological Center (ECBC) that allows these improvements to be made on two ECBC-owned sensors. Based on testing conducted at Dugway from 2008 to 2010, the sensor unit is currently assessed at a TRL of 6 for fixed site operation and a TRL of 3 for on-the-move operation. In addition, ARO recently made a new award to PSI supported by funding provided jointly by the U.S. Army Night Vision Electronic Sensors Directorate (NVESD) and the SBIR Commercialization Pilot Program (CPP) to develop a lower cost and higher reliability replacement for the current Integrated Detector Dewar Cooler Assembly (IDDCA) utilized on the AIRIS-WAD sensor, and additionally updates electronics that will reduce electronics costs, achieve required data transfer rates, enable the implementation of a 16 target set algorithm, and address component obsolescence issues. These technology upgrades are needed by the NGCSD program to provide fixed site protection against chemical vapor and aerosol attack for ports, airfields, etc, and on-the-move reconnaissance capability via the Stryker NBCRV. PSI achievements were also recognized by receipt of the 2011 Army SBIR Achievement award for CB Defense.

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. PN Nanojunctions in Compound Semiconductors

Professor Gary Wicks, University of Rochester, Single Investigator Award

The goal of this research project is to test the hypothesis that conventional electronics break down at nano-sizes because the electronic processes become dominated by surface effects rather than the bulk effects seen at micro-scale dimensions. It is well known that the Fermi level is pinned at the surface in semiconductors and this level is independent of the doping (see FIGURE 14). Fermi level pinning at the surface can occur at the conduction band (shown), at the valance band, or in the bandgap. It is possible for a semiconductor to change type at the surface, where a p-type doped semiconductor changes to n-type at the surface. If surface effects dominate at the nanoscale (~30 nm), then nano pn junctions will depend on the Fermi level rather than doping.

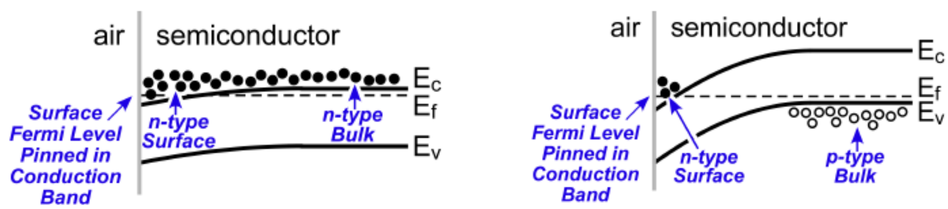

FIGURE 14

Fermi Level Pinning. Left, an n-type doped semiconductor which pins n-type will retain its properties at the surface. Right, a p-type doped semiconductor which pins n-type will have different properties at the surface.

It is anticipated that in FY12 the research team will test this thesis and create nano pn junctions that are based on surface effects. If successful, this development will open the door to a wide collection of nano-devices, such as nano-rectifiers, nano-LED's, nanophotodiodes, nano-bipolar-transistors, and nano-photo-transistors. The particular emphasis in this is antenna-coupled photodiodes. Antenna coupling has shown to enhance the signal of bolometers in the micro regime but it has not been attempted in the nano regime where bolometers are too large and pn junctions do not work.

B. Integrated Analysis of Piezoelectric Resonators as Components of Electronic Systems

Professor Haifeng Zhang, University of North Texas, Single Investigator and DURIP Awards

Professor Zhang is studying quantitative analysis software tools that link materials and advanced design to piezoelectric resonator performance in communication, navigation and surveillance systems. The technical objectives of this work are to integrate existing modeling techniques into a software package that can calculate resonator vibration characteristics important to system performance, extend the present modeling capability to include materials with strong piezoelectric coupling and to include the effects of dynamic accelerations and relatively large accelerations, and measure the third-order material constants and the first-order temperature derivatives of the second-order material constants of langasite (LGS), langanite (LGN), and langatate (LGT), collectively referred to as the LGX family of crystals.

As essential components of military electronics systems, crystal resonators are always in need of improvement with respect to new materials and/or new designs. This research program will combine modeling with experimental research. For the modeling aspect, an integrated design analysis will be performed that links materials, components, and systems. It is anticipated that in FY12, the software analysis package will be capable of calculating the basic vibration characteristics, the frequency-temperature behavior, and the acceleration sensitivity of the resonator given the specific cut of a crystal. When new materials and new resonator designs are considered, the software will allow efficient optimization of resonator design, quick prediction of system behaviors, as well as their implications in system performance. It will make possible rapid benchmarking and early evaluation of system performance. Experimental techniques will include the method of transit time and the method of resonator/capacitor to measure the second- and third-order material constants of common and new resonator crystals and the temperature derivatives of the second-order material constants. These material parameters are needed in the proposed and future resonator analyses. This research may greatly improve the efficiency of the design cycle of military electronic systems.

C. 1.55 micron In(Ga)N Nanowire Lasers on Silicon
Professor Zetian Mi, McGill University, STIR Award

The goal of this project is to build on prior groundbreaking work using In(Ga)N in the visible region to make high-efficiency light emitters for solid state lighting. Professor Mi is is attempting to expand the new epitaxial growth technique into the short-wave infrared (SWIR) to make 1.55 micron lasers on a silicon substrate for use in silicon photonics, i.e. for potential integration with silicon integrated circuits. Although a number of groups have demonstrated III-V lasers on silicon, none have proven reliable enough to push to high technology readiness levels. Nanowire lasers have this potential because their growth is substrate invariant. In other words, perfect crystalline quality can be obtained without lattice matching. Professor Mi has already demonstrated InN nanowires with perfect crystalline quality, and by coupling with his prior In(Ga)N doping and heterostructuring techniques within the nanowires, lasers become possible. It is anticipated that this result will contribute to a true breakthrough in silicon-based lasers. Another important factor though to make the lasers compatible with growth-temperature limitations (*e.g.*, for silicon CMOS production). The anticipated growth temperatures of molecular beam epitaxy grown nanowires are in the 500-600 °C rangem which may be possible to incorporate with CMOS (although the target temperature would be around 400 °C) with careful processing studies.

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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 2011* is to provide information on the programs and basic research efforts supported by ARO in FY11, 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 FY11.

A. Scientific Objectives

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

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

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

B. Program Areas

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

Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY11, the Division managed research efforts within these three Program Areas: (i) Atmospheric Science, (ii) Terrestrial Sciences, and (iii) Habitation Science. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

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

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

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

C. Research Investment

The total funds managed by the ARO Environmental Sciences Division for FY11 were \$14.8 million. These funds were provided by multiple sources and applied to a variety of Program Areas, as described here.

The FY11 ARO core (BH57) program funding allotment for this Division was \$2.8 million. 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 \$9.3 million provided by the Defense Advanced Research projects Agency (DARPA). The Small Business Innovation Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided \$1.0 million for awards in FY11. Finally, \$0.9 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

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

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). 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. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. The 14th International Symposia on Long Range Sound Propagation (Baltimore; 17-18 March 2011). This symposium is held every two years, rotating between U.S. and European locations. This symposium provided researchers with a forum to discuss recent developments in the field. The goals of the symposia are to exchange information on current research, identify areas needing additional work, and coordinate further research activities, including co-operative experimental and modeling efforts. Presentations included ongoing work on infrasound for monitoring, wind noise suppression and impulsive source propagation. Approximately 50 participants from academia and federal agencies attended.

2. The 9th International Conference on Military Geosciences: Desert Warfare - Past Lessons - Modern Challenges (Las Vegas, Nevada; 20-24 June 2011). The overarching theme of this 2011 meeting in Las Vegas was the role of deserts in past and modern warfare, issues with management of military lands in desert regions, and how desert environmental conditions can impact military equipment and personnel. Topics and areas of specific interest included geospatial intelligence, historical military geography and military cartography, and situational awareness in the battlespace.

3. Workshop for Developing Standardized Design and Testing Procedures for Benchmarking Bio-electrochemical System Advancements (State College, PA; 14-15 September 2011). This workshop, sponsored jointly by ARO and the USACE, brought together experts in microbial fuel cells to focus on developing standardized testing protocols to enable proper benchmarking of advancements in bio-electrochemical systems. There has been considerable research on this technology over the past decade, with each research group having their preferred designs, media, enrichment strategies, and performance evaluations. The lack of standardized protocols resulted in an accumulation of published data that do not allow for direct comparison; therefore, an emphasis of this workshop was the development of standardized testing protocols.

C. Multidisciplinary University Research Initiative (MURI)

No projects were active in FY11.

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

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as was discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Real-Time Chemometrics and Sensor-Fusion (RT-CSF) Technology. A Phase II SBIR contract was awarded to ChemImage, Inc. to develop a means of combining spectroscopic data information from LIBS and Raman to enhance the individual performance of these two sensor technologies in the difficult problem of remote detection of explosives. Specifically, the effort is addressing the problem of fusing LIBS and Raman sensor data using a combination of chemometric and advanced multivariate statistical analysis-based spectral signal processing techniques. A prototype system is being developed that operates in real-time that allow testing of algorithm performance in limited field testing. Embedded processors or other hardware acceleration will be used to offer near real-time operation. Under a FY11 SBIR Program Commercialization Pilot Program award, ChemImage is bringing this sensor system to the point where it is ready for commercialization and conducting the necessary field tests to demonstrate environmental operability.

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

No new starts were initiated in FY11.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) – 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). The FY11 new starts within these programs are described here, while the missions of each of these programs were described *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Core HBCU/MI: High-Sensitivity MEMS Biosensor for Monitoring Water Toxicity. A new Core HBCU/MI award was granted to Professor Ioana Voiculescu at the City College of New York to characterize endothelial cell responses to toxicants and to test these as a model system for a field-portable toxicity device that is highly sensitive to toxicants in water. The approach is to develop a system with a biosensor that will record impedance and resonant frequency measurements from endothelial cells after toxicant exposure and will give information about the cells shape, growth and viability, and an integrated micro-incubator for the culture of endothelial cells equipped with an automated media delivery system. The development of a toxicity sensor that can rapidly detect a wide variety of contaminants would be a critical new capability for the Army.

2. PIRT: Lower Atmospheric Research Using Lidar Remote Sensing. This five-year PIRT project was awarded in FY11 to a team led by Professor Michael McCormick of Hampton University. The goal of this project is to expand the LIDAR research capabilities.

This research project focuses on i) data assimilation and integration of elastic lidar measurements of clouds and clear-sky scenes, ii) empirically-derived cloud lidar ratios that reduce errors and reliance on modeling through a fractal-based analysis to calculate and study the fractal dimensions of the planetary boundary layer and compare them with aerosol physical properties, and iii) synthesis of higher-level data products. This research is directly relevant to the DoD's objective to develop LIDAR-based measurement capabilities for environmental monitoring. Routine retrievals of temperature and water vapor concentrations can assist in regional weather forecasting and visibility assessment over a future battlefield.

3. DoD TCU Instrumentation Awards. As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the TCU program aims to enhance science, mathematics, and/or engineering education programs and/or research capabilities through the acquisition of equipment and/or instrumentation that will augment existing facilities, enhance curricula, or help develop new laboratories, programs, and capabilities in these areas. In FY11, the Environmental Sciences Division managed two new TCU projects. The equipment purchased with these awards is promoting education and research in areas of interest to ARO, including efforts to inventory natural resources, water quality, the flora, and fauna of targeted environments, and to provide instruction of engineering technology associated with renewable resource use, specifically wind farm development.

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

No new starts were initiated in FY11.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY11, the Environmental Sciences Division managed four new DURIP projects, totaling $0.6 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies to explore including studies to explore fluvial processes, improved infrastructure design, maintenance and protection and behavior of micro/nano-particles in the terrestrial environment.

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

The ARO Environmental Sciences Division is serving as agent for the DARPA MANTRA program. The goal of this program is to demonstrate a prototype seawater desalination system that produces high rates of potable water from seawater while achieving two orders of magnitude reduction in size and weight and one order of magnitude reduction in power compared to existing systems. The research efforts supported through this program are investigating and designing large-area membranes with substantially reduced defects for improved fluid transport by increasing the use of CNTs or other gatekeeper molecules in the membrane, while preserving the salt rejection at 98%. However, research pursuing evolutionary improvements to the existing state of practice for the rapid development of more advanced membrane concepts is excluded. This program moved into its second phase during FY11.

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

The goal of this Congressionally-mandated project is to explore military testing and training in support of the Army Yuma Proving Ground Natural Environments Test Office. Five distinct research efforts are being pursued: (i) Multiple Master Environmental Reference Sites (MERS) for comprehensive characterization of soil processes will be established at sites that represent prevalent terrain conditions critical for military operations and testing (*i.e.*, different military operating environments; MOE), (ii) data analysis of the established MERS will be initiated to evaluate the temporal dynamics of energy fluxes under both natural and disturbed conditions in different climatic regimes, (iii) techniques and methods will of incorporating data on soil and soil surface processes and conditions in the development and testing of technologies for the detection and defeat of IEDs will be studied and a set of recommended approaches developed, (iv) terrain conditions at primary testing and training installations will be characterized to determine terrain analogs for areas of current and future strategic interest, and (v) a military environments reference database will be created that compiles soil and terrain data and related literature to increase availability of global terrain data to the testing and training community. The research proposed is directly relevant to the Army's test and evaluation mission and has extremely high relevance to Army requirements gaps and material technical shortcomings. Providing better insight and understanding of actual military operating environments worldwide to the Army test community will lead to improvements in test procedures and methodologies for Army materiel and systems and aid in improving the performance of sensors and multi-sensor systems used for explosives detection.

K. Multi-Sensor Detection of Obscured and Buried Objects Program

This program is sponsored by CERDEC-NVESD, Countermine Division and the goal is to develop new algorithmic approaches for detecting obscured and buried objects using multi-sensor systems. The research will primarily explore systems that use some combination of Ground Penetrating Radars (GPR), Electro-Magnetic Induction (EMI) sensors, and Electro-Optical (EO) Systems, including broad-band cameras, as well as multi- and hyper-spectral imaging systems. A broad program of signal processing research that focuses on the development and enhancement of feature-extraction and classification algorithms will be pursued. In the area of GPR, the effort will investigate, develop, and test Hidden Markov Model discrimination algorithms based on Gabor features. The utility of using differential data-driven and model-based techniques to process Argand diagrams of wideband EMI systems will be investigated. The use of a random set method for providing context-based cueing from an airborne multi- or hyper-spectral system to a ground-based GPR or GPR/EMI system will be explored. The use of Bayesian methods for combining multiple experts as a means of accommodating strengths and weaknesses of different sensors will be studied. Finally, modeling class preference relations for rank-based fusion will be investigated. The work to be undertaken is highly relevant to current Army countermine and explosive object detection programs at CERDEC-NVESD, all of which have a critical need for advanced signal processing algorithms.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. Turbulence Fine Structure, Intermittency, and Large-Scale Interactions in the Stable Boundary Layer and Residual Layer: Correlative High-Resolution Measurements and Direct Numerical Solutions

Dr. David Fritts, Northwest Research Associates Inc., Single Investigator Award

The objective of this project is to perform a correlative and highly integrated study addressing the sources, scales, intensities, and intermittency of turbulence in the stable nocturnal boundary layer (SBL) and the residual layer (RL). Ongoing efforts merge state-of-the-art measurement and direct numerical simulation (DNS) capabilities, with DNS guiding and being guided by previous and anticipated SBL and RL measurements. Using instrumentation enhancements, the research team significantly improved the measurement capabilities of the airborne platform, to provide: improved altitude stability, greatly improved roll stability, careful temperature calibration (thermistor and cold wire), humidity sensing, completely autonomous operation, launch to landing, broadband (cold-wire) turbulence measurement capability, extended-range telemetry capability, development of a triple failsafe abort capability for flight safety, and balloon-launch capability for higher-altitude studies. A recent field campaign in Paracas, Peru provided a rich dataset for analysis (see FIGURE 1).

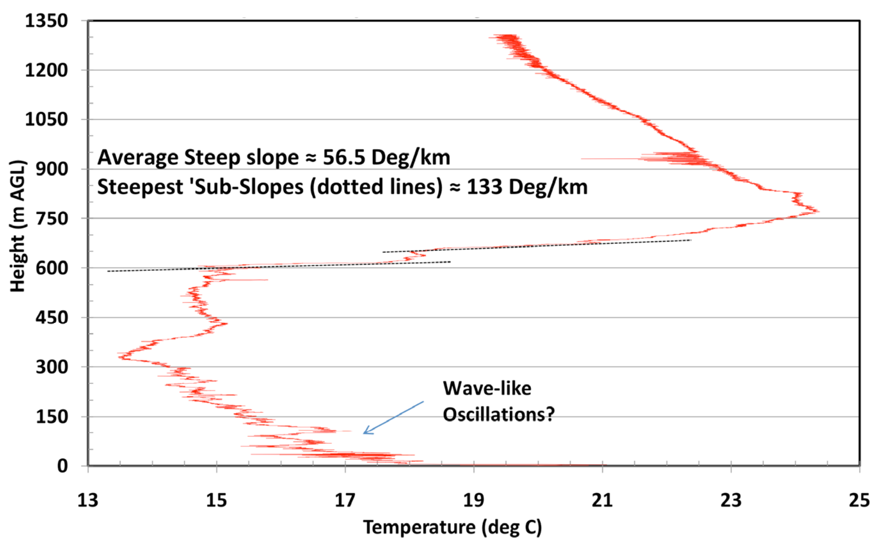

FIGURE 1

Experimentally measured temperature profile over Paracas, Peru: High-resolution temperature profile showing a strong inversion and significant small-scale structures from 0 to ~ 1300 m. The sample temperature measurements were taken from the automated DataHawk vehicle.

The investigator's modeling studies were found to complement the experimental observations. A suite of DNS of multi-scale interactions that we believe illustrate a range of SBL dynamics containing residual fine structure (FS) in the wind field due to previous mixing events and larger-scale gravity waves (GWs) which interact and mutually deform each other. The effect of shear on GWs has been a major undertaking for the research team (see FIGURE 2).

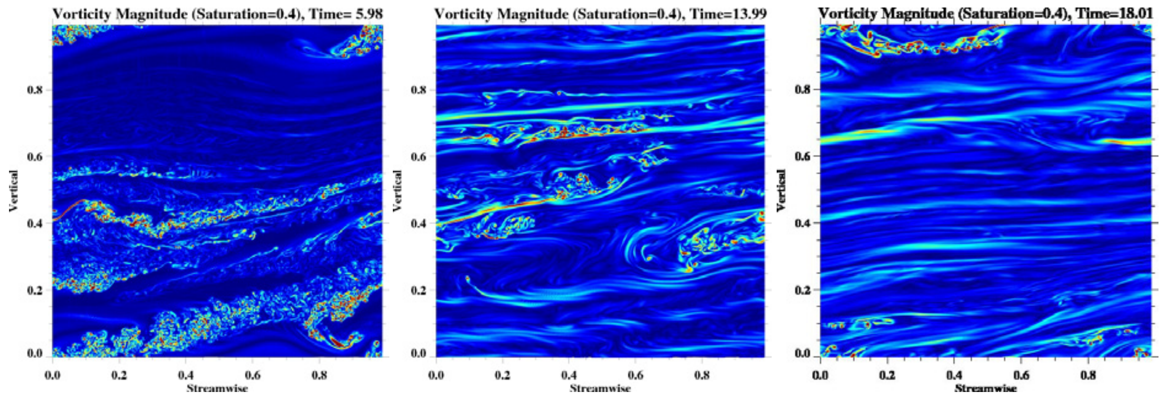

FIGURE 2

Streamwise-vertical vorticity cross sections of DNS. (x,z) cross sections of vorticity magnitude through the center of the computational domain at t = 6, 14, and 18 *Tb*. Vorticity is saturated at 40% of the maximum value, the domain is inclined along the GW phase, and group velocity is to the left (slightly above horizontal).

B. Autonomous Mini-Glider for Sampling Small-Scale Atmospheric Structure in the Atmospheric Boundary Layer

Professor Ben Balsley, University of Colorado, STIR Award

The goal of this previously-completed research project was to develop a simple, inexpensive method for obtaining very high vertical resolution *in situ* atmospheric measurements from ground to above 3 km. The method consisted of constructing a slow-descent-rate, GPS-controlled, pre-programmed, mini-glider. This glider system evolved into a remote-controlled motorized aerial vehicle capable of obtaining real-time temperature, humidity, pressure, and high-resolution turbulence measurements using cold-wire probes. Relative to a conventional radiosonde balloon system, the technique provides: (i) 10-100 times improved vertical-resolution needed for direct comparison with emerging high-resolution models of breaking atmospheric gravity waves and turbulence generation, (ii) unique information on atmospheric gravity wave structure (wave-front direction, slope, and width), and (iii) true vertical profiles in contrast to conventional systems, where the balloon is carried many km downwind by the wind. These gliders can be constructed for approximately $1,000 and provide a low-cost means of obtaining *in situ* data for incorporation into atmospheric models (see FIGURE 3).

FIGURE 3

DataHawk glider with Dr. Dale Lawrence. The DataHawk is capable of providing real-time in situ measurements of the atmosphere. The glider can be launched on the ground or by balloon for high-altitude measurements.

Field tests were recently completed at Dugway Proving Grounds, Utah, Smoky Hill, Kansas, and in Paracas, Peru. Surprisingly, the DataHawk provided data that does not conform well with current theory. Circular flight paths measured using GPS at approximately 100m heights were found to have an anomalous feature at the location of a ~1 m gully (see FIGURE 4A-B). This anomaly is apparently the result of a gravity wave extending much higher than expected. This feature is confirmed in temperature measurements (FIGURE 4C).

FIGURE 4

Flight paths and measurements reveal that gravity waves extend much higher than models predict. (**A**) The flight path of the DataHawk determined with GPS. (**B**) The presence of a gully is visible in Google Earth images. (**C**) An enhanced temperature upsurge is measured.

This accomplishment contrasts with, but is complementary to, the research performed by Dr. David Fritts, Northwest Research Associates. The research by Dr. Fritts aimed to characterize the tendency for instability in multi-scale NBL flows, to understand of instability dynamics driving large and small scale turbulence, including external atmospheric gravity waves, to understand the missing and transport mechanism in the NBL, to test theoretical predictions for scaling parameters in stratified atmospheric turbulence, and guide improvement of parameterizations of these processes in larger scale models. The research led by Professor Ben Balsley led to the development of tools for the directed measurements of wind, temperature, pressure, and moisture at high vertical resolution through the atmospheric boundary, which subsequently resulted in the Dr. Fritts success when these research tools were applied.

C. Using Maximum Entropy Principle as a Unifying Theory for Characterization and Sampling of Multi-Scaling Processes in Hydrometeorology

Professor Rafael Bras, Georgia Institute of Technology, Single Investigator Award

This project is exploring the idea that the concept of maximum entropy (MaxEnt) can be utilized as a unifying principle to characterize and understand multi-scaling behavior in hydrometeorology o characterize multi-scaling parameters such as rainfall and soil moisture. Two important scientific questions are being addressed: (i) Can known multi-scaling laws can be derived from the MaxEnt theory and (ii) how does MaxEnt help in designing a network for sampling multi-scaling processes. The ultimate goal of the research is to develop an effective first-principle-based sampling scheme of environmental conditions (*e.g.*, rainfall, soil moisture and topography) to meet the demands of Army operations.

In FY11, building on previous research, the project focused on deriving the maximum entropy (MaxEnt) distributions of Type I and II multi-scaling processes (*i.e.*, self-similar process with constant parameters and multi-fractal processes with variable parameters, respectively) to establish the links between the multi-scaling distributions and the aggregated properties of the corresponding field variables and on developing a model of evapotranspiration over the land surfaces using the Principle of Maximum Entropy Production (MEP). Following the MaxEnt formalism, the probability distribution of a Type I multi-scaling process has been derived under the constraints of given multi-scaling moments and geometric mean of the incremental process. The MaxEnt distributions have been validated against empirical histograms of soil moisture and topographic fields (see FIGURE 5). Derivation and validation of MaxEnt distributions also have been derived and validated for Type II multi-scaling processes, where the parameters are described by probability distributions has also been derived, where an additional constraint of multi-fractal condition to those of multi-scaling moments and geometric mean was imposed.

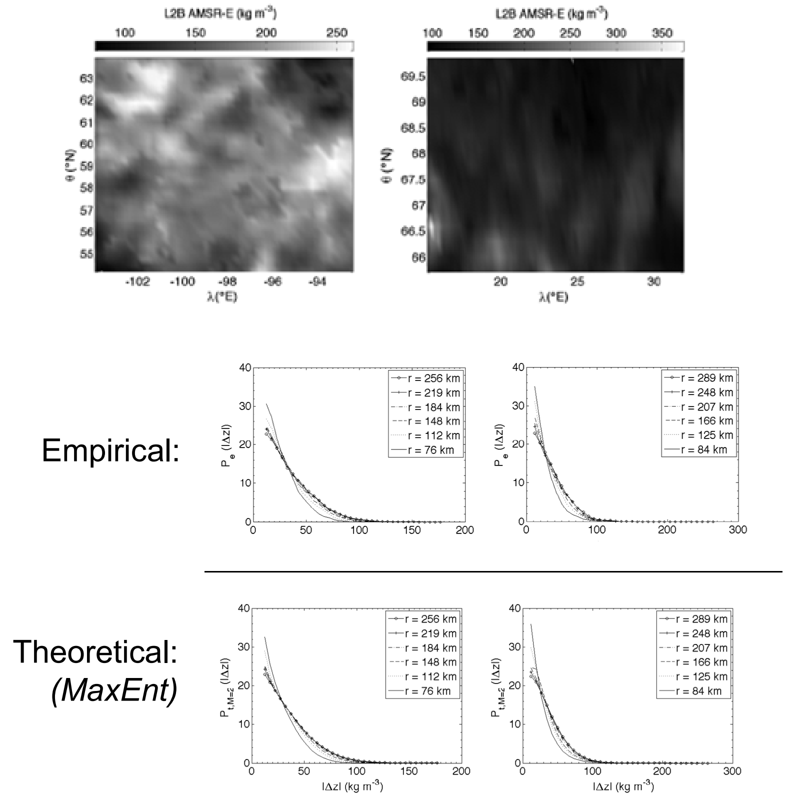

FIGURE 5

Validation of MaxEnt theory through AMSR-E soil moisture measurement. The top panels display soil moisture maps (38-km resolution) for October 2009, and bottom panels display the probability distributions of incremental soil moisture fields at various separation distances.

D. Optical Information for Tactical Tracking and Its Training
Professor James Staszewski, Carnegie Mellon University, Single Investigator Award

This research brings together two disparate disciplines - human cognition and optical remote sensing - to create new fundamental knowledge and understanding about how optically-available terrestrial information is perceived and used by human experts in tactical tracking. The ultimate goal of the effort is to quantify, systematize, and ultimately augment and partially automate the tracking of small-scale human movement within deserts and other poorly vegetated, environments. The effort aims to describe in detail, both qualitatively as well as quantitatively, the optical information resulting from disturbance of ground by human movement and the manner in which information capable of supporting tracking changes as a function of time and exposure to the natural environment. The investigation focuses explicitly on problems and contexts that have immediate implications for application. The physical and mineralogical effects of disturbance, both immediate effects and the aging of these effects, were characterized. The extent of photometric techniques, such as enhanced backscatter and polarization over visible through shortwave infrared wavelengths, were investigated and thermal and reflected illumination techniques were used to examine and quantify surface roughness. The investigator is using these data to understand the selective perception and use of available information by an individual who is an expert tracker and trainer of trackers.

E. Model Reduction in Groundwater Modeling
Professor William W.-G. Yeh, University of California at Los Angeles, Single Investigator Award

Simulation models are used as tools for decision making in environmental cleanup and water resources planning. The complex simulation models currently in use are computationally expensive, particularly if they have to be repeatedly called during a model simulation run. The computational demand can be reduced by approximating the full model with a reduced model that captures the physics and the dominant variance of the full model, but runs considerably faster than the full model. Proper Orthogonal Decomposition (POD) is an efficient model reduction technique based on the projection of the original model onto a subspace generated by full-model snapshots. This project will develop a methodology that can be used to select the optimal temporal model simulation snapshots. The selection criterion is the maximization the minimum eigenvalue of the snapshot covariance matrix. The reduced model can also be used for parameter estimation. The inverse algorithm combines POD with quasilinearization and quadratic programming. In this application, POD is used to reduce the size of the linearized model, thereby considerably reducing the computational burden of solving the associated quadratic programming problems.

In FY11, research to select the optimal snapshot selection criterion for model reduction on a one-dimensional test problem was validated. The selection strategy can then be employed to determine the optimal snapshot set for a unit, dimensionless model, with the resulting snapshot set then translated to any complex, real-world model based on a simple, approximate relationship between dimensionless and real-world times. The model reduction methodology developed was to a real-world problem in which the full model was reduced from a system of more than 222,000 to 10 ordinary differential equations. The results show that that the reduced model runs 1000 times faster than the full model. The POD approach was then applied to a real-world parameter-estimation problem after testing the inverse algorithm that integrates POD, quasilinearization, and quadratic programming on a 1D aquifer system. Subsequent application to a 2D version of a real-world model with about 30,000 computation nodes where as many as 15 zones of hydraulic conductivity were estimated correctly.

F. User-Generated Terrain Information

Professor M. Goodchild, University of California at Santa Barbara, Single Investigator Award

Research being conducted by Professor M. Goodchild at the University of California at Santa Barbara is seeking to understand the role of crowd-sourcing in the creation and maintenance of terrain information. This research is evaluating the role of social networks in engaging and facilitating observers, examining the integration of information acquired from disparate sources that include both experts and non-experts, and assessing data quality and assurance. To date, research methods have been developed for the synthesis and analysis of disparate crowd-sourced information from diverse sources and with variable quality.

Geographic information created by amateur citizens is often known as volunteered geographic information (VGI). A model has been created of the process of acquisition of geographic information that explains the advantages of VGI over traditional methods. Also, methods were developed for the analysis of VGI in text form, culled from narrative sources. Methods of analysis were developed for measuring and improving data quality based on concepts of horizontal and vertical context (see FIGURE 6).

Wikipedia entry on UC-Santa Barbara: 135 authors,
719 revisions, signature distance = 533 km.

Locations of individuals who either contributed to or edited the Wikipedia entry on UC-Santa Barbara.

Frequency of contributions and edits versus distance between a Wikipedia article subject and its contributors

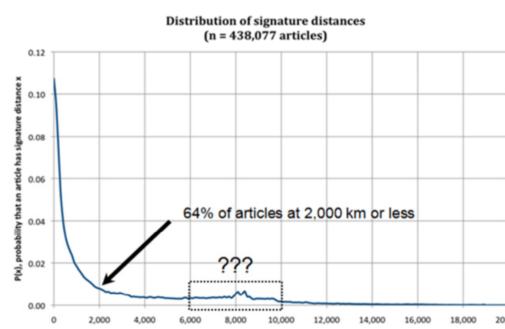

FIGURE 6

Analysis of spatial interaction models that account for the non-uniform distribution of people. The analysis of VGI revealed that the curve is a mixture of (i) a distance-based negative-exponential decay and (ii) a uniform distribution that reflects the irrelevance of distance in the virtual world.

G. Accounting for Hydrologic State in Ground-Penetrating Radar Classification Systems

Professor Stephen Moysey, Clemson University, Single Investigator Award

Professor Moysey of Clemson University is undertaking a fundamental study aimed at understanding the how water in the near-surface environment affects the performance of ground penetrating radar. The objective is to evaluate the hypothesis that shifts in GPR signatures occurring as a result of changes in environmental conditions can be predicted using hydrologic models and integrated into decision systems to improve detection of targets and assessment of environmental risk. During the past year, a laboratory study conducted in tanks packed with soils and using automated GPR data collection systems evaluated the radar signatures of target and clutter objects in heterogeneous media during successive water infiltration events. Computationalmodeling research is exploring neural network analysis as an approach to normalizing GPR signals to a hydrologic "reference" state that is independent of site conditions, thereby making current classification methods more general in character.

IV. TECHNOLOGY TRANSFER

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

A. Improved Measurement System for Atmospheric Studies

Investigator: Yannick Meillier, University of Colorado, Single Investigator and DURIP Awards
Recipient: ARL-CISD (Battlefield Environment Division)

The objective of the research project led by Professor Meillier, which led to a notable FY11 transition, is to construct basic meteorological system for temperature , humidity, position and data acquisition to examine high resolution, in situ, vertical profiles of turbulence, temperature, wind and humidity in nocturnal atmospheric boundary layers. In FY11, Professor Meillier of the University of Colorado began transferring a Tethered Lifting System (TLS) with sensors and high-wind blimps to ARL-CISD researchers in addition to training in its use. The TLS consists of an aerodynamic blimp with a suspended line of multiple sensors to make measurements at either fixed altitudes or by profiling from the ground up to many kilometers altitude. Each of the multiple sensors consists of low-frequency temperature, velocity, pressure and humidity sensors, in addition to newly available low-noise high frequency hot-wire and cold-wire sensors for fine-scale measurements in the challenging low turbulence conditions of the night time boundary layer. Low-frequency information from the TLS is transmitted to a ground station for real-time input into measurement planning as well as hazard avoidance. The high wind blimp will permit observations for wind energy research and turbulence studies. Recipients of the TLS and training are turbulence researchers ARL-CISD Battlefield Environment Division. The researchers will use the system to make atmospheric observations for input in turbulence models.

B. Determination of soil water content at intermediate spatial scale using cosmic-ray neutrons

Investigator: Marek Zreda, University of Arizona, Single Investigator Award
Recipient: USACE

Under joint ARO and NSF basic research support, Dr. M. Zreda of the University of Arizona and his former doctoral student D. Desilet, developed a novel method to quantitatively determine soil moisture passively and non-invasively at a horizontal scale of half a kilometer averaged over depths of 15-70 centimeters based upon measurement of cosmic-ray neutron flux above the ground surface. Low-energy cosmic rays constantly bombard the planet and travel into the soil, where they are moderated and then emitted from the soil back into the atmosphere. A sensor is elevated above the ground and measures the low-energy neutrons emitted from the soil, whose intensity is inversely proportional to water content. The COSMOS technology, which is presently being commercialized, can be deployed at a site for continuous soil moisture monitoring at a fixed site or be operated from a vehicle for large area measurement.

C. Geo-Spatial Enabled Dynamic Network Analysis

Investigator: Professor Kathleen Carley, Carnegie Mellon University, Single Investigator Award
Recipient: USACE

As highlighted in a recent radio announcement on National Public Radio on 10 December 2010, military commanders in are turning to the use of social network analysis to identify the key players in the groups responsible for the omnipresent hazard of improvised explosive devices. The underlying idea is that an IED is seldom the work of a single individual, but rather takes a network to build the devise, undertake the site surveillance, and emplace the device. At the Counter-IED Operations Intelligence Center in Baghdad, Major Ian McCulloh, a former PhD student of ARO Terrestrial Sciences program is using the 'Organizational Rank Analyzer' (ORA) to attack the IED network. ORA links geospatial and network analytics to identify key actors based on movement and asses shifts of groups in different geographic regions thus providing critical information for planning facilitating tactical missions. This tool was developed at the Carnegie Mellon University

Computational Analysis of Social and Organizational Systems (CASOS). Professor Carley has trained a number of government groups in how to use ORA and the new geo-spatial network tools that are now incorporated into ORA. In FY11, this transition continued as a one-week class in "Advanced Network Analysis and Targeting" was presented at Ft. Bragg to a group of soldiers departing for Iraq.

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. Workshop: Weather in Mountainous Terrain

Professor Harindra Fernando, University of Notre Dame, Conference Award

The atmospheric effects resulting from complex terrain are highly variable and unpredictable. They also have great consequence. A major part of the Earth's land surface is covered by complex topography, and it drastically affects the weather as well as related quality-of-life issues such as air pollution, energy production, transportation and security. Air flow over terrain begets a host of important phenomena, for example, inertio-gravity waves, wind gusts, canyon flows, Venturi effects, stagnation, rotors, cold air pooling, up/down drafts, slope and cross flows, fog, snow/ice, convective clouds and lightning. As such, the weather in mountainous areas is highly variable and unpredictable. In the context of security, many areas of current U.S. engagement are located in complex terrain, as well as the U.S.-Mexican border, and the aerial platforms used for surveillance, reconnaissance and combat are highly weather sensitive. In addition, dispersion of contaminants and obscurants on the ground has far reaching health and security implications. The results of these campaigns will have a major impact on the way the weather will be modeled in these difficult regions and it is anticipated these will drive the development of a new generation of weather models.

B. Physics-Based Modeling of Bridge Foundation Scour: Numerical Simulations and Experiments

Professor Panos Diplas, Virginia Polytechnic Institute & State University, Single Investigator Award

Hydrological research being led by Virginia Tech, the St. Anthony Falls Laboratory of the University of Minnesota, and the USACE-ERDC Waterways Experiment Station, and that is jointly but independently funded by ARO and the NSF Hydrologic Sciences Program, continues to develop and validate the first 3-D, unsteady state numerical model capable of accurately producing bridge foundation scour. The aim of the work is to integrate the latest developments in the numerical modeling capable of resolving 3-D coherent hydrodynamic structures of turbulent juncture flows with state-of-the art laboratory experimentation in which simultaneous measurements are made of instantaneous flow quantities and pressures within the progressive spatial and temporal development of a scour hole. Other fluvial hydrologic research will examine turbulent flow and sediment transport in meandering rivers and in rivers near dike structures of various geometries through an integrated program of laboratory experiments, numerical modeling, and field application. The result will be a feasible design of dike structures that can effectively reduce sediment deposition and maintain a favorable flow condition during winter low flows in the island. In addition, research at the Colorado School of Mines will be completed that is aimed at understanding of the non-isothermal, multi-phase flow processes of water, water vapor and air in the shallow subsurface, the research program will test the hypothesis that the differences in local hydrological/geohydrological conditions and thermal properties of target objects result in a distinct difference or evolution in water saturation or temperature in the direct vicinity of the target object, under different environmental conditions. A variety of different controlled laboratory experiments will be conducted under transient conditions using soil columns and tanks with accurately known hydraulic/thermal properties. The experimental data will be used to test existing theories and appropriate numerical models, providing new insights into mass flux and thermal process interactions. Also, concurrent hydrological research at Clemson University is evaluating the hypothesis that shifts in the signatures obtained by ground penetrating radar that occur as a consequence of changes in environmental conditions can be predicted using hydrologic models. This problem will be investigated by performing a series of sand-box experiments designed to simulate a variety of common hydrologic scenarios. If validated, the effort will integrate this new knowledge into decision systems to improve detection of buried targets and the assessment of environmental risk.

C. Whole-cell Modeling and Integrated Experimentation of Bioelectrochemical Systems
Professor John Regan, Pennsylvania State University, Single Investigator Award

Progress in the field of bioelectrochemical systems depends on establishing a fundamental research foundation for an experimentally validated whole-cell bioelectrochemical system (BES) model that converges microbial, electrochemical, and transport characterizations. It is anticipated that in FY12, progress will be made in this regard by the examination of how catalyst density in anode and cathode impacts biofilm system performance in a time-varying manner. Once a fundamental examination is complete, researchers can explore how the mechanism of extracellular electron transfer affects biofilm architecture and the maximum power and current densities of mixed cultures, how anode potential can be used to predictably tailor biofilm development and system performance, and how the balance of microbial, physical, and chemical constraints can be fundamentally predicted in different BES configurations.

VI. DIVISION STAFF

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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 2011* is to provide information on the programs and basic research efforts supported by ARO in FY11, 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 FY11.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Life Sciences Division supports research efforts 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 possible non-invasive methods of monitoring cognitive states and processes during normal activity; basic research to understand antimicrobial resistance mechanisms; microbial community interactions including biofilm formation, cell-to-cell communications, population dynamics and host-pathogen/symbiont interactions; studies of organisms that are not culturable; studies of organisms at the single cell or mixed population (*e.g.*, metagenomic) level; studies of organisms that have adapted to grow or survive in extreme environments; identification and characterization of gene function, gene regulation, genetic interactions, gene pathways, gene expression patterns, mitochondrial regulation and biogenesis, nuclear and mitochondrial DNA replication, mutagenesis, oxidative stress, DNA repair, and regeneration; studies in structural biology, protein and nucleic acid structure-function relationships, molecular recognition, signal transduction, cell-cell communication, enzymology, cellular metabolism, and synthetic biology; and research to understand human behavior across different temporal, spatial and social scales. The results of these research efforts will lay a foundation for future scientific breakthroughs and will enable new technologies and opportunities to maintain the technological and military superiority of the U.S. Army.

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

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Life Sciences Division frequently coordinates and leverages efforts within its Program Areas with many other agencies, including the Defense Threat Reduction Agency (DTRA), the Defense Advanced Research Projects Agency (DARPA), the Joint Improvised Explosive Device Defeat Organization (JIEDDO), the Army Natick Soldier Research Development and Engineering Center (NSRDEC), the U.S. Army Corps of Engineers (USACE), the Army Research Institute (ARI), the Army Medical Research and Materiel Command (MRMC), the Center for Disease Control (CDC), the National Institute of Health (NIH), the Intelligence Advanced Research Projects Agency (IARPA), the Department of Homeland Security (DHS), 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 also coordinates efforts with the Materials Science Division to pursue the design and development of new biomaterials. The Life Sciences Division also coordinates extensively with the Mathematical Sciences Division to develop new programs in bioforensics. In addition the Division coordinates with the Materials Science and the Mechanical Sciences Divisions to understand the effects of blast on synapses. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

To meet the long-term program goals described in the previous section, the Life Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY11, the Division managed research efforts within these six Program Areas: (i) Genetics, (ii) Neurosciences, (iii) Cultural and Behavioral Science, (iv) Biochemistry, and (v) Microbiology and Biodegradation, and (vi) Institutional and Organizational Science. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Genetics. The goal of this Program Area is to understand and characterize genes and genetic networks, particularly genetic pathways that affect warfighter performance and survival. This program also emphasizes mitochondrial regulation and biogenesis, nuclear and mitochondrial DNA replication, mutagenesis, oxidative stress, DNA repair, regeneration, mine detection, and biological causes of social instability. Research is expected to lead to new avenues for reducing warfighter mortality and for improving warfighter physical and mental performance. This Program Area is divided into two research Thrusts: (i) Soldier Performance, and (ii) Soldier Protection. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. Research within these Thrusts focuses on human performance and protection under normal conditions and when affected by a variety of stressors that are likely to be encountered in battlefield situations, such as dehydration, heat, cold, sleep deprivation, fatigue, caloric insufficiency, microbial factors, and psychological stress. Potential long-term effects on the Army include improved warfighter performance, the ability to maintain warfighter performance at peak capacity when needed, a reduction in cognitive errors, reduced warfighter mortality, and the ability to heal without scarring and to regenerate missing or damaged limbs or organs as needed.

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

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

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

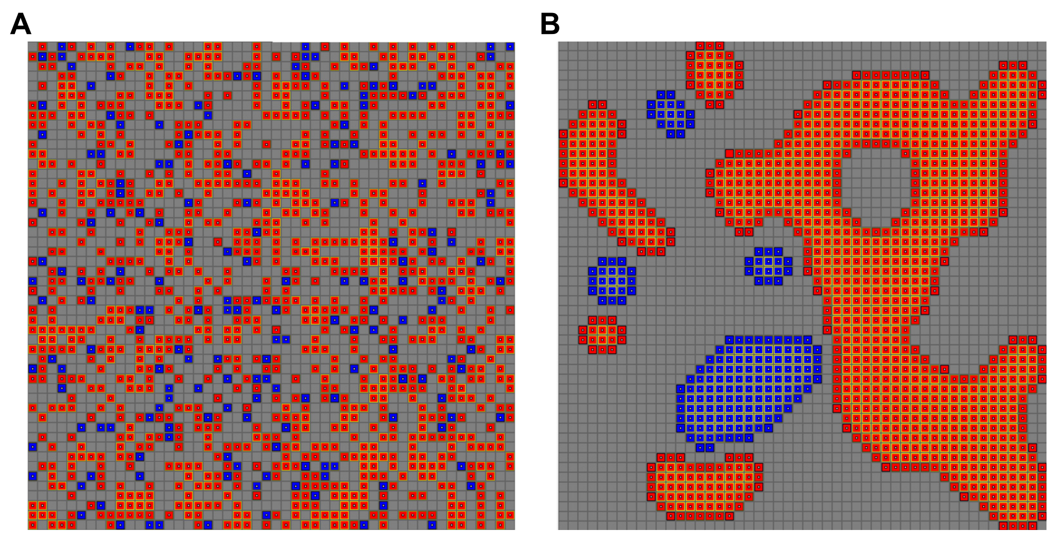


FIGURE 1

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

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

4. Biochemistry. The goal of this Program Area is to elucidate the mechanisms and forces underlying the function and structure of biological molecules. Research in this program may enable the design and development of novel materials, molecular sensors and nanoscale machines that exploit the exceptional capabilities of biomolecules. This Program Area supports two research Thrusts: (i) Biomolecular Recognition and Specificity, and (ii) Biomolecular Assembly and Organization. Within these Thrusts, innovative research efforts are identified and supported in pursuit of the vision of this program. Efforts in the Biomolecular

Recognition and Specificity Thrust aim to understand and control biomolecular activity, to identify the determinants of the specificity of molecular recognition, and to modulate and control this specificity through protein engineering and synthetic biology approaches. Research in the Biomolecular Assembly and Organization Thrust aims to explore the fundamental principles governing biological self-assembly to understand and control the interactions and forces operating at the interface between biological molecules and abiological materials, and to identify innovative approaches for supporting biological activity outside of the cellular environment.

The research efforts supported by this program promote 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.

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

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

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

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

C. Research Investment

The total funds managed by the ARO Life Sciences Division for FY11 were $97.7 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY11 ARO Core (BH57) program funding allotment for this Division was $5.9 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $7.7 million to projects managed by the Division. The Division managed $37.6 million provided by the Defense Advanced Research projects Agency (DARPA), and $22.5 million provided by other agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.2 million for contracts in FY11. The Institute for Collaborative Biotechnologies received $13.1 million in FY11. Finally, $10.2 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

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

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). 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. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. 2011 International Conference on Social Computing, Behavioral-Cultural Modeling, and Prediction (College Park, MD; 29-31 March 2011). Social computing harnesses the power of computational methods to study social behavior and social context. Behavioral-cultural modeling refers to representing behavior in the abstract and is a convenient and powerful way to conduct virtual experiments and scenario planning. Both social computing and behavioral-cultural modeling are techniques designed to achieve a better understanding of complex behaviors, patterns, and associated outcomes of interest. This conference provided an opportunity for behavioral and social science researchers to come together with computational and computer scientists and other related disciplines and seeks to attract researchers, practitioners, program staff from federal agencies and graduate students in disciplines such as sociology, behavioral science, psychology, cultural study, health sciences, economics, computer science, engineering, information systems, physics, and operations research. The conference included invited speakers from government, industry, and academia, research presentations and discussions, poster and paper sessions in addition to focused pre-conference tutorial sessions and post-conference cross-fertilization workshop.

2. 2011 ARO-DTRA Microbial Adaptation Workshop (Alexandria, VA; 27 July 2011). Bacteria adapt to changes in their environment by changing the complement of genes being expressed, and/or by inducing mutational pathways to modify their genetic makeup. In either case, the resulting bacterial cells contain information about the organism's history. ARO and DTRA are funding programs to develop the necessary fundamental scientific principles and approaches to determine factors that are necessary and sufficient to predict how an organism was grown (*e.g.*, *in vitro* vs. *in vivo*, growth media, environmental growth conditions), processed, and where it may have originated with the goal of providing a foundational understanding for a microbial forensics capability. This workshop brought together ARO- and DTRA-funded microbial adaptation researchers who presented recent findings from their projects. Discussions following the presentations generated collaborative and synergistic approaches to understand microbial adaptation, and identified gaps in current research efforts that will guide future research directions.

C. Multidisciplinary University Research Initiative (MURI)

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

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

The long-term goal of this research is to uncover the materials and methods required to establish functional and structural connections between living limb segments and nonliving devices. The MURI team is exploring the interface between living and non-living structures, including bone, skin, muscle and nerve. Setting prosthetic materials research on a firm theoretical foundation, based in physiological interfaces and principles, will enable the current art of anatomical and physiological compensation to be on a scientific rather than an empirical foundation. The research team has already developed a method for directly connecting with peripheral nerves using a soft, electrically conductive scaffold that can be filled with muscle cells to act as targets for propagating axons (see FIGURE 2). As a result of these results, the research has led to a spin-off project currently being considered for separate funding in order to advance the state of knowledge to the point of clinical trials. The ability to design and build intelligent, adaptive, active devices using such engineered biological/non-biological interfaces could ultimately permit a complete return to duty for military personnel with no diminution of ability. In addition, it will produce a body of knowledge enabling the augmentation of limited function to normal or even enhanced levels of performance.

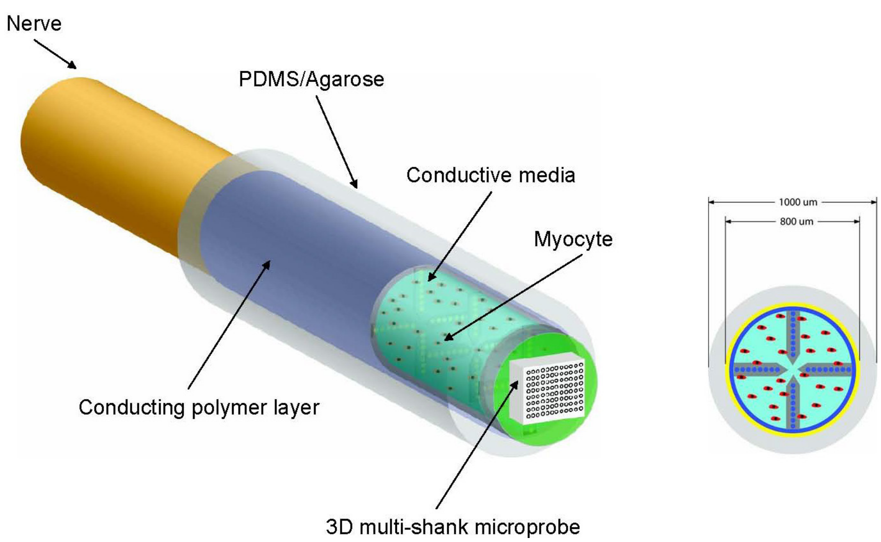


FIGURE 2

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

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

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

Preliminary results from the research teams have revealed that the EEG can be used to detect imagined speech rhythm and that 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 activated as part of motor planning for physical orienting (see FIGURE 3). EEG signals generated during lateralized covert attention resemble strongly those used in conventional BCIs to signal left and right through lateralized motor imagery.

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

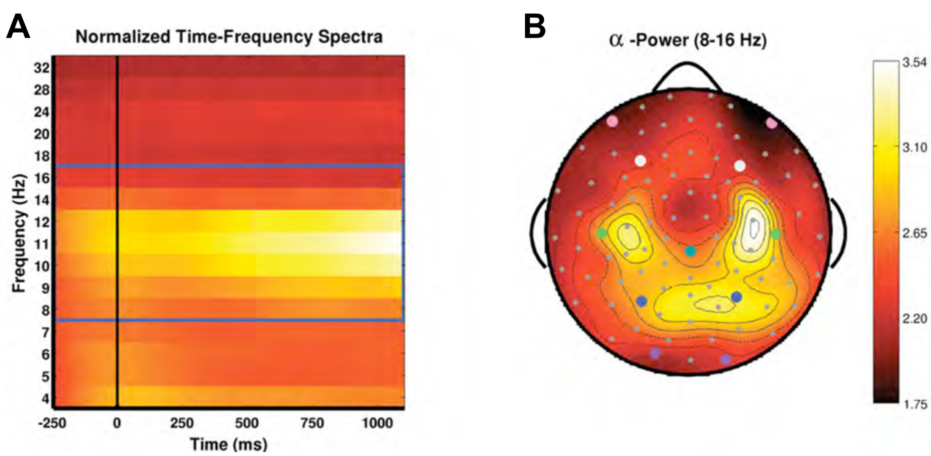


FIGURE 3

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

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

FIGURE 4

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

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

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

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

FIGURE 5

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

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

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

6. Modeling Cultural Factors in Collaboration and Negotiation. This MURI began in FY09 and was awarded to a team led by Professor Katia Sycara at the 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 already made interesting discoveries in these studies, including the observation of certain values called “sacred values” that are considered as essential to the identity of a given social group, thereby leading members of the group to respond defensively when these values are seen to be challenged or threatened. One example of sacred values includes the observation that the Iranian nuclear program is treated as sacred by some Iranians, leading to a greater disapproval of deals that involve monetary incentives. In addition the team is exploring how humiliation may contribute to regulating relationships within Muslim countries. Humiliation seems to result in clashing behavioral tendencies that offer no regulatory strategies. Participants in the study motivated to change the status quo underestimated the extent to which the out-group moralized the domains of harm, care, fairness and justice. Further, participants motivated to maintain the status quo accurately identified that the out-group moralized harm, care, fairness and justice to the same extent that they themselves did. The investigators will replicate these studies in India and Israel/Palestine in the coming year.

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

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

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

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

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

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as was discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Ultrasound for Neuromodulation and Control of Post-trauma Pain. A Phase I SBIR contract was awarded to Synsonix, LLC to demonstrate the feasibility of safely reducing or eliminating the perception of pain through the use of peripheral nervous system ultrasonic modulation of neurons. Pain management has been a significant challenge for military healthcare providers throughout the history of human conflict. Recently, innovative approaches for battlefield anesthesia and analgesia, such as regional anesthesia, total intravenous anesthesia, and novel drugs or drug mixtures have been welcome additions to the existing armamentarium of opioids and general anesthetics. Ideally, pain control would be complete yet the patient's cognitive and perceptive abilities should be maintained. Additionally, analgesics would exhibit a low abuse potential and not require close monitoring that in turn requires committed personnel to be near the bedside/stretcher. Although these goals can be partially met with existing technologies (*e.g.*, regional anesthesia of extremity trauma), there remain many injuries that may not be amenable to these methods. The use of ultrasound as an analgesic tool and neuromodulator may provide a modality for ideal analgesia. It has been known for several decades that tissues and now neurons could be activated or inhibited by sound waves. Recent ultrasound technology has been developed that allows precise delivery of ultrasonic energy through the spine or skull in a manner that could potentially safely be used to modulate neurons. Ultrasound systems are also now sufficiently small to allow use at home or in a field environment by people with minimal medical training. If successful, this research may ultimately result in the development of a prototype system that could be easily used to manage post-trauma pain by a medic or other healthcare provider, even with limited training.

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

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Rugged Automated Training System. Three Phase I STTR contracts were awarded to Barron Associates Inc., Coherent Technical Services Inc., and Strategic Feasibilities Inc. to develop and validate a machine that will reliably train small animals to detect explosives or other compounds of interest, and to provide an objective unbiased measurement of the animal's sensitivity and accuracy. De-mining is often necessary to restore farm land to agricultural use, and to enable societies to economically stabilize after war. Although dogs are the most commonly used animal for mine detection, it has been demonstrated that other animals can reliably smell mines and may have advantages over dogs in some situations. The cost of training animals to detect mines is primarily due to the human labor involved. The investigators are working to design a system to reliably train small animals to detect mines and to objectively evaluate and score their performance. The ultimate goal of this research is to build prototype systems used to train animals to detect mines to restore mined land to civilian use.

2. Rapid Ethnographic Assessment and Data Management Integration Toolkit. Two Phase I STTR contracts were awarded to Charles River Analytics, Inc. and Perceptronics Solutions, Inc. to develop and validate an integrated software tool for the collection, management, analysis, and visualization of ethnographic data in high-risk areas. The collection and analysis of socio-cultural data is becoming increasingly important for the conduct of effective military operations. The production of more scientifically valid models of human behavior has become increasingly dependent on the available forms of socio-cultural data. The ability to rapidly collect social and cultural data in field settings is challenging under most circumstances, and in conflict, denied, or high-risk areas these challenges become even more pronounced. The investigators are attempting to design software that will incorporate a number of ethnographic methods for the rapid collection of cultural, social,and economic data based on structured and semi-structured interviews, qualitative text sources, or unobtrusive observations. If successful, this research may ultimately provide U.S. organizations with an enhanced ability to mine, collect, analyze and manage social media data.

3. High-capacity and Cost-effective Manufacture of Chloroperoxidase. Three Phase I STTR contracts were awarded to Infoscitex, Co., Agave BioSystems, Inc., and IMPACT Technology Development, Inc. to develop a fungal protein expression system with an integrated purification scheme for low-cost production of purified, functional chloroperoxidase in kilogram quantities. Chloroperoxidase (CPO) is an enzyme produced by certain fungal species that catalyzes a diversity of biochemical reactions. For example, the CPO produced by the filamentous fungus *Caldariomyces fumago* catalyzes the non-specific halogenation, including chlorination, bromination and iodation, of electrophilic organic molecules. In the absence of halide, CPO is similar to the cytochrome P450 enzymes in its epoxidation and hydroxylation of olefins and organic sulfides. A CPO recently identified in the fungus Agrocybe aegerita has been shown to carry out both benzylic and aromatic hydroxylation. The versatile catalytic properties of CPO have application in paper bleaching and potential application as active ingredients in cleaning supplies and in detection and inactivation of chemical agents or products on environmental surfaces. These projects aim to develop and validate a fungal expression system and purification scheme to produce milligram quantities of CPO at a purity of 90% or greater, and ultimately to develop a high-capacity cost-effective fungal production system for chloroperoxidase that can support capabilities in enzymatic-based field technologies.

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

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). FY11 new starts within these programs are described here, while the missions of each of these programs were described *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Center of Excellence in Infection Genomics. A REP Center of Excellence award was granted to Professor Bernard Arulanandam at the University of Texas - San Antonio to establish a new research and educational center focused on infection genomics. Beginning in FY11 and funded through FY15, this new center supports research and education in microbiology to determine the biological characteristics and functional properties of infectious organisms, particularly intestinal and respiratory pathogens and fungal infections. This grant will provide exceptional opportunities and commitment to student education and training related to STEM activities of relevance to DoD, directly through participation in DoD-relevant research and indirectly, through increased interest in science and technology and the training of future scientists in these disciplines.

2. Center of Excellence in Renewable Energy. A REP Center of Excellence award was granted to Professor Kai Griebenow at the University of Puerto Rico - Rio Piedras to establish a new research and educational center focused on renewable energy. Beginning in FY11 and funded through FY15, this new center focuses on algae-based biofuels produced from harvested cells using thermochemical and anaerobic digestion processes, and will make use of the climate advantages Puerto Rico offers in growing algae, namely light intensity and marine location. This center will be a major new tool for teaching both undergraduate and graduate students in STEM fields and will provide a vehicle to accelerate the training of a competent workforce required by this new high-technology industry.

3. DoD REP Awards. As described in more detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, REP awards aim to enhance or increase the programs, capabilities, and graduates in scientific and engineering disciplines in universities serving underrepresented minorities. In FY11, the Life Sciences Division managed seven new REP projects (including two centers of excellence), totaling $9.9 million. The equipment purchased with these awards is promoting education and research in areas of interest to ARO, such as studies to assess integrated wastewater treatment and algal growth process as a means for both wastewater remediation and production of value-added products, and to determine the molecular mechanism of action for anti-inflammatory proteins using biochemical and structural biology approaches.

4. DoD TCU Instrumentation Awards. As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the TCU program aims to enhance science, mathematics, and/or engineering education programs and/or research capabilities through the acquisition of equipment and/or instrumentation that will augment existing facilities, enhance curricula, or help develop new laboratories, programs, and capabilities in these areas. In FY11, the Life Sciences Division managed two new TCU projects. The equipment purchased with these awards is promoting research in areas of interest to ARO, including the use of motion capture system for studies in animation, simulation, virtual reality, biomechanics, computer science and engineering.

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

1. Nanofluidic Analysis of Protein Transport, Adsorption and Kinetics. The objective of this PECASE, led by Professor Sumita Pennathur at the University of California - Santa Barbara is to investigate protein behavior and interactions in confined channels.

The unique physics and phenomena afforded by nanochannels enable novel fundamental studies of biomolecules that cannot otherwise be achieved. Nanofluidics has the potential to analyze, separate, concentrate, manipulate and detect biomolecules with superior sensitivity, throughput, and ease relative to conventional methods. Professor Pennathur is investigating and determining the behavior and interactions of proteins in confined nanochannels, which may ultimately provide a new method of biomolecule analysis. This research could enhance capabilities through rapid elucidation of binding affinity and specificity of peptides to biothreat proteins of interest. A future nanofluidic bioanalysis platform could potentially screen a large pool of candidate binders within hours, with minimal protein modification required, significantly reducing the time needed to fully characterize a high-affinity binder for an emerging threat. Nanofluidic biomolecular systems could also enhance capabilities in electrochemical energy conversion and storage, electrokinetic flow, electrocatalysis, photovoltaics, biomolecule sensors, water purification, and lab-on-a-chip analyses.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY11, the Life Sciences Division managed eight new DURIP projects totaling $1.1 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including efforts to study self-assembling DNA nanostructures, to explore etho-genetic variation, and to monitor the function of the microcirculation within tissues.

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

The ICB is managed 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 $13.1 million was allocated to the ICB in FY11, which was the third year of a $70 million contract that was renewed in FY09 for a five-year period. Of these FY11 funds, $8.9 million was allocated for 6.1 basic research and $4.2 million was allocated for five 6.2 projects, including two new projects.

In FY11, the ICB supported 58 faculty, 90 graduate students, and 44 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.

J. DARPA Revolutionizing Prosthetics Program

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

K. DARPA Soldier Centric Imaging via Computational Cameras (SCENICC) Program

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

L. JIEDDO Rapid Development of Counter-IED Capabilities Program

The goal of this program is to establish new approaches and capabilities for countering IEDs, from initial detection to mitigation of the effects following detonation. The ARO Life Sciences Division is co-managing two programs covering the development of experimental models of post-traumatic stress disorder and research for updating physiological diagnostics and interventions following injury by IEDs, including minimal traumatic brain injuries.

M. DARPA Seven Day Program

In recent years global surveillance networks have determined that the frequency and diversity with which new infectious microorganisms are emerging is increasing. While these increases are in part due to better reporting, there are multiple examples demonstrating this increase is promulgated by changes in natural systems and potentially the activities of humans. Examples of factors implicated in the increase in new, emerging and re-emerging pathogens include: increased animal-human interface; increased population densities and co-location of vulnerable species with pathogen reservoirs; climate change, particularly affecting migration and spread of vectors; and narrowing of genetic diversity among food animal stocks. The expansion of biomedical technologies on the global stage is also suspected to increase the risk of orthogonal and highly diverse microorganisms. One growing concern is the potential risk posed by the proliferation of genetic engineering technologies that can be easily redirected from beneficial to offensive purposes or for covert biological industrial sabotage of food animals. Together, these natural occurring and synthetic threat agents challenge current detection methods and could possibly defeat traditional medical countermeasures.

No group is at greater risk of exposure to new international pathogens, to bio-sabotage of food supply lines, or to attack from biological threat agents, than the U.S. Military. The traditional medical response for responding to large scale infectious disease outbreaks is to (i) quarantine exposed personnel (hours to weeks), (ii) identify and characterize the agent (usually within 0-90 days), (iii) develop a vaccine or therapeutic (1-14 years), and (iv) stockpile, distribute, and administer treatment. In cases where the pathogen is unknown or difficult to characterize, victims are likely to succumb before an effective therapy or vaccine can be developed, distributed and administered. The objective of this program, co-managed by the ARO Life Sciences Division and DARPA, is to develop highly innovative approaches to counter any known, unknown, naturally occurring or engineered pathogen. The goals are to investigate novel technologies to prevent infection, extend survival until a curative response is available, provide transient immunity, and increase the onset of adaptive immunity.

N. DARPA Enabling Stress Resistance Program

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

O. DARPA Physical Intelligence Program

The goal of this program, parts of which are co-managed by the Life Sciences Division and DARPA, is to establish the physical foundations of intelligence using a coordinated effort that includes theory, implementation, and analysis. The objective of the theory domain is to develop and validate a physical formalism that unifies and expands ideas from diverse domains such as evolution, thermodynamics, information, and computation. The objective of the implementation domain is to demonstrate the first human-engineered open thermodynamic systems that spontaneously evolve non-trivial "intelligent" behavior under thermodynamic pressure from their environment. The objective of the analysis domain is to design analytical tools to support the development of human-engineered physically intelligent systems and to understand physical intelligence in the natural world. The Division currently co-manages a project within this program that is developing a unified formalism of physical intelligence from two complementary theories, will validate these theories and demonstrate physical intelligence in engineered chemical and electronic prototypes, and will develop analytical methods to quantitatively assess the intelligence of the prototype systems. If successful, this program will provide the foundations to enable novel engineered systems that exhibit physical intelligence.

P. DARPA Fundamental Mechanics of Gliding Flight in Snakes Project

The objective of this project is to determine the fluid mechanics, musculoskeletal anatomy, and tissue mechanics required to produce gliding flight in snakes. The project is co-managed by the Life Sciences Division and DARPA. The project will achieve its goals using integrated experimental and computational modeling studies. Experimental investigations will utilize 1:1 scale snake models and a low speed water tunnel. To investigate the dynamics and control of snake gliding, detailed 3D kinematics will be determined using previously obtained videographic data and dynamical modeling will be used to reproduce the snake's body movements and overall trajectory. The musculoskeletal anatomy and tissue mechanics important for snake gliding will be assessed by comparing preserved specimens of well-gliding vs. poor-gliding vs. non-gliding snakes. The flying snake under investigation in this project (*Chrysopelea paradisi*) is one species of very few that can move across all terrains (*i.e.*, air, water and land) with exceptional efficiency. Understanding the basic mechanisms behind the snake's flight ability may enable the future development of novel biologically-inspired reconfigurable unmanned vehicles that will be effective in air, water or land.

Q. DARPA Phytoremediation of Atmospheric Methane Project

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

R. DoD-funded Microbial Forensics Program

Bacteria adapt to changes in their environment by altering gene expression. They also respond to different environmental conditions by permanently changing their DNA, in a process known as DNA mutation. DNA mutations persist and are readily detectable and the types, distribution, and frequency of these mutations depend on the specifics of the bacteria's environment. The goal of this program is to disentangle mutations and identify patterns of mutations so that the information about the bacteria's history inherent in its DNA can be decoded. This program is managed by the ARO Life Sciences Division, in cooperation with DTRA, DARPA, DHS, and other agencies. This basic research is anticipated to create new capabilities for forensics, biometrics, national security, and Army operations.

S. DARPA Eukaryotic Synthetic Biology

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.

T. Minerva Research Initiative (MRI): 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, with proposal evaluation and funding selection scheduled for FY12.

U. Minerva Research Initiative (MRI) Project: 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, with proposal evaluation and funding selection scheduled for FY12.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. Efficient, Rapid, and Economical Protein Purification Method

Professor David Wood, Ohio State University (formerly at Princeton University), Single Investigator Award

Professor David Wood has recently devised a novel method for the reliable, economical, and large-scale expression and purification of enzymes, which will greatly benefit DoD-wide research efforts, as well as academic basic research, medicine, and the chemical and biotechnology industries. Professor Wood and his colleagues are attempting to purify organophosphate hydrolase (OPH) and then study its unique mechanism of action to better understand how biological catalysis could be employed to rapidly decompose hazardous molecules. While pursuing this objective, the researchers faced a significant obstacle before they could obtain sufficient enzyme for subsequent study. A long-standing problem in biochemistry and protein science is how to produce and purify large quantities of a large enzyme or multi-protein system without compromising its catalytic activity. Although many approaches for protein expression and purification are available, such as affinity tag-based purification and high-performance liquid chromatography, these methods can lead to the inadvertent inactivation of an enzyme and are difficult to scale up for the production of large quantities of enzyme.

The researchers successfully devised and demonstrated a self-purifying protein purification method that employs elastin-like polypeptide (ELP) and intein tags (see FIGURE 6). The researchers demonstrated that attaching this tag to a protein of interest (via standard genomic tagging methods) enabled the simple purification of the protein by increasing salt concentration or gently heating the solution, which precipitates the ELP tag. As a result, the researchers could easily "pull" an attached enzyme of interest out of solution without the need for expensive and time-consuming liquid chromatography equipment (see FIGURE 7). The researchers also combined a version of the tag with engineered inteins, which allows the separation of the ELP tag from the protein of interest when subjected to a mild pH shift. This approach provides a much simpler and cheaper method for the reliable and high-yield purification of a given enzyme. The researchers' preliminary versions of this method have already led to more than a dozen peer-reviewed publications, three patent applications, over ten lectures at international bioprocess conferences, and over one hundred requests for the technology from academic and industrial researchers worldwide. This purification approach may enable the rapid and economical purification of OPH or other enzymes that could drive research for a variety of potential applications for the Army, including the degradation of lethal nerve agents, the neutralization of industrial waste products, and the development of new therapeutic proteins.

FIGURE 6

Schematic of ELP-Intein tag. To produce an ELP-intein-tagged protein, the researchers used standard cloning methods to add the ELP and intein sequence ahead of the coding DNA for the enzyme/protein of interest. The enzyme of interest can then be purified by heating (causing precipitation via ELP tag) and then cleaving the Intein tag via a mild pH shift, resulting in an easily-purified enzyme without the loss of activity characteristic of other more complex purification methods.

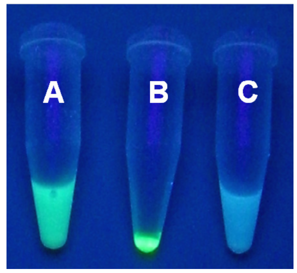


FIGURE 7

Demonstration of protein purification using ELP-intein tags. Using standard genomic tagging methods, ELP-intein tags were fused to green fluorescent protein (GFP), which provided an easily-visualized demonstration the progress of the purification process. First, cells expressing the ELP-intein-GFP fusion were lysed. Note that the resulting cell lysate fluoresces due to the presence of GFP (Tube A). Salt was added to precipitate the ELP tag with the fused target protein, and then the lysate was centrifuged to produce a pellet of the tagged target protein (GFP; Tube B). The remaining supernatant (Tube C) fluoresces only slightly, demonstrating that the majority of GFP was concentrated into the pellet. The precipitated protein was resuspended and the pH shifted to begin the intein self-cleaving reaction. After the intein cleavage was complete, subsequent separation and analysis revealed that the vast majority of the ELP-intein tag was separated from the target protein.

B. Sensory-Based Diagnostics for Assessing Cortical Information Processing

Professor Mark Tommerdahl, UNC-Chapel Hill, Single Investigator Award

Unique quantitative sensory testing methods, based on information obtained from neurophysiological studies of the nonhuman primates, have led to a library of cerebral sensory cortical responses to a variety of modes of natural skin stimulation. The sensory testing methods and apparatus enable objective evaluation of the elaborate neuroanatomical connectivity that subserves the neuronal communication between adjacent and near-adjacent regions within the sensory cortex that is widely recognized to be essential to normal sensory function. Although this intra-cortical communication involves numerous mechanisms, the tests appear specifically sensitive to the status of mechanisms generally accepted to play major roles in the disorders of sensory cortical information processing often seen in patients with mild traumatic brain injury (mTBI).

The investigator and his collaborators have developed a prototype device/testing approach that appears sensitive to a number of commonly-prescribed drugs. Coupled with quantitative-assessment protocols, this testing approach may enable non-invasive and objective assessment of the efficacy of drugs or other treatments for neurologically-compromised individuals. Other advantages of the new method are: (i) the device is portable and reproducible, (ii) the protocols are fast (longest protocol in the current test battery lasts between 3-5 minutes, depending on the subject), (iii) the protocols are relatively simple for the subjects to understand, (iv) the method is noninvasive, and (v) the tests have a rapidly growing subject database for comparison. Multiple clinical research collaborations have been initiated in a number of areas to continue examining this testing approach, including investigations in the research areas of autism, chronic pain, alcoholism, and aging. This research could have a significant impact on a number of areas which are currently being explored and could eventually be used as a diagnostic tool by not only medical practitioners, but by primary health care providers for obtaining measures of central nervous system disorder and/or assessment of efficacy of therapeutic strategies. In addition, quantitative dosimetry of exposure to blast-related trauma is an important aspect of Soldier protection, yet it is currently a difficult, if not impossible task. The development of a field-deployable lightweight and portable diagnostic sensory testing system would allow commanders to protect personnel from excessive blast exposure by reassignment as appropriate in each individual case. When environmental and medical interventions have been set in place, the system could one day allow for the quantitative tracking of the efficacy of treatment.

C. Investigating the Mechanics of the Adhesive Properties of Ivy Nanoparticles

Professor Mingjun Zhang, University of Tennessee, Single Investigator Award

The goal of this research effort is to characterize and understand the mechanical properties of ivy adhesive at both the microscopic and macroscopic levels, and to relate the microscopic features of the adhesive to its macroscopic properties. Understanding the adhesive mechanisms used by biological species may provide exciting opportunities for the future development of biomimetic systems with unique capabilities. While some biological adhesive systems have been widely studied, including the gecko and the sea mussel, the physical properties that allow ivy to cling to and climb surfaces have been widely neglected. Charles Darwin reported that a single ivy adhesive disc weighing 0.5 milligram could support a weight of two pounds. Thus, the force supported by the ivy adhesive disc is about 1.8 million times greater than its own weight, and the adhesive force of mature ivy may be even greater. Professor Mingjun Zhang's research group at the University of Tennessee recently discovered that the adhesive secretion produced by ivy rootlets contains protein-based nanoparticles. This effort involves elucidation of the biological process leading to the generation of ivy adhesive, characterization of the intra- and inter-molecular bonding forces between the components of the adhesive (nanoparticles and adhesive matrix) and between the adhesive and the affixing surface, as well as determination of structure-function relationships through the systematic alteration of adhesive components.

In FY11, the investigators characterized the mechanism of ivy adhesive secretion in significant detail using a real-time video microscopy system combined with atomic force microscopy (AFM) analysis and have successfully discerned the key stages of attachment of ivy rootlets to a surface (see FIGURE 8). The initial stage of attachment is contact with the surface by the rootlet tip, rather than the root hairs. Following contact with the surface, there is an increase in the number of root hairs, which also show an increased growth rate. However, no root hairs were observed on the root tip. This initial contact was also found to stimulate the production of additional rootlets. These results suggest that the rootlet tip acts as a pressure sensor signaling not only the production of root hairs on the attaching rootlet, but also triggering increased rootlet production. The second stage of attachment consists of parallel bending of the rootlet to the substrate, which brings the root hairs into close contact with the surface. As rootlet bending occurs, the root hairs begin to secrete adhesive, even when they are not in contact with the surface. These results indicate that shear force is not necessary for deposition of adhesive, as was previously hypothesized.

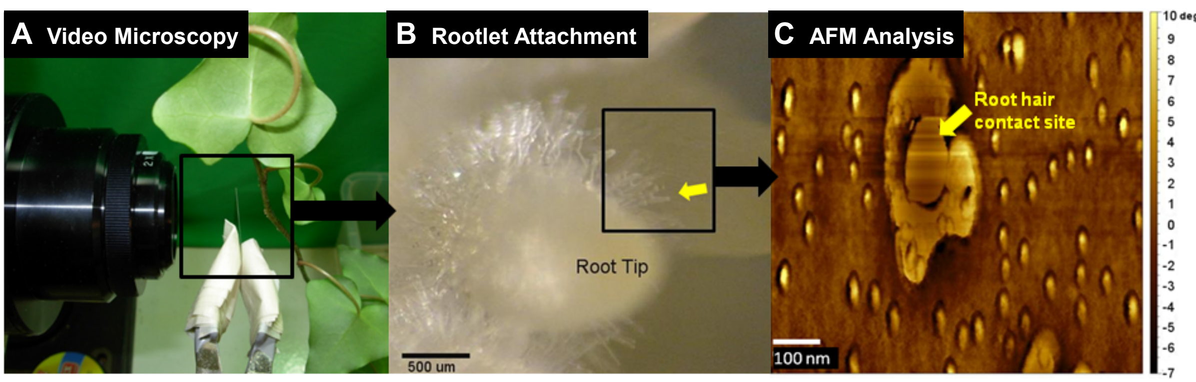


FIGURE 8

Analysis of Ivy Adhesive Secretion. Video microscopy was used to visualize attachment of the ivy to a surface in real time. (**A**) The coverslip acted as the surface for monitoring via video microscopy. (**B**) Time-lapse imaging was conducted to discern the roles of the root tip and the root hairs (yellow arrow) in attachment and secretion. (**C**) The surface containing secreted adhesive was then analyzed using AFM to determine the abundance and distribution of nanoparticles within the adhesive.

The investigators will next explore the intra- and inter-molecular bonding forces (i) between nanoparticles, (ii) between the nanoparticles and the adhesive polymer matrix, and (iii) between the nanoparticles and the affixing surface, using atomic force microscopy and nanoindentation. These analyses will be performed by attaching purified ivy nanoparticles to the tip of an AFM probe. In support of these planned experiments, the team recently developed a procedure to reliably purify the protein-based nanoparticles using trichloroacetic acid.

Elucidation of the chemical composition and mechanical properties of the ivy nanoparticles may enable future work in which the adhesive polymer matrix and/or the nanoparticles are altered to create new material properties. This research may also inspire biomimetic approaches for the design of new materials with superior surface adhesion for military applications.

D. Bacterial Programmed Cell Death as a Population Phenomenon

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

Programmed cell death (PCD) is recognized as an essential mechanism in multi-cellular organisms. For example, the cells that make up the webbing between the fingers during human embryogenesis must die to free the individual digits. The first single cell PCD was described by Prof Engelberg-Kulka in the mid-1990s. She and colleagues identified a novel communication chemical, termed extracellular death factor (EDF), which signals bacteria to "commit suicide." They further showed that a toxin-antitoxin system (*maz*EF) is involved in mediating cell death. The goal of this project is to understand the fundamental mechanisms of PCD to determine how the sensing of EDF results in loss of viability.

During the course of this study, the investigators made a breakthrough in understanding not only PCD, but how bacteria survive stress conditions. They demonstrated that *maz*EF is a stress-induced toxin-antitoxin module. 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 9). 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.

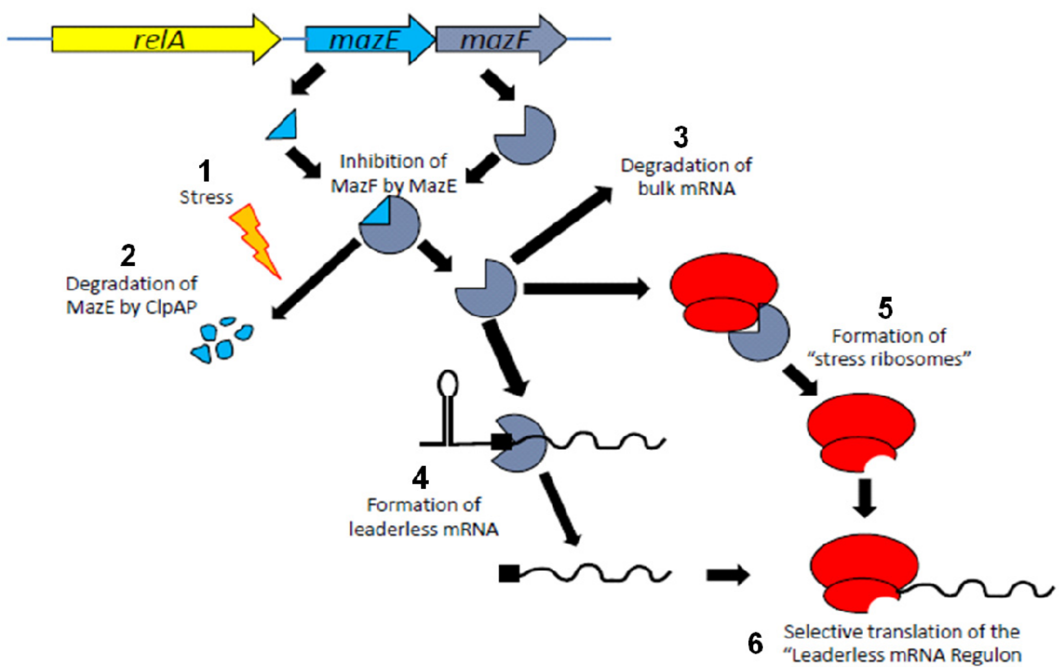


FIGURE 9

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."

E. Vaccine Design Using MicroRNA-mediated Viral Attenuation

Professor Benjamin tenOever, Mt. Sinai School of Medicine, PECASE Award

The objective of this research is to determine how host-generated microRNA molecules interact with invading viruses. The investigator is testing the hypothesis that viruses can be attenuated by modifying the viral genome to be an exact complement to a microRNA expressed in the host tissue of interest.

Influenza A virus is a seasonal pathogen responsible for the deaths of over 50,000 people in the U.S., annually. The viral life cycle in humans begins when the virus enters lung bronchial epithelial cells. The eight individual non-coding strands of RNA comprising the viral genome migrate to the host cell nucleus where individual strands are transcribed by a viral RNA-dependent RNA polymerase (see FIGURE 10). The transcripts are then transported to and translated in the cytoplasm. At a later point in time, the RNA-dependent RNA polymerase switches from viral genome transcription to replication. Newly synthesized genome segments are then packaged into viral capsids using the previously synthesized proteins.

Due to the high rate of mutation and segment exchange, live, attenuated influenza A vaccine virus strains must be developed annually to provide an effective method of controlling the virus. Attenuation is normally achieved by conferring temperature sensitivity upon the virus. These viruses are then grown to high titers in chicken eggs, purified, and mixed with other influenza strains to comprise the final multivalent influenza vaccine. The investigator proposed developing a microRNA strategy for virus attenuation. MicroRNAs are known to be present and to influence RNA stability and translatability in a wide range of eukaryotic cells, often in a species- or tissue-specific manner.

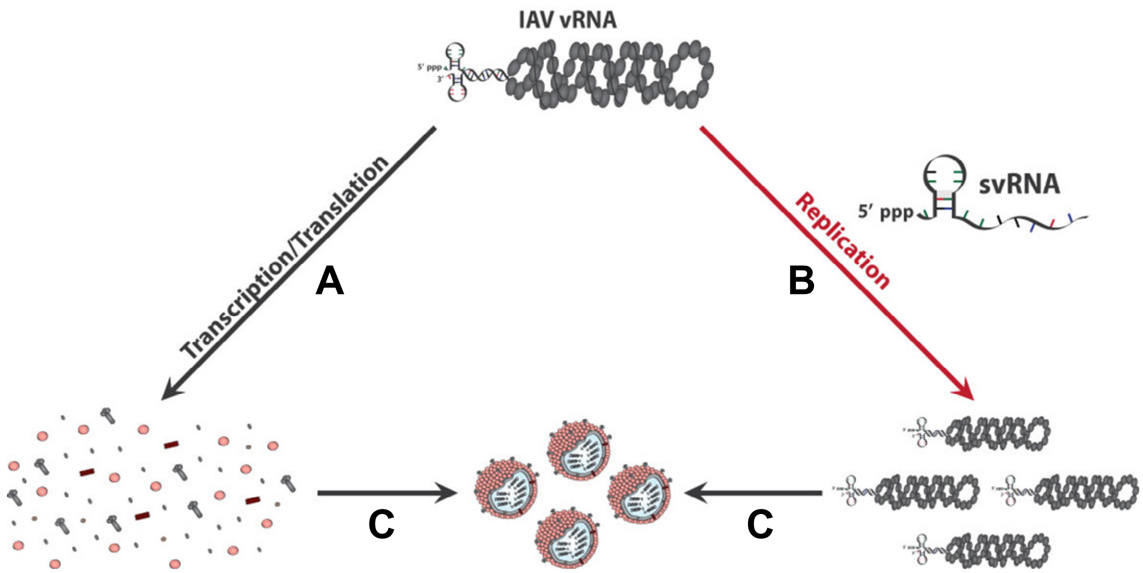


FIGURE 10

Small viral RNA (svRNA) impact on virus life cycle. (A) Influenza A virus (IAV) viral RNA (vRNA) is initially transcribed to mRNA which is translated to produce proteins required for viral capsid formation. (B) svRNAs are synthesized at a low rate and as they accumulate they interact with the viral genome strands and switch them from being transcribed to being replicated to produce new IAV vRNA genomes. (C) The new genomes and proteins are then assembled into virions.

The investigators discovered that modifying the highly-conserved virus protein coding sequences in the influenza genome, to make them complementary to mammalian bronchial epithelial cell microRNAs, resulted in attenuated viruses that induced a robust immune response in the mouse. While confirming these results by deep sequencing of microRNAs isolated from mouse bronchial epithelial cells infected with the modified viruses, a small RNA was found that is complementary to a highly conserved sequence present at the 5' end of all eight individual strands of RNA that comprise the viral genome.

Further investigation of the small viral RNA (svRNA) showed that it is produced in cells from multiple host species infected with influenza A virus. They showed that svRNA accumulates during infection and biases the RNA-dependent RNA-polymerase (RdRp) machinery from transcription towards genome replication. Depletion of svRNA was shown to result in a dramatic decrease in the amount of progeny produced. These and other data led them to conclude that svRNA acts as a surrogate promoter for RdRp and shifts the activity from viral transcription to viral replication. Therefore, svRNA acts as a mechanistic switch and is required for the virus's natural life cycle and represents a new target that could be exploited for *universal* anti-influenza A virus-based therapeutics.

F. Novel Semiconductors Integrated with Biological Membranes

Professor Guillermo Bazan, University of California - Santa Barbara, ICB (UARC)

Professor Guillermo Bazan has recently developed a novel and simple approach to directly mediate extracellular electron transfer in living microorganisms. As part of the Institute for Collaborative Biotechnologies (ICB) at UCSB, researchers discovered a specialized class of water-soluble, semiconducting molecules called conjugated oligoelectrolytes (COEs) that have the ability to readily and nondestructively insert into the phospholipid bilayer membranes of living microorganisms or synthetic liposomes in a very reproducible and ordered way. These membrane-incorporated COEs exhibit a range of unique optical and electronic properties that could have immense implications for bioenergy production, bioremediation of waste water effluents, biosensing, biological imaging and fundamentally understanding signal transduction across the biological-inorganic interface in bioelectronic devices.

While these COEs were initially developed by Professor Bazan's research group for application as two-photon absorption fluorophores useful for biological imaging, it soon became apparent that these molecules could preferentially insert themselves into lipid bilayer membranes and, because of the electronic properties of the COEs, allow for the direct and reversible shuttling of electrons across electrically insulated biological interfaces (see FIGURE 11). This result is powerful, especially because the process of incorporating COEs into microbial cell membranes is trivial, and because these molecules, as semiconductors, create an efficient and direct conduit for electron transfer between the interior of living microorganisms and their environment without the need for electron-accepting proteins or molecules that typically act to mediate this process.

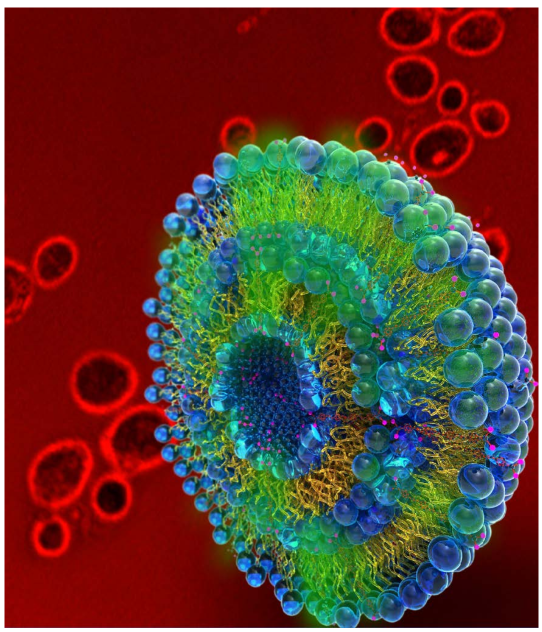


FIGURE 11

Microbial vesicle and COEs incorporated into yeast membranes. Shown in the foreground is a cross-section of a vesicle, a non-biological model of a microorganism, revealing several lipid bilayer membranes with the inserted conjugated oligoelectrolytes (COEs): the blue spheres represent the polar, water-soluble, heads of the lipids, which have yellow non-polar hydrocarbon tails attached to them; the incorporated COEs are colored in pink. The background illustrates the fluorescence of the membranes of yeast cells that have incorporated COEs.

Microbial fuel cells (MFCs) function on the principle that electrons from the metabolic cycle of many anaerobic and facultative organisms known as exoelectrogens can generate a useful electrical current as they transfer electrons from cell respiration directly to electrode surfaces. Understanding and controlling electron transport physics at the biological-inorganic interface is critical to improving the power density of fuel cells that function directly by consuming biomass. MFC's also provide for a potentially simple and practical means to convert biomass to electricity while purifying waste water streams. As such researchers at the ICB, in collaboration with scientists at ARL-SEDD, have demonstrated that yeast MFCs with incorporated COEs exhibited a nearly 5-fold increase in performance relative to MFCs that require electron-transporting molecules (ETMs) to mediate electron transfer (see FIGURE 12). Remarkably, this level of performance was achieved using concentrations of COEs that were two orders of magnitude lower than that of commonly used ETMs, and without any noticeable effects on yeast cell viability. An ICB collaboration with ECBC demonstrated that MFCs can function by simply adding COEs to waste water effluents using the microbial populations already present. An additional joint collaboration between ECBC and ARL-SEDD has demonstrated that the processing of cellulosic waste occurs more rapidly and with a greater reduction in total organic content relative to dark fermentation when using MFCs that have been charged with microbes and COEs. These efforts are ongoing and should continue to provide more fundamental insight into the processes that are relevant to the integration of biological systems to electronic devices.

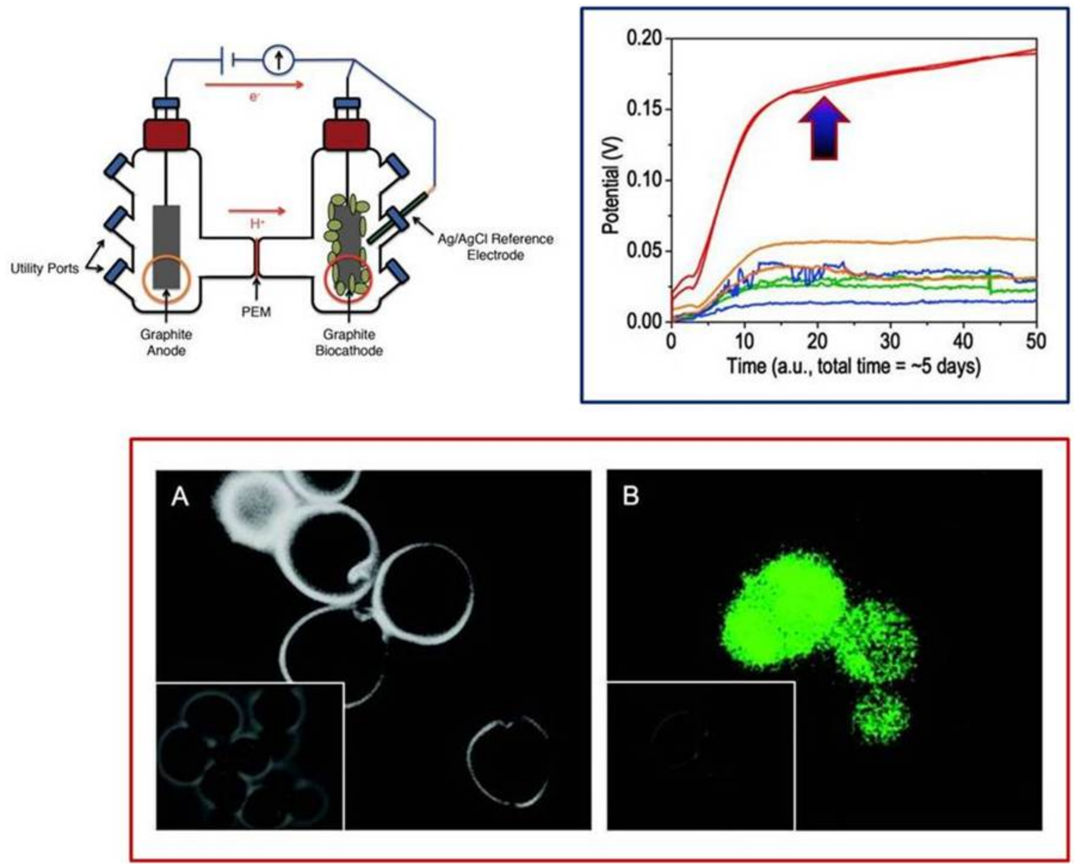


FIGURE 12

COEs incorporated into yeast MFCs provided nearly 5-fold increase in performance. (Top Left) Schematic of a typical MFC illustrating several key components: 1) a chamber with a graphite anode; 2) a chamber with a graphite cathode that has a biofilm growing on its surface; and a polymer electrolyte membrane (PEM) separating both chambers. (Top Right) Plots of yeast MFC voltage production as a function of time show a notable increase in MFC performance when using COEs, as indicated by a 5-fold increase in the voltage produced compared to common electron transport mediators and despite being at much lower concentrations. (Bottom) COEs maintained within cell membranes of subsequent yeast generations born over the course of MFC operation during this study: A) fluorescence images of yeast cells on day 1; B) fluorescence images of yeast cells on day 4, after exponential growth of yeast cells.

G. Actionable Variation in Human Genes

Professor Jasper Rine, University of California - Berkeley, Single Investigator Award

The objective of this project is to leverage the value of the Human Genome Project by identifying human genetic variants that are responsible for suboptimal performance of individual enzymes, and then identifying those genes and downstream functions that are amenable to metabolic tuning. Professor Rine's preliminary data indicates that the average human has five mutant enzymes whose enzymatic performance could be improved by vitamin or mineral supplements. The team has interrogated the known non-synonymous single polynucleotide polymorphisms (SNPs) in five prototypical B6, niacin, riboflavin, and thiamine dependent enzymes for functional impact and vitamin responsiveness. The investigators created a *Saccharomyces cerevisiae* complementation assay that coupled the functions of the two enzymes responsible for cysteine biosynthesis via the transsulfuration pathways: cystathionine beta-synthase and cystathionine gamma-lyase. The team discovered that variants of both proteins that appear fully functional in each single assay had functional impacts in specific combinations in the coupled assay. This result provides support to the hypothesis that interactions between variants in different genes, when characterized, could one day be used as the basis for low-cost individualized performance optimization. If successful, this research could provide a validated, individualized approach to manage a variety of potential nutritional or metabolic deficiencies faced by military and civilian personnel.

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. Lateralized neuro-feedback for display data control and apprehension

Investigator: Dr. Leonard Trejo, Pacific Development and Technology LLC, Single Investigator Award
Recipient: ARL-HRED

In FY11, the transition of a neuro-feedback system to ARL-HRED began. This system will use the electroencephalography (EEG; measurement of brain electrical activity) and electrooculography (EOG; measurement of eye movements) signatures of personality, performance, cognitive workload, and fatigue in order to test whether optimized hemispheric input and selective hemispheric activation with EEG neurofeedback can be used as a training aid and/or as an operational tool. The goal is to prevent performance degradation or mission failure due to fatigue and/or information overload by directing attentional loads to different brain hemispheres. This collaborative research uses a continuous lateralized presentation system enabled by an eye tracker and a gaze-contingent display controller. The system will be used to approximate natural visual tracking conditions (via EOG) in the laboratory, which is also relevant to the field. The system incorporates the Lateralized Attention Network Test (LANT), which measures components of attention in each cerebral hemisphere. Using these tools, the investigators will have a map of the visual targeting movements (measured via EOG) and the corresponding brain-to-eye muscle control signals (measured via EEG). These data may allow the investigators to determine the relationships between the complexity of a task (*i.e.*, information-processing overload) and any resource limitations due to fatigue (*e.g.*, during sleep deprivation) while a subject sights targets across the visual field. In addition, a QUASAR EEG system previously received by ARL as part of a prior transition and developed in part by Dr. Trejo and Pacific Development and Technology (PDT), will be tested for use in this new collaborative effort. The system is designed to enable and optimize attentional resources in information comprehension tasks.

This research has the potential to be used in command and control systems or other stationary environments where cognitive workload/overload and/or fatigue affect performance. This work may enable integration of previously transitioned QUASAR EEG workload analysis systems and advanced display technologies for workstation ergonomic design. Independent of this, observations using the gaze-contingent display controller also may be useful in soldier-crewstation interaction such that alerts or targets of interest are re-represented and directed to the brain hemisphere most suited for the required cognitive processing, taking into account the aptitude, personality, cognitive status, and mood of the operator.

B. Stress and Performance in Working Canines

Investigator: Professor Mike Davis, Oklahoma State University, Single Investigator Award
Recipient: U.S. Marine Corps.

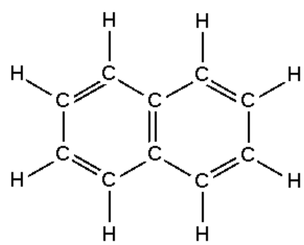
The objective of the project leading to this transition was to determine biological mechanisms enabling extreme performance in Iditarod dogs. This race covers over 1000 miles in grueling Artic conditions. Although the primary focus of this research project was to investigate the mechanisms of enhanced oxidative substrate uptake as a metabolic strategy to reduce fatigue during sustained submaximal exercise, the investigator made the unexpected discovery that gastric ulcers are common in the Iditarod dogs. As a result of this research, mushers now proactively treat their dogs with Prilosec® (omeprazole magnesium) to prevent gastric ulcers and this is credited with reducing canine deaths during extreme racing approximately ten-fold. Recent interest from military dog trainers and dog handlers has led to follow on work demonstrating that gastric ulcers are also common in military working dogs and that the weight loss, lack of appetite, and stamina problems observed in military working dogs can be largely negated using Prilosec® to prevent gastric ulcer formation. These results have transitioned to the U.S. Marine Corps for prophylactic treatment of IED detection dogs, which are retrievertype dogs that work on- or off-leash on daily patrols in deployment areas in southwest Asia often requiring long periods of physical stress.

C. Naphthalene Dosimeter

Investigator: Photon Systems, Inc., SBIR contract
Recipients: DARPA; MRMC; National Institute for Occupational Safety and Health (NIOSH), USACE

Naphthalene is a byproduct of the fuel refining process and is found in many fuels, including the fuel refined to the Jet Propellant 8 (JP-8) standard. Naphthalene is an aromatic compound that rapidly vaporizes (see FIGURE 13). This chemical has been identified as a serious health hazard for personnel working with JP-8 and other fuels containing naphthalene. A SBIR contract with Photon Systems, Inc., has been focused on designing and creating a dosimeter capable of accurately assessing naphthalene exposure levels. Regulatory changes are expected that will require DoD personnel working with JP-8 to be able to monitor exposure in real time in order to be able to keep personnel exposures below NIOSH limits. In addition naphthalene exposure will enable human data to be obtained; the EPA decision to classify naphthalene as a likely carcinogen is based on rodent data. The shape of rodent noses and differences in the p450 pathway make it difficult to extract rodent data to humans and direct measurements on humans are necessary.

Other agencies, including DARPA, NSF, USACE, OSD, NIEHS, and NIOSH, have invested in transitioning this research to both validate the dosimeter with human testing and to expand the range of measurable analytes. This SBIR project and the collaborating agencies expect to build a dosimeter capability that will enable DoD to protect warfighters working with JP-8 and will enable the continued use of JP-8 containing fuels. Given that DoD uses 5.5 billion gallons of JP-8 each year and exposure to JP-8 represents the single largest source of chemical exposure to DoD personnel, this investment will lead to improved Soldier health and protection.



Naphthalene
$C_{10}H_8$

FIGURE 13

Structure of naphthalene. JP-8 and other military-grade fuels contain naphthalene. A naphthalene dosimeter, for use in measuring levels of personnel exposure to the compound is being developed by this SBIR contract. Based on the progress and potential of this work, DARPA, MRMC, NIOSH, USACE, and others are actively investing time, expertise, and funds to transition the dosimeter to operational use.

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. Multisensory Navigation and Communications System

Engineering Acoustics, Inc. (EAI), SBIR Contract

Combat environments can subject personnel to extreme conditions, testing the limits of both their physical and cognitive abilities. EAI previously designed and demonstrated a proof-of-concept system that enables investigation of multisensory navigation and communication among dismounted soldiers. The prototype Active Tactile Array Cueing Navigation and Communication (ATAC-NavCom) system provides GPS-derived tactile navigation cues integrated with a prototype mobile visual map display (see FIGURE 14). The design framework facilitated demonstration of intuitive tactile representation on a wearable, scalable Hybrid Tactile Array (HTA), for navigation, situational awareness, and communication tasks. It is anticipated that in FY12 the system will be refined and enhanced to implement a networked, multi-user multisensory navigation and communication system for evaluation and optimization in a realistic military environment. The resulting system will have the potential to greatly improve the dismounted warfighter's individual and team performance and survivability by improving situational awareness and communication in the combat environment. Success in the program will result in a system that can integrate with, and augment, battlefield-visualization techniques currently in use, and enable commanders to effectively provide critical information to the dismounted soldier to improve navigation, communication and situational awareness in the battlefield. Many non-military users, including first-responders, firefighters, and search and rescue personnel could potentially benefit from this technology.

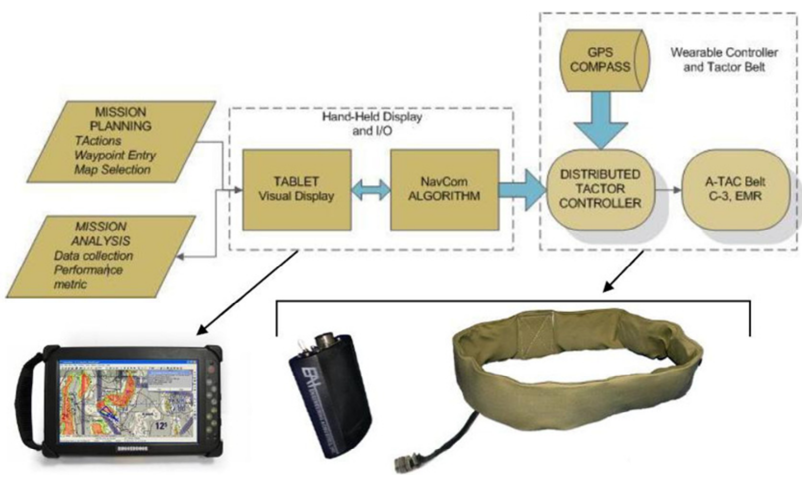


FIGURE 14

ATAC-NavCom system. The system comprises visual display hardware, EAI tactor controller and belt array, a GPS / compass sensor interfaced directly to the controller and a number of software components. Management (mission planning and analysis) software is located on a server employing conventional WiFi networking.

B. Engineering Synthetic Ribosomes

Professor Michael Jewett, Northwestern University, Single Investigator Award

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

Professor Michael Jewett's research group at Northwestern University is using methods in synthetic biology to harness the extraordinary synthetic capability of the ribosome to assemble polymers containing non-biological building blocks (see FIGURE 15). Expanding the repertoire of ribosome substrates is a challenging task because the requirement of cell viability severely constrains the mutations that can be made to the ribosome. In practice, these constraints make the natural ribosome un-evolvable and so far, there is not a generalized method for modifying the catalytic active site of the ribosome to incorporate substrates beyond those found in nature. The keystone of this effort will be an innovative ribosome engineering platform designed by Professor Jewett that will be used to select and evolve synthetic ribosomes that are programmed to efficiently synthesize sequence-defined polymers containing multiple types of non-natural monomers. In addition to synthetic ribosomes, this effort will also require the creation of non-natural building blocks and a code that directs the ribosome to polymerize these monomers in a specific sequence.

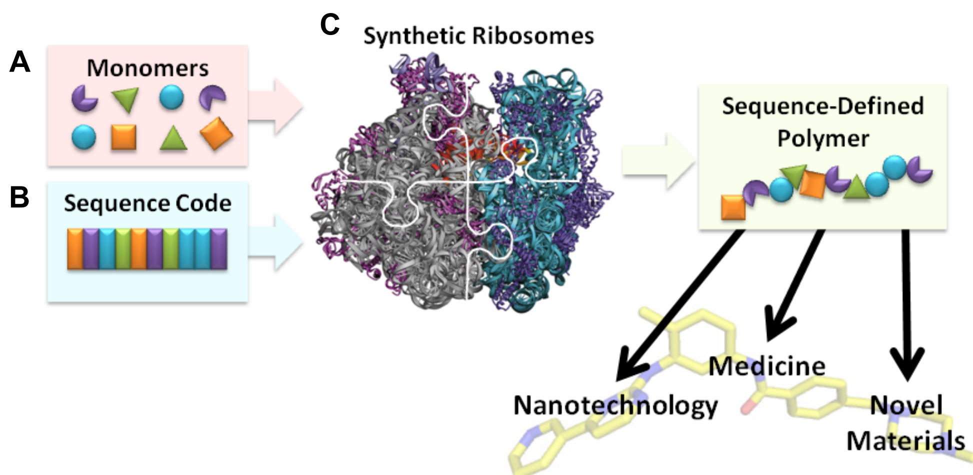


FIGURE 15

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

The research team is currently generating monomers with vinyl building blocks attached to enable their selective incorporation into a growing polymer chain. The team will also initiate efforts to reprogram the genetic code by replacing redundant codons with novel codons directing the insertion of non-biological monomers. In nature, 64 triplet codons signal either the incorporation of a natural amino acid or the termination of peptide polymerization. In order to synthesize peptides using monomers beyond the natural amino acids, one or more codons must be reprogrammed to specifically accept non-natural building blocks. Traditionally, codon reprogramming has been accomplished by reassigning one of the termination codons to incorporate a non-natural monomer. However, this approach results in the ability to incorporate only a single additional building block. Dr. Jewett's vision is to enable incorporation of multiple non-natural building blocks by rationally reducing the redundancy of the genetic code. Multiple codons direct incorporation of the same amino acid, therefore eliminating this redundancy will free several codons for the incorporation of non-natural monomers.

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

C. Rugged Automated Training System (RATS)
Barron Associates Inc., Coherent Technical Services Inc., and Strategic Feasibilities Inc., STTR Contracts

There is an increasing trend towards the use of non-metal based mines, necessitating the use of direct detection of explosive vapors instead of the simpler metal detectors. Direct detection of vaporized explosive compounds is accomplished either by explosive vapor detector equipment or with animals. Although not rigorously quantified, it is apparent that trained animals are capable of detecting explosives at levels lower than abiotic systems such as gas chromatography / mass spectrometry. The U.S. DoD currently relies on dogs for animal-based explosive detection; however, a Dutch organization has demonstrated that rats can be used to reliably find mines. Rodents have multiple advantages over dogs for the detection of explosives: (i) rodents are more acceptable to use than dogs in some cultures, (ii) humans do not typically have the emotional attachment to rodents as to dogs, (iii) rodents do not have the emotional attachment to humans that dogs do; therefore, rodents will work for anyone and not just a selected trainer, (iv) rodents are smaller, enabling transport in a backpack and allowing searches in smaller spaces, (v) rodents can climb trees, (vi) rodents need less food, less space, less medical care, and less logistical support than a dog. Although it is not the intent of these efforts to replace military working dogs with military working rats, it is desirable to develop a rodent capability to complement existing dog capabilities. In addition to detecting mines, trained rodents could also be used to find humans or bodies after natural disasters such as earthquakes, and can be used to search in caves, sewers, walls, and other spaces too difficult for dogs to access. Rats are also more conducive to operating in stealth mode than dogs; they are common sights in many environments and they are quiet (see FIGURE 16). Three newly-initiated STTR projects are working to develop and validate a machine that will reliably train small animals to detect explosives or other compounds of interest, and to provide an objective unbiased measurement of each animal's sensitivity and accuracy.

FIGURE 16

African giant pouched rat in training to detect mines in Tanzania. The goal of these projects is to design and validate a system to reliably train small animals in mine detection.

D. Fundamental Studies on Lensfree Microscopy and Tomography
Professor Aydogan Ozcan, University of California - Los Angeles, Young Investigator Program (YIP) Award

Optical microscopy is undergoing a renaissance with various innovative technologies being developed to overcome the fundamental barriers that limit resolution. However, the complexity of these systems makes them expensive to build and maintain, and highly trained technical personnel are required to take advantage of the new capabilities. Professor Ozcan is taking advantage of rapid advances in digital technologies and 2D solid state detector arrays with the goal of eliminating optical lenses and their limitations. His research group has developed a lens-free image capturing system that has 2 μm micrometers resolution, which is comparable to high magnification of an optical microscope (see FIGURE 17). This system also has dramatically-increased fields of view and depths of field.

It is anticipated than in FY12, this research will lead to fundamentally-new design architectures based on lens-free on-chip imaging of complex biological systems, and basic performance limitations of these new lens-free architectures will be characterized. This research will be transformational in the microscopic imaging field and lead to lens-free imaging systems that exceed theoretical limits of resolution obtainable by optical microscopes for a fraction of the cost. Further, with the increased field of view and depth of field, tomography with an imaging volume of >80 mm^3 is predicted. If attained, this will enable imaging of microbial biofilms, mammalian cells, and other biological materials *in situ* and provide never-before-seen 3D details of the workings of living cells.

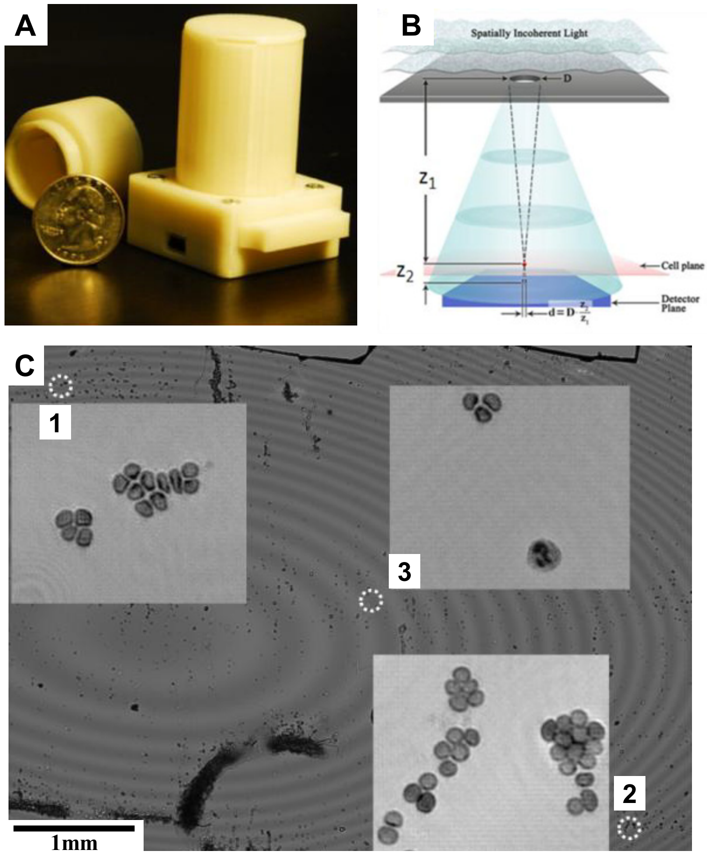


FIGURE 17

Lens-less Ultra-wide-field Cell monitoring Array platform based on Shadow (LUCAS) Imaging. In FY12, researchers will explore new lens-free on-chip imaging concepts imaging system building on the LUCAS imaging system previously developed in the Ozcan laboratory. (**A**) The LUCAS-based lens-free holographic microscope weighs ~ 45 grams (<1.6 ounces). The system utilizes a simple light-emitting diode (LED) at 591 nm with an aperture of ~50-100 µm in front of the imaging source. The LED and the sensor are powered through a side USB connection. The target objects within the sample volume interact with the illuminated light through scattering, absorption and refraction processes. This interaction creates the holographic shadows of the objects on the digital sensor array, containing their "fingerprints" and permitting digital recognition and microscopic image reconstruction within <1 sec. (**B**) Schematic of the holographic LUCAS microscope shown in (A). (**C**) High-resolution (~0.6 µm) imaging of a blood sample using pixel super-resolution over a field of view 24 mm^2. Regions 1-2 show RBC clusters and region 3 shows the sub-cellular features of a WBC. This performance constitutes >200X increase in FOV compared to a conventional microscope that has a similar resolution.

E. Toolkit for Ethnographic Assessment and Data Management Integration

Charles River Analytics, Inc. and Perceptronics Solutions, Inc., STTR Contracts

The collection and analysis of socio-cultural data is becoming increasingly important for the conduct of effective military operations. The production of more scientifically valid models of human behavior has become increasingly dependent on the available forms of socio-cultural data. The ability to rapidly collect social and cultural data in field settings is challenging under most circumstances, and in conflict, denied, or high-risk areas these challenges become even more pronounced. It is anticipated that in FY12, two recently-initiated STTR contracts will design algorithms incorporating ethnographic methods for the rapid collection of cultural, social, and economic data based on structured and semi-structured interviews, qualitative text sources, or unobtrusive observations. If the software development and validation is completed in future STTR contracts, this software may provide U.S. organizations with an enhanced ability to mine, collect, analyze and manage social media data, which will ultimately enable better decision-making at various levels (*e.g.*, policy, combat operations).

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CHAPTER 8: MATERIALS SCIENCE DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2011* is to provide information on the programs and basic research efforts supported by ARO in FY11, 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 FY11.

A. Scientific Objectives

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

2. Potential Applications. In addition to advancing and exploiting worldwide knowledge and understanding of new materials to achieve unprecedented properties, the research efforts 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 leverage of new materials discoveries worldwide, the Division collaborates with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the Defense Advanced Research Projects Agency (DARPA), and across federal-funding agencies (*e.g.*, Nanoscale Science and Engineering Technology subcommittee, Reliance 21 Community of Interest for Materials and Processes), and in international forums (*e.g.*, the Technical Cooperation Program). The Materials Science Division is also very active in pursuing other ARO Divisions to co-fund research, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. In particular, ongoing collaborations exist with the ARO Chemical Sciences, Electronics, Life Sciences, Mechanical Sciences, Mathematical Sciences, and Physics Divisions.

B. Program Areas

To meet the long-term program goals described in the previous section, the Materials Science Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY11, the Division managed research efforts within these four Program Areas: (i) Materials Design, (ii) Mechanical Behavior of Materials, (iii) Physical Properties of Materials, and (iv) Synthesis and Processing of Materials. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

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

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

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

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

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

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

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

These research Thrusts are expected to provide new materials that will provide revolutionary solutions to the 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 FY11 were \$45.6 million. These funds were provided by multiple sources and applied to a variety of Program Areas, as described here.

The FY11 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 \$11.9 million to projects managed by the Division. The Division also managed \$19.6 million from the Defense Advanced Research Projects Agency (DARPA). The Small Business Innovative Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided \$1.1 million in FY11. Finally, \$6.8 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

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

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). 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. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. Armor Ceramic Symposium (Daytona Beach, FL; 23-28 January 2011). The goal of this symposium was to discuss new ideas and needs pertaining to the development and incorporation of ceramic materials for armor applications. The topics covered at the symposium included nondestructive characterization, high-rate real-time characterization, nanotechnology and microstructural design for enhanced armor ceramics, impact mechanics and phenomenology, multi-scale modeling, and manufacturing.

2. Biological Materials Science Symposium (San Diego, CA; 27 February - 3 March 2011). The goal of this symposium was to provide an annual forum for the presentation and discussion of emerging scientific opportunities and breakthroughs at the intersection of materials science and biology. The topics covered at the symposium included (i) bio-inspiration and bio-inspired materials (both hard and soft biomaterials), (ii) surface engineering and biological interactions, (iii) biomedical materials, implants, and devices, and (iv) mechanical behavior of biological materials. Student participation was a particular emphasis of this symposium, and included a very successful student poster contest to increase student participation and interaction with senior investigators.

3. Directed Self-Assembly of Materials Workshop (Nashville TN, 28 September - 1 October 2011). The goals of the workshop were to review the current state-of-the-art in the directed self assembly of materials, and identify breakthrough strategies and enabling technologies that may facilitate the future design and self assembly of multi-component 3D structures with precisely-engineered electronic and optical properties. The conference was led by Dr. John Prater of the ARO Materials Science Division. The topics covered at the workshop included (i) cluster growth and template preparation methods leading to tailored properties and functionality, (ii) control of the assembly process, (iii) strategies for performing staged assembly and demonstrations of sequential assembly processes that lead to architectures with new and unique properties, (iv) avenues for the capture, conversion, and/or transduction of various forms of energy which may drive the assembly and/or reconfiguration processes, (v) theoretical tools and computational methods capable of modeling the self-assembly process and identifying optimal assembly pathways to interesting hierarchical architectures and functionality, (vi) theoretical and experimental approaches for predicting the range of dynamic behavior that can be achieved in these systems, and (vii) novel characterization methods for probing the 3D structure and properties of self-assembled systems.

C. Multidisciplinary University Research Initiative (MURI)

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

1. Investigating Superatoms as Building Block of New Materials. This MURI began in FY06 and was granted to a team led by Professor A. Welford Castleman at the Pennsylvania State University. The objectives of this research are to (i) synthesize atomic clusters of tailored composition, structure, and size, and (ii) self-assemble these clusters into condensed films and solids at the micrometer length scale that retain the distinct properties of the clusters.

The electronic structure of small clusters of free-electron metallic and metalloid atoms is fundamentally different from the bulk. This gives unique "superatom" bonding properties to these clusters that resemble atomic bonding, but are distinctly different in character from any of the elements, which could result in novel properties for assembled solids formed of these clusters. Once assembled into solids, the objective is to characterize the mechanical and electro-optical properties of the films and solids and compare them to the current theoretical understanding of these systems. This should validate the current theoretical understanding and lead to sufficient model fidelity to begin activities on the exploration of devices based on cluster materials. Exploration of these materials is only just beginning and, aside from the C_{60}-based materials, assembled cluster solids at this scale are unknown. A number of significant contributions could be achieved if the research team is successful in developing synthesis routes for different classes of clusters into macroscopic specimens, analogous to fullerenes, as proposed. Since the available variables are greatly extended by exploration of the periodic table beyond carbon, the properties of the clusters could be tailored for device requirements with electronic and optical devices expected to be the first applications of the science to technology.

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 with the ARO Chemical Sciences Division.

Electroactive materials are materials that exhibit a physical response, usually a change in shape, under activation by an electrical potential. These materials are useful in a number of applications including MEMS, stimuli-responsive structures, energy harvesting, micro-sensors, chem-bio protection, and portable power. The main technological limitations of these materials, which limit their usefulness, are their relatively slow response time and low actuation authority (the maximum force they can apply). The focus of the research is on molecular design, synthetic methodology, nanoscale morphological control, property measurements, modeling, and characterization of device performance. The specific research areas of this project include the study of (i) free radical, step growth, and condensation, (ii) polymer structure characterization using atomic force microscopy (AFM), scanning transmission electron microscopy (STEM), small angle X-ray scattering (SAXS), dynamic mechanical analysis (DMA), transmission electron microscopy (TEM), and standard polymer characterization techniques, such as nuclear magnetic resonance (NMR) and gel permeation chromatography (GPC), (iii) the synthesis of zwitterionic monomers using step- and chain-growth polymerizations to form membranes and crosslinked networks, and (iv) the 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. Spin-Mediated Coupling in Hybrid Magnetic, Organic, and Oxide Structures and Devices. This MURI began in FY08 and was granted to a team led by Professor Michael Flatte at the University of Iowa. The objectives of this research are to (i) improve the field's understanding of spin behavior in hybrid systems where magnetic semiconductors and/or organics are integrated with ferromagnetic metals and multiferroic oxides, and (ii) develop the engineering expertise needed to exploit spin-mediated processes to establish nanoscale control over spin transport, local magnetic order, and electrical/optical/magnetic properties of hybrid magnetic systems.

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

5. 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. More specifically, the goals of this research effort 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 enable lightweight military hardware with dramatically enhanced survivability to serve the Soldier in the battlespace of the future, in addition to new paradigms for insensitive munitions.

6. 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.

7. 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. The goal of this MURI 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.

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 to be investigated. One goal of this research effort is to establish an ability to selectively disassemble and reconfigure these pathways through judicious exposure to heat, pH or light. The research also includes aspects of self-limiting growth of superclusters. The experimental program is complemented by a very strong theoretical component. Research approaches include the sequential staged self-assembly of nano-particles into complex and hierarchical architectures, the development of theoretical tools and computational algorithms to model the self-assembly process, identification of stable self assembly pathways that lead to the targeted hierarchical structures, and finally prediction of the final properties of the assembled material. Ultimately the research will focus on the derivation of tailored properties and functions within highly complex or hierarchical materials. This research effort may ultimately revolutionize the materials capabilities for building increasingly complex, functional materials of the future.

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

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

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

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

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

No new starts were initiated in FY11.

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

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESRIPTIONS AND FUNDING SOURCES.*

1. A Novel Oxygen Separation and Storage Apparatus for Underwater and High Altitude Fuel Cell Applications. A Phase II STTR contract was awarded to Enogetek, Inc. to explore room temperature ionic liquid, organometallic oxygen carrier, and support optimizations to realize novel oxygen transport membranes. The research team will build upon the facilitated oxygen transport (FOT) oxygen separation membrane fabrication and process optimization efforts established under the Phase I effort. Under the Phase II project, the team will design, fabricate, evaluate and optimize hollow fiber membrane modules based on the previously demonstrated membrane process technology. Extensive testing work will be carried out to evaluate membrane operation stability and durability under nominal operation conditions. Hydrophobic all-silica DDR-type zeolite membranes will also be fabricated and characterized as an alternative high efficiency membrane for oxygen separation from air, and both flat and hollow fiber type membrane will be fabricated and evaluated. A detailed analysis and comparison will be made between FOT membranes and DDR-type zeolite membranes. Based on these results, a prototype compact oxygen separation and storage system will be designed and constructed. The successful development of a low cost and high energy efficient oxygen extraction technology is expected to have tremendous economic impact on the steel, paper, and wastewater treatment industries.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) – 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). The FY11 new starts within these programs are described here, while the missions of each of these programs were described *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. DoD REP Awards. As described in more detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, REP awards aim to enhance or increase the programs, capabilities, and graduates in scientific and engineering disciplines in universities serving underrepresented minorities. In FY11, the Materials Science Division managed seven new REP projects, totaling $6.8 million. The equipment purchased with these awards is promoting research in areas of interest to ARO, such as the study of new methods for fracture mechanics analysis and characterization of novel single phase and multilayer multiferroic materials.

2. DoD TCU Instrumentation Awards. As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the TCU program aims to enhance science, mathematics, and/or engineering education programs and/or research capabilities through the acquisition of equipment and/or instrumentation that will augment existing facilities, enhance curricula, or help develop new laboratories, programs, and capabilities in these areas. In FY11, the Materials Science Division managed two new TCU projects. The equipment purchased with these awards is promoting education and research in areas of interest to ARO, including studies of the concentration and impact of heavy metal release into lakes and rivers using atomic fluorescence spectroscopy, and the mapping of subsurface structures using ground penetrating radar.

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

No new starts were initiated in FY11.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY11, the Materials Science Division managed six new DURIP projects, totaling $1.1 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies to explore thermoelectric materials, magnetocaloric materials and oxide heterostructures.

I. DARPA Nanostructured Materials for Power (NMP) Program

The DARPA NMP program seeks to exploit advanced nano-structured materials for revolutionary improvements in power applications of DoD interest. The ability to decouple and independently control physical, chemical, electromagnetic, and thermal phenomena through nanoscale design, is being tapped to enable improvements in the energy product of permanent magnets and the efficiency of future thermoelectric devices. The Materials Science Division currently co-manages projects within this program. The goals of these projects are ultimately to provide new nano-structured magnetic and thermoelectric materials with enhanced figures of merit for development of higher performance compact power sources in the future.

J. DARPA Bioinspired Photonics (BIP) Program

The goal of the DARPA BIP program is to harness innovative bioinspired synthetic organic and inorganic approaches to drive improved photonic material capabilities. Nature's hierarchical structures, scaling from micron to nanometer level, achieve remarkable optical functionality through complex scattering, reflection and absorption phenomena. The Bioinspired Photonics program draws inspiration from the best of nature's photonic structures to demonstrate tunable reflectors and volatile organic vapor sensors capable of operating in the visible and near infrared. The Materials Science Division currently co-manages projects within this program with the goal of identifying new approaches to the design and fabrication of future high performance photonic systems.

K. DARPA Low-Cost Light Weight Portable Photovoltaics (PoP) Program

The goal of the DARPA PoP program is to provide low-cost light-weight portable photovoltaics to DoD. The Materials Science Division currently co-manages projects within this program with the goal of exploring new materials solutions that can meet these goals.

L. DARPA Advanced Structural Fiber (ASF) Program

The goal of the ASF program is to develop and produce a fiber that offers at least a 50-percent 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 Materials Science Division currently co-manages projects within this program seeking to explore and optimize the most promising fiber compositions and processing strategies and to establish new paradigms for revolutionary fiber precursors.

M. DARPA Chemical Communications Program

The DARPA Chemical Communications program is exploring innovative methods to develop self-powered chemical systems that can encode an input string of alphanumeric characters (*i.e.*, a message), convert the message to a modulated optical signal, and transmit repetitively to a receiver. The ultimate goal of this program is to develop a small replicator device, with the form factor of a personal digital assistant or cell phone that will enable warfighters to generate disposable optical transmitters in real time, each with a user-specified message. The Materials Science Division currently co-manages projects within this program exploring various chemical phenomena capable of generating unique approaches to optical transmissions and communications.

N. DARPA Chemical Robots (ChemBots) Program

The goal of the ChemBots program is to create a new class of soft, flexible, mesoscale mobile objects that can identify and maneuver through openings smaller than their dimensions and perform various tasks. This program seeks to create a convergence between materials chemistry and robotics through the application of any one of a number of approaches, including gel-solid phase transitions, electro- and magneto-rheological materials, geometric transitions, and reversible chemical and/or particle association and dissociation. The Materials Science Division currently co-manages projects within this program seeking to demonstrate a new functional form of matter to enable an entirely new approach to robotic sensing and data collection.

O. DARPA Feedback Regulated Automatic Molecular Release Program

The goal of the DAPRA Feedback Regulated Automatic Molecular Release program is to develop biodegradable self-regulating drug delivery systems that enable feedback-regulated release in response to a biomarker(s) correlated with drug efficacy and/or toxicity. These systems will enable Soldier self-care through the development of drug delivery methods that assure, in the combat environment, the delivery of a therapeutic dose while eliminating the possibility of drug overdose. Delivery systems for one or more of the therapeutics classes that are currently used in tactical field care or battlefield medicine are of particular interest. The early objectives of this project are to demonstrate that the release rate of the drug from the new system is sufficient to achieve therapeutic levels, but can be reduced by an amount sufficient to avoid toxicity (*e.g.*, >10:1) in the presence of a biomarker correlated to a toxic effect. The Materials Science Division currently co-manages projects within this program seeking to realize novel approaches to battlefield drug delivery systems based upon novel molecular structures and materials architectures.

P. 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 resorbable by-products 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 the elimination of infection and secondary fractures. The Materials Science 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.

Q. DARPA Instant Fire Suppression (IFS) Program

The DARPA IFS program seeks to establish the feasibility of a novel flame-suppression system based on destabilization of flame plasma with electromagnetic fields, acoustics, ion injection or other novel approaches. The key to transformative firefighting approaches may lie in the fundamental understanding of fire itself. Fire suppression technologies have largely focused on disrupting the chemical reactions involved in combustion. Yet from a physics perspective, flames are cold plasmas consisting of mobile electrons and slower positive ions, and by using physics techniques rather than combustion chemistry, it may be possible to extinguish and/or manipulate flames. To achieve this goal, key scientific breakthroughs are needed to understand and quantify the interaction of electromagnetic and acoustic waves with the plasma in a flame. IFS research results will be used to determine the scalability of potential techniques, and if scaling is achievable, the program will design and construct a prototype fire suppression system for Class A and B fires inside of a ship or HUMVEE-sized compartment. The Materials Science Division currently co-manages a project within this program seeking to understand and demonstrate new paradigms for flame suppression and control.

R. 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.

S. DARPA PowerSwim Program

The DARPA PowerSwim program is developing highly-efficient, human-powered swimming devices for use by combat and reconnaissance swimmers. This program explores a new concept in swimming propulsion that uses the oscillating foil approach to swimming that is exhibited by many fish and aquatic birds. This propulsion approach is more than 80% efficient in conversion of human motion to forward propulsion. Typical recreational swim fins are no more than 15% efficient in their conversion of human exertion to propulsive power. This dramatic improvement in swimming efficiency will enable subsurface swimmers to move up to two times faster than is currently possible, thus improving swimmer performance, safety, and range. The Materials Science Division currently co-manages a project within this program exploring novel materials and designs to provide revolutionary enhancements to the swimming propulsive efficiency of combat swimmers.

T. DARPA Programmable Matter Program

The goal of the DARPA Programmable Matter program is to demonstrate a new functional form of matter, based on mesoscale particles, which can reversibly assemble into complex 3D objects upon external command. These 3D objects will exhibit all the functionality of their conventional counterparts. Programmable Matter represents the convergence of chemistry, information theory, and control into a new materials design paradigm referred to as "InfoChemistry," which involves building information directly into materials. Of critical importance are radical new material architectures that maximize the efficiency of information processing/transfer, and design rules for the optimal number, size, and shape of particles required to create objects of a specific size and spatial feature resolution. The Division currently co-manages projects within this program exploring a wide range of materials systems, compositions, and structures to provide reversible assembly and robust control.

U. DARPA Revolutionizing Prosthetics Program

The DARPA Revolutionizing Prosthetics program will create, within this decade, a fully-functional (motor and sensory) upper limb that responds to direct neural control. This revolution will occur by capitalizing on previous DARPA investments in neuroscience, robotics, sensors, power systems, and actuation. DARPA has delivered a prosthetic for pre-clinical trials that is far more advanced than any device currently available. This prosthetic enables many degrees of freedom for grasping and other hand functions, and will be rugged and resilient to environmental factors. This program now seeks to deliver a prosthetic for clinical trials that has function almost identical to a natural limb in terms of motor control and dexterity, sensory feedback (including proprioception), weight, and environmental resilience. The results of this program will allow upper limb amputees to have as normal a life as possible despite their severe injuries. The ARO Materials Science and Life Sciences Divisions currently co-manage a project within this program with the goal of optimizing materials and controling architectures to realize maximum capabilities in upper-arm prostheses.

V. 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.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. A New Family of Solitary Waves in Granular Dimer Chains

Professor Alexander Vakakis, University of Illinois - Urbana Champaign, MURI Award

The objective of this effort is to establish a new class of material systems that have the ability to mitigate adverse effects of stress wave propagation by exploiting wave tailoring phenomena in highly nonlinear inhomogeneous granular media. The research 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.

Researchers at the University of Illinois at Urbana Champaign recently discovered a new family of solitary waves in general one-dimensional dimer chains with elastic interactions between beads obeying a strongly nonlinear Hertzian force law. These dimers consist of pairs of 'heavy' and 'light' beads without the application of pre-compression forces. The solitary waves discovered can be considered analogous to the solitary waves in general homogeneous granular chains, in the sense that they do not involve separations between beads, but rather satisfy special symmetries or, equivalently anti-resonances in their intrinsic dynamics. These solitary waves appear to be the direct products of a countable infinity of anti-resonances in the dimer. Simulations indicate that the solitary waves in the dimer propagate faster than solitary waves in the corresponding homogeneous granular chain obtained in the limit of no mass mismatch between beads. This finding, which may at first appear counter-intuitive, indicates that under certain conditions nonlinear anti-resonances can increase the speed of disturbance transmission in periodic granular media, through the generation of new ways for transferring energy to the far field of these media. In addition, resonances were determined to produce a much more efficient pulse attenuation in these dimmers than in their compressed (weakly nonlinear) counterparts (see FIGURE 1).

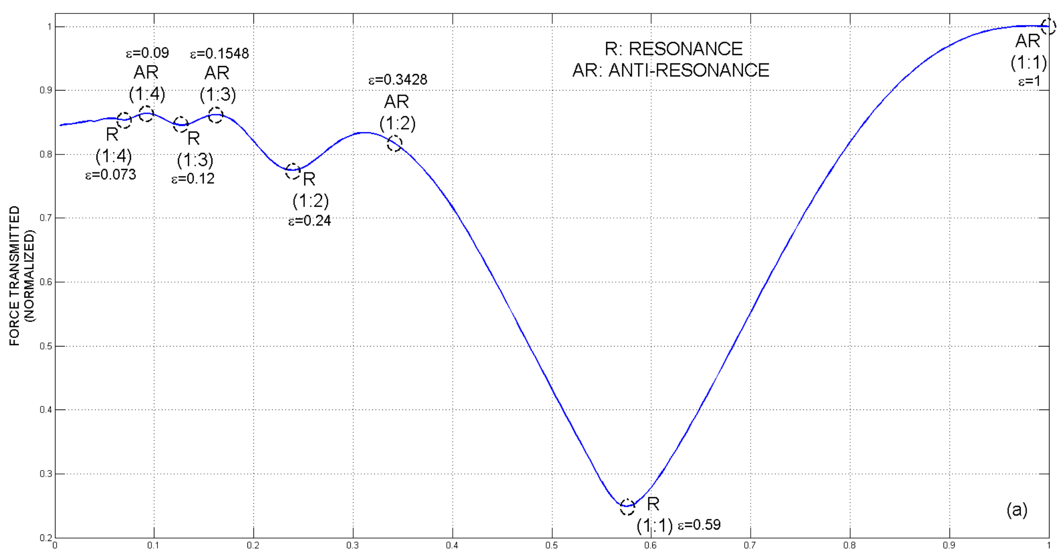

FIGURE 1

Resonances produce more efficient pulse attenuation in recently-discovered dimmers vs. compressed counterparts. Normalized force transmitted to the end of the granular dimer, with anti-resonances (AR) and resonances (R) indicated. Note that each point also indicates the number ratio of the "heavy" beads to "light" beads in the chain (*i.e.*,1:1 corresponds to the homogeneous granular chain) and ε is the normalized mass ratio of the "heavy" beads to the "light" beads.

As shown in the figure, the discrete values where solitary waves (anti-resonances) are realized are evidenced as peaks (local maxima), indicating that the formation of solitary waves provides a mechanism for effective transmission of energy through the dimer. Valleys (local minima) correspond to optimal (local) scattering of the energy of the pulse by the dimer, hinting on realizations of resonances at these values of ε. Moreover, each anti-resonance is preceded and followed by a resonance and vice versa. Discrete values of ε where valleys are realized corresponding to locally minimal transmitted forces. From a practical point of view, this result can have interesting implications in applications where granular media are employed as shock transmitters or attenuators.

B. First-ever Demonstration Of Deformation Twin Activation in Nanocrystalline Mg

Professor Yuntian Zhu, North Carolina State University, STIR Award

The objective of the STIR project, now completed, that led to this noteworthy FY11 accomplishment, was to understand twinning mechanisms in nanostructured hcp metals and their alloys. More specifically, the researchers probed two fundamental deformation-related mechanisms (deformation twinning and solution clustering) with an aim of producing ultra-strong Mg alloys with good ductility. While deformation twinning has not previously been reported in nanocrystalline (nc) hcp alloys, this effort aimed to enable deformation twinning, to provide both strength and ductility enhancements, in the Mg alloy system by precision alloying to lower the stacking fault energy.

This research led to the successful demonstration of the activation of twinning in an nc hcp Mg–Ti alloy. Nanocrystalline Mg with 10 wt% Ti samples were prepared by ball milling, using a steel vial and balls. Starting materials were elemental powders of Mg (99.9%) and Ti (99.5%). X-ray analysis revealed Bragg peaks corresponding to the hcp Mg phase after 24 h milling, indicating no new phases were formed and the Ti formed a solid solution with Mg. High-resolution electron microscopy images were captured for two deformation twins in the as-processed nc Mg–Ti alloy (see FIGURE 2).

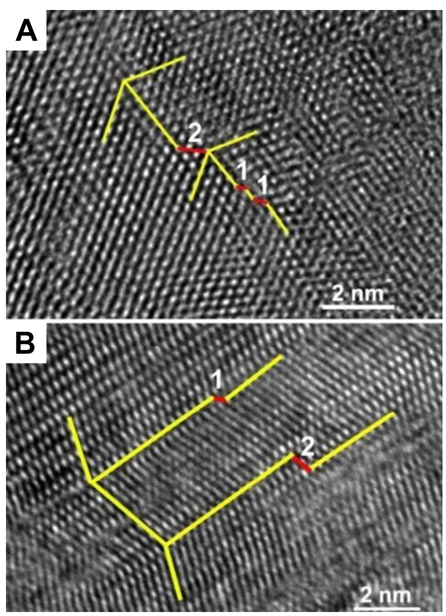

FIGURE 2

High-resolution transmission electron micrographs of twins in nanocrystalline MgTi alloy. The twin system in both micrographs is {10$\underline{1}$1}<10$\underline{12}$>. (**A**) An HREM micrograph showing deformation twin in the nc Mg-Ti alloy, viewed along a [11$\underline{2}$3] zone axis, A two-atomic-layer step and two one layer steps are on the twin boundary. (**B**) HREM micrograph showing another deformation twin with a two-layer step on the lower twin boundary and a one-layer step on the upper twin boundary. The two-layer steps are consistent with the zonal twinning dislocation predicted by MD simulation.

The images shown in the figure are viewed from a [1123] zone axis. Coherent twin boundaries and mirror images of atomic arrangements are clearly shown, verifying that they are indeed twins. The {1011}<1012> deformation twins observed are consistent with the twinning mode observed in MD simulation of Mg under compression. These simulations predicted that {1011}<1012> deformation twins grow by the slip of a zonal twinning dislocation, ½ • ½ <1012>, on the coherent (1011) twin boundary, followed by atomic shuffling. This zonal dislocation involves two (1011) planes, forming a two-layer step on the twin boundary. The MD simulations also predicted that the one-layer steps are immobile, and the four-layer steps are unstable and can spontaneously dissociate into two two-layer steps. Consistent with these predictions, one-layer steps were observed experimentally (see FIGURE 2), while no four-layer steps have been observed.

C. Self-Limiting Growth of Monodisperse Supraparticles

Professor Sharon Glotzer, University of Michigan, MURI Award

The objective of this MURI project is to uncover the scientific foundations and technical know-how to create an entirely new class of self-assembled, reconfigurable colloidal materials with radically increased complexity and functionality. Professor Glotzer and her collaborator, Professor Nicholas Kotov, have discovered that a delicate balance of atomic forces can be used to self assemble nanoparticles into superclusters of a uniform size. This is an important attribute for many nanotechnology applications. This self-limiting growth process is accomplished by establishing a balance between electrostatic repulsion and van der Waals attraction among the nanoparticles, and is actually improved when a broad polydispersity of size and shape of the constituent nanoparticles is present. The diameter of the supraclusters, which can be controlled easily over the range of 20-50 nm, was found to be a simple function of growth time and temperature (see FIGURE 3).

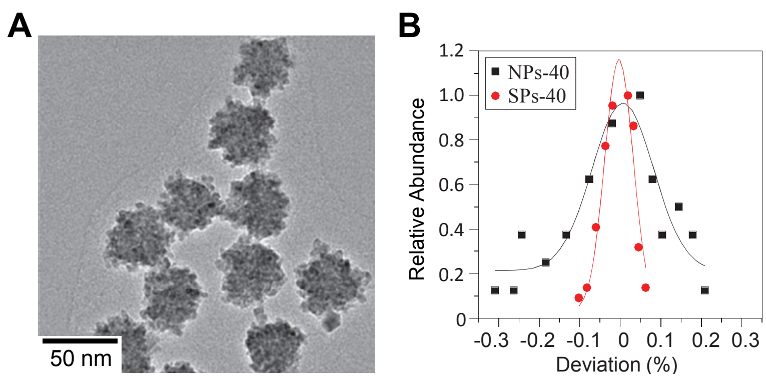

FIGURE 3

Self-limiting growth of nanoparticles. This study revealed that the diameter of supraclusters is a function of growth time and temperature. (**A**) The micrograph reveals set of 42 ±3.5 nm CdSe supraclusters that were grown in solution for 1080 minutes at 80˚C using short-chain citrate organic molecules to stabilize the nanoparticles. (**B**) Comparison of the relative size distributions for the nanoparticles and the supraclusters. The difference highlights the self organizing principles that distinguish this process from those reported previously. These inorganic superclusters share many of the same attributes possessed by simple life forms, including size, shape, core-shell structure and the ability to assemble and dissemble.

D. NMR Investigations of Atomic Structure and Dynamics of Bulk Metallic Glasses

Professor Yue Wu, University of North Carolina - Chapel Hill, Single Investigator Award

The great challenge to the applications of bulk metallic glasses (BMGs) is their limited plasticity. Since dislocations are absent in BMGs, an issue of central importance is the fundamental understanding of the deformation mechanism. To successfully achieve this objective, a thorough investigation of changes in local atomic structure imparted by deformation and thermal relaxation is essential. In this project, the investigator used ^{27}Al NMR to capture, for the first time, atomic scale rearrangements after preloading below yield strength at room temperature in $La_{50}Ni_{15}Al_{35}$ metallic glass.

NMR Hahn-Echo experiments were used to explore how changes of structural ordering at ^{27}Al sites depend on uniaxial preloading time and pressure. The Hahn-Echo intensity is measured as a function of 2nd pulse duration. This allows one to quantitatively determine the electric-field-gradient (EFG) since ^{27}Al is a quadrupolar nucleus. The NMR fitting parameter obtained from these experiments is the *quadrupolar frequency,* ω_Q , which depends on the EFG or symmetry of the external charge distribution. The investigator found that compression below the yield strength, in comparison with the as-cast state, enhanced structural symmetry (*i.e.*, lowered the quadrupolar interaction or ω_Q) around ^{27}Al atoms and is proportional to the loading time (see FIGURE 4). In addition, the structural symmetry for the annealed state (20 deg below glass transition, Tg.) shown in the figure reveals that thermal relaxation does not compromise the metallic glass structure. These results demonstrate that structural symmetry is an important and essential order parameter for understanding the mechanism of deformation in metallic glasses.

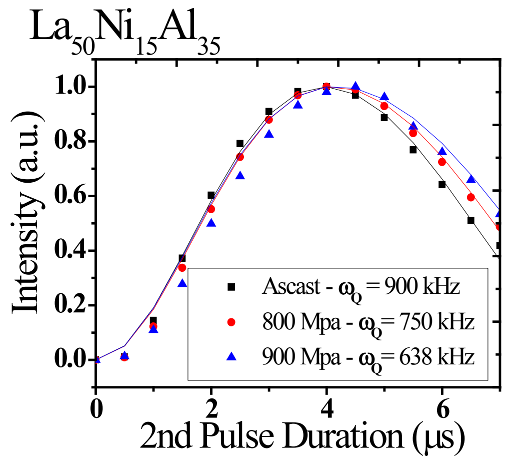

FIGURE 4

NMR Hahn-Echo analysis for $La_{50}Ni_{15}Al_{35}$. This data plot reveals the enhancement of structural symmetry (quadropolar interaction) in the BMG after compression of the sample below the yield stress.

E. Millimeter and Sub-millimeter Wave Magnetoelectric Interactions in Layered Multiferroics: Phenomena and Devices

Professor Gopalan Srinivasan, Oakland University, Single Investigator Award

The research is aimed at a new class of low-loss, miniature, tunable ferrite signal processing devices for 1-110 GHz for use in the next generation of radars and communication systems. The approach is to synthesize novel ferrite-ferroelectric layered composites, investigate the nature of interaction between the sub-systems, and design and characterize *electric field* tunable ferrite resonators, filters and phase shifters. Magnetic field tuning of ferrite devices is often slow, noisy, and requires kW power for operation. Composite based devices are planar, miniature in size, require mW power for operation, and can be integrated with semiconductor devices. In FY11, studies of microwave magnetoelectric (ME) effects over 8-25 GHz in bilayers of single crystal Y-type hexagonal ferrite $Ba_2Zn_2Fe_{12}O_{22}$ and single crystal lead magnesium niobate-lead titanate (PMN-PT), revealed evidence for strong ME coupling (see FIGURE 5). In addition, the investigator designed and characterized a ferrite/PMN-PT based phase shifter (see FIGURE 6). Data on phase shift vs. E revealed a phase shift of 50 deg, a linear variation in the phase shift with E and low insertion loss.

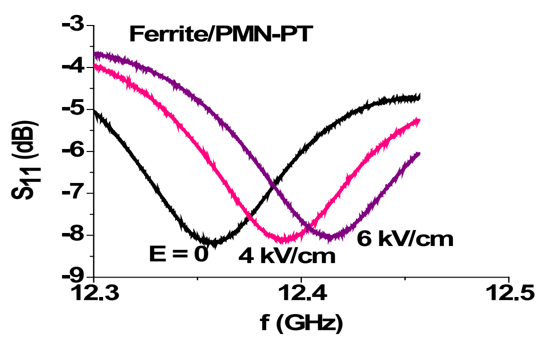

FIGURE 5

Electric field-tunable ferrite. Electric field E tuning of magnetic resonance in hexaferrite/PMN-PT bilayer indicating ME strong interaction in the system. Ferrite devices such as 8-25 GHz resonators that are usually tuned with a magnetic field can be tuned with a DC voltage.

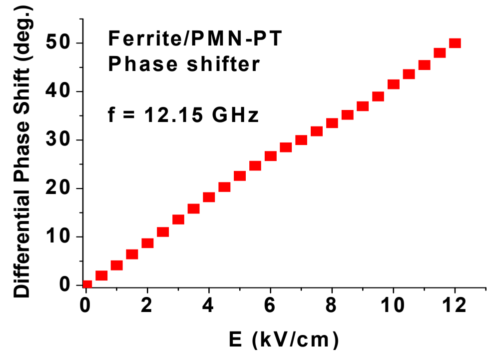

FIGURE 6

Differential phase shift vs. *E* at 12.38 GHz for ferrite/PMN-PT. Data on phase shift vs. *E* revealed a phase shift of 50 deg, a linear variation in the phase shift with *E* and low insertion loss.

F. Domain Wall Evolution in Phase Transforming Oxides

Professor Jacob Jones, University of Florida, PECASE Award

The objective of this project is to enhance the basic understanding of mechanistic contributions to properties of ferroelectric materials. The PI and his team took an approach to utilize advanced, real-time characterization techniques including high-resolution and high-energy *in situ* X-ray and neutron diffraction experiments to measure and quantify subtle changes in crystallography and microstructure during electric field or temperature change. The researchers determined that the contribution of ferroelectric domain wall motion to the macroscopic piezoelectric strain coefficient, d_{33}, exceeds 50% in certain compositions of lead zirconate titanate (PZT) materials (see FIGURE 7). This measurement was insightful because it was the first direct measurement of the contribution of domain walls to this property. Prior indirect measurements could only quantify the irreversible contribution of domain walls moving across pinning centers by evaluating the field-amplitude dependence of the property coefficient. However, the diffraction experiments measured the additional reversible motion of domain walls between pinning centers. The team also demonstrated in this work that previously ignored intergranular interactions account for a surprisingly large portion of the d_{33} value. These results demonstrate that electromechanical coupling in polycrystalline aggregates is substantially different from that observed in single crystalline materials.

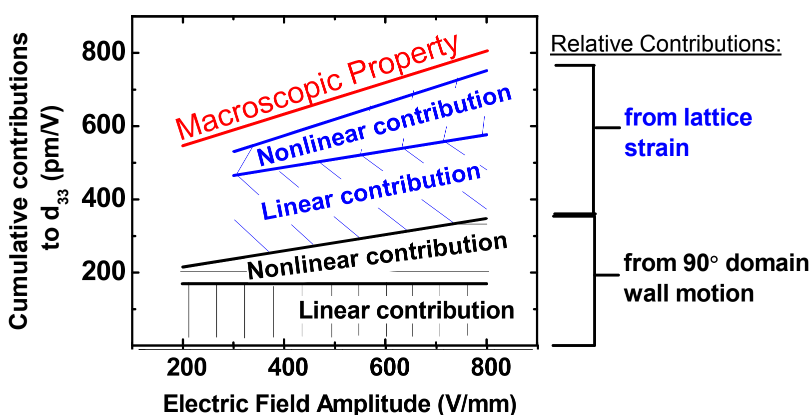

FIGURE 7

Relative contributions to the piezoelectric coefficient, d_{33}. Field-amplitude independent domain wall contributions are only measurable using this technique. Total domain wall contributions approach 50% of the total property coefficient.

Another significant accomplishment of this project includes understanding structure of Pb-free ferroelectrics. Sodium bismuth titanate ($Na_{0.5}Bi_{0.5}TiO_3$, or NBT) is a Pb-free component in several solid solutions currently under investigation to replace PZT and provides a useful contrast. Its structure has been assumed to be rhombohedral with space group *R*3*c* and $a^-a^-a^-$ octahedral tilting at room temperature. However, the PIs high-resolution X-ray diffraction measurements of NBT confirmed the monoclinic space group *Cc* with $a^-a^-c^-$ octahedral tilting. Prior work in PZT has suggested that the monoclinicity of the crystal structure is the reason for the high piezoelectric coefficient. However, the present measurements show that a different monoclinic crystal structure exhibits a small piezoelectric coefficient (~80 pm/V). These measurements further reinforce the idea that domain wall motion contributes significantly to the piezoelectric coefficient in ferroelectric materials. Piezoelectric materials are used in several military applications and devices including surveillance, reconnaissance, navigation, frequency filters, surface acoustic wave devices, accelerometers, sensors, nonlinear optics, ultrasonics, sonar, microphones, and hydrophones.

G. Lattice Engineering for Novel Materials and Devices

Professor E.A. Fitzgerald, MIT, Single Investigator Award

The objective of this project is to systematically explore and advance the creation of new, composite electronic materials via defect science and heteroepitaxy for demonstrating and exploiting novel optical and electronic properties. Professor Fitzgerald and a co-investigator, Professor Ringel at Ohio State University, have investigated combined epitaxy of III-V and IV compounds on a single platform (Si). The MIT-OSU team used both Molecular Beam Epitaxy (MBE) and Metal Organic Chemical Vapor Deposition (MOCVD) growth methods to explore these materials and interfaces (see FIGURE 8).

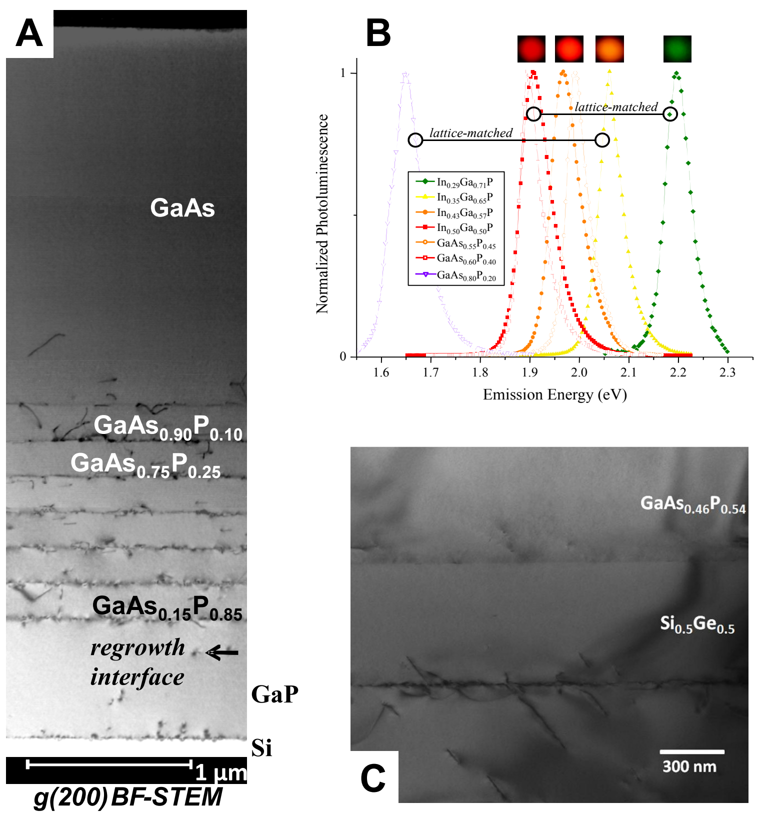

FIGURE 8

MBE and MOCVD to explore epitaxy of III-V and IV compounds on Si. (A) First high quality GaAsP grades on Si out to GaAs; achieved via MBE; (B) first demo of strong light emission from red to green on Si (room temp PL of bare III-V layers on Si by MBE); (C) first high quality GaAsP/SixGe1-x interfaces; achieved by MOCVD.

The researchers addressed relaxation of stress of GaAsP/Si by using GaAsP and SiGe composition-graded layers that introduce defects through controlled nucleation and propagation. The heterovalent interfaces between III-V and IV semiconductors were explored in the lattice-matched interfaces of GaP/Si or GaAsP/SiGe. The defect and lattice structure was explored through characterization techniques like TEM, x-ray diffraction, AFM etc. The researchers have been able to create high quality heterovalent interfaces in both GaP/Si and GaAsP/SiGe. In the case of GaAsP/SiGe/Si, the researchers found that the growth conditions must be such that some As and P exposure occurs, but not significant enough exposure that the single-domain SiGe surface (on off-cut wafer) is substantially altered. For GaP/Si, there is no growth window in which this is possible, and therefore they preserve the step-structure by depositing Ga-first at low temperatures. In combination with graded composition SiGe or GaAsP layers, the team demonstrated interfaces with low defect density for GaP/Si and for GaAsP/SiGe/Si for As concentrations greater than approximately 50%. Photoluminescence results revealed that LEDs on silicon were observed across the visible range from red to green. The GaAsP band gaps mentioned here, and their lattice-matched InGaP complements, can be used to form high efficiency multi-junction solar cells on silicon, resulting in lower cost, high efficiency, lightweight solar cells for remote power applications and high performance low-cost multi-spectral cameras.

H. Electrical Switching of Ferromagnets Using Spin Currents Generated By Spin Hall Effect

Professors Dan Ralph, Cornell University and David Awschalom, UCSB, MURI Award

Following upon the recent discovery at UCSB of the Spin Hall effect in semiconductors, researchers at Cornell University have found that even stronger effects can be obtained in platinum. The investigators also showed that these currents can be large enough to switch a ferromagnetic element. The Spin Hall effect allows spin currents to be generated without the use of ferromagnetic spin polarizers, due to electrons flowing in a nonmagnetic material containing heavy elements, in which spin orbit coupling can cause spin up and spin down electrons to be deflected in opposite directions (due to either different scattering processes or band structure effects). Thus, a charge current in one direction produces a perpendicular pure spin current. Professor Ralph and colleagues have shown that the pure spin current generated by the Spin Hall effect can be used to apply a spin transfer torque to a ferromagnet to efficiently switch the magnetization of a perpendicularly-polarized magnetic layer. This is an appealing strategy for many applications because it enables a lateral charge current to produce a vertically-flowing spin current to apply a spin torque, and avoids the need to send large charge current densities vertically through delicate tunnel barriers as in magnetic tunnel junctions controlled by conventional spin transfer torque.

I. Thermodynamic Stabilization of Powder-Route Nanocrystalline Tungsten Alloys

Professor Christopher Schuh, Massachusetts Institute of Technology (MIT), Single Investigator Award

One of the major challenges with nanocrystalline metallic materials is their tendency to undergo grain growth at moderately elevated temperatures wherein any advantageous properties are compromised. The goal of the project is to develop a tungsten-rich alloy powder that can be produced readily in a nanocrystalline form that is sufficiently stable to resist significant structural change during high-temperature consolidation to full density. To achieve this goal, the researchers have employed theoretical modeling to identify candidate alloys with improved stability in the nanocrystalline state.

The Regular Nanocrystalline Solution (RNS) model, developed under ARO funding in previous work by Professor Schuh, can predict the existence of a nanocrystalline phase that is stable against grain growth via grain boundary segregation. A second consideration for the stability of a nanocrystalline alloy is its stability against second phase precipitation. To quantify the stability of a nanocrystalline binary alloy with respect to second phase formation, the Gibbs free energy of the predicted (from RNS) stable NC phases to the free energy of secondary phases is compared. Varying the materials parameters in the RNS model across the range of appropriate values, a nanocrystalline behavior map with three regions was produced (see FIGURE 9). These results revealed one region where there is no NC phase that is stable in the particular system, one in which a NC phase exists that is stable against grain growth but not phase separation, and one in which the NC phase that exists is stable against both grain growth and phase separation. The suitability of tungsten based alloys can be evaluated at first pass using this map. The property space thus far examined by the RNS model involves only binary alloys with positive enthalpies of mixing, denoting phase separating materials. Using this model, W-Ti was selected as the most promising binary systems; the Ti additive is introduced because it has a low tendency to phase separate, but can segregate to grain boundaries and lead to nanostructure stabilization.

The discovery of a methodology to produce stable full-density nanocrystalline tungsten could have significant potential in kinetic energy penetrator applications where a high-density and self-sharpening via shear localization are critical top optimal performance.

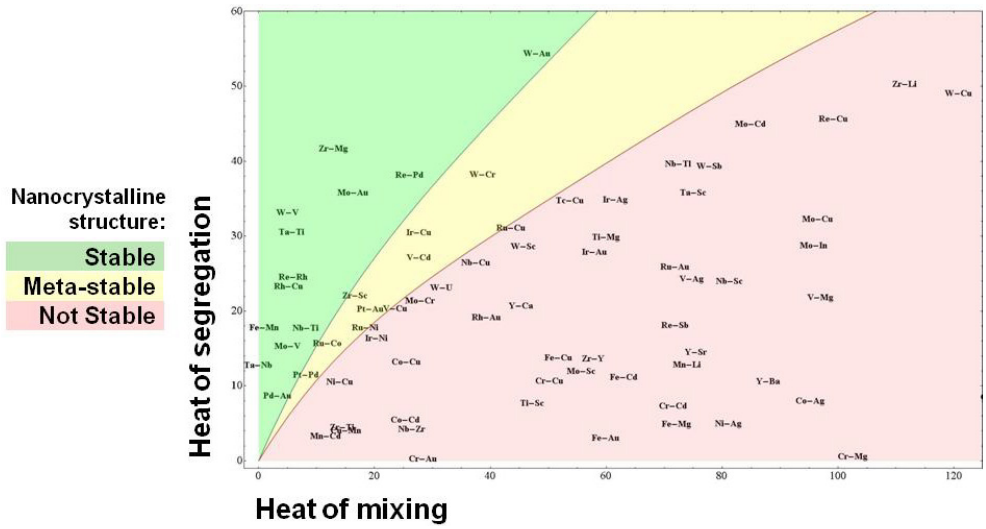

FIGURE 9

New thermodynamic model describing segregation of solute to nanoscale grains. For certain combinations of material properties (green area), the system exhibits a minimum in the free energy, indicating a stable nanocrystalline grain size. For many phase separating systems, a minimum does not exist, and stable nanocrystalline grains are not achievable (pink area.)

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. Bicontinuous Battery Electrode

Investigator: Professor Paul Braun, University of Illinois at Urbana Champaign, MURI Award
Recipient: Xerion Advanced Battery Corp

The objective of the research effort that led to this technology transfer is to advance discoveries in the areas of interference lithography, single crystal III-V heterostructured 3-D photonic crystals, and holographic patterning in IR transparent chalcogenide glasses to realize unprecedented 3D photonic crystals. Rapid charge and discharge rates have become an important feature of electrical energy storage devices, but cause dramatic reductions in the energy that can be stored or delivered by most rechargeable batteries due to their limited energy capacity. Supercapacitors do not suffer from this problem, but are restricted to much lower stored energy per mass (*i.e.*, energy density) than batteries. Recently, researchers developed a storage technology that combines the rate performance of supercapacitors with the energy density of batteries by demonstrating very large battery charge and discharge rates, with minimal capacity loss by using cathodes made from a self-assembled three-dimensional bicontinuous nanoarchitecture consisting of an electrolytically active material sandwiched between rapid ion and electron-transport pathways (see FIGURE 10). Rates of up to 400°C and 1,000°C for lithium-ion and nickel-metal hydride chemistries, respectively, have now been achieved (where a 1°C rate represents a one hour complete charge or discharge), enabling fabrication of a lithium-ion battery that can be 90% charged in 2 minutes. These results formed the basis for a new battery that transferred to a new start-up company, Xerion Advanced Battery Corporation, for further development.

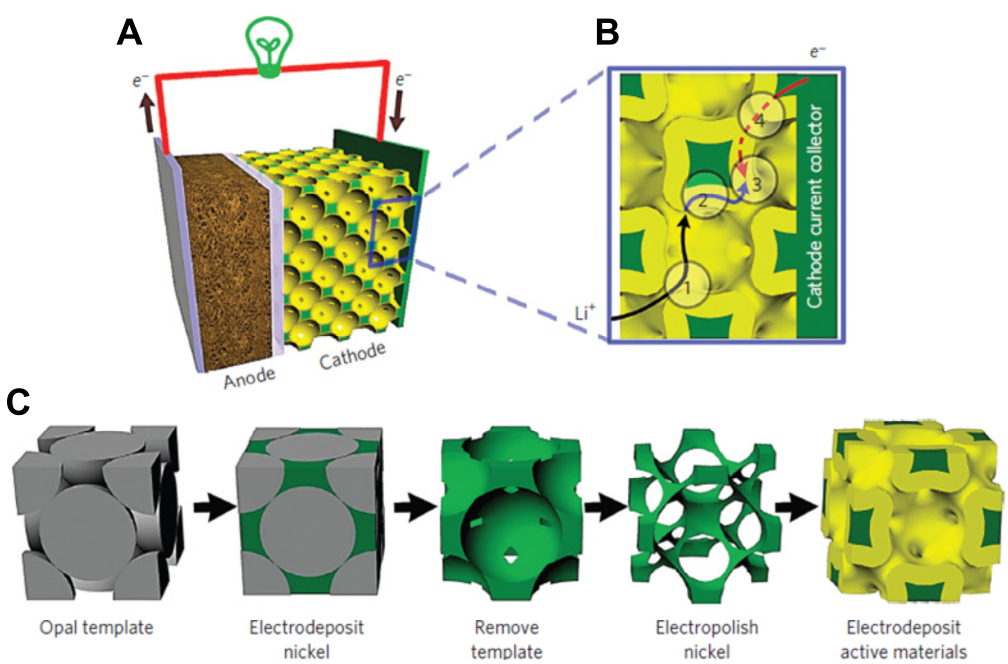

FIGURE 10

New battery design consisting of self-assembled three-dimensional bicontinuous nanoarchitecture. The panels illustrate (**A**) schematic of a battery containing a bicontinuous cathode, (**B**) the four primary resistances in a battery electrode, and (**C**) the bicontinuous electrode fabrication process. The electrolytically active phase is yellow and the porous metal current collector is green. The electrolyte fills the remaining pores.

B. Defect Engineering for the Development of Ultra-Low Loss Microwave Dielectrics
Investigator: Professor Nate Newman, Arizona State University, Single Investigator Award
Recipients: Freescale Inc. and Trans-tech Inc.

The objective of the current research project that led to this transition is to establish a fundamental understanding of microwave loss mechanism and the defect's contribution in dielectric materials. This is expected to facilitate development of dielectric materials with large ε, reduced tan δ and a zero temperature coefficient of resonant frequency. The investigators have used fundamental principles involving defect engineering and modern solid state methods to develop a fundamental understanding of microwave loss.

Professor Newman and co-investigator Professor Mark van Schilfgaarde, discovered that $Ba(Zn_{1/3}Ta_{2/3})O_3$ (BZT) and $Ba(Cd_{1/3}Ta_{2/3})O_3$ (BCT) exhibit the unusual combination of a large ε and a small tanδ at microwave frequencies. Ab-initio electronic structure calculations show this comes from charge transfer between cation *d*-orbitals providing covalent directional bonding and facilitates a more rigid lattice with higher melting points, enhanced phonon energies and thus low microwave loss. Also, *ab initio* DFT was used to calculate BZT and BCT phonon resonant frequencies, and a good agreement with experimental data was found. This observation allowed identifying the nature of each phonon mode in the optical spectra. The researchers also found that microwave loss in BZT occurs under three different regimes. First, at high temperatures, the dominant mechanism comes from resistive loss resulting from carriers generated by oxygen-defect complexes. Optical absorption studies on these same sample show that the magnitude of this electrical conduction scales with the defect concentration. Second, at cryogenic temperatures, the dominant loss comes from paramagnetic absorption from dopant's unpaired electrons. Transition metal dopants with unpaired electrons (*e.g.*, Ni & Mn) degrade Q in direct proportion to their concentration. However, impurity dopants such as Cd and Mg can actually enhance the quality factor to a record for high dielectric constant materials of 200,000 @ 2 GH (see FIGURE 10). Lastly, at moderate temperatures, including the ever-important room temperature, several different mechanisms can absorb microwave radiation. However, for high-quality materials, absorption from anharmonic multiphonon processes dominate the loss. It is found that when the anharmonic phonon line width (proportional to the lifetime) is measured, it strongly correlates to the microwave performance (*e.g.*, Q) of the material in both undoped and intentionally doped materials. This research has transitioned to Freescale Inc. and Trans-tech Inc. for developing practical microwave devices, such as ceramic injection molded BZT microwave filters and resonators for next-generation radar and communication systems.

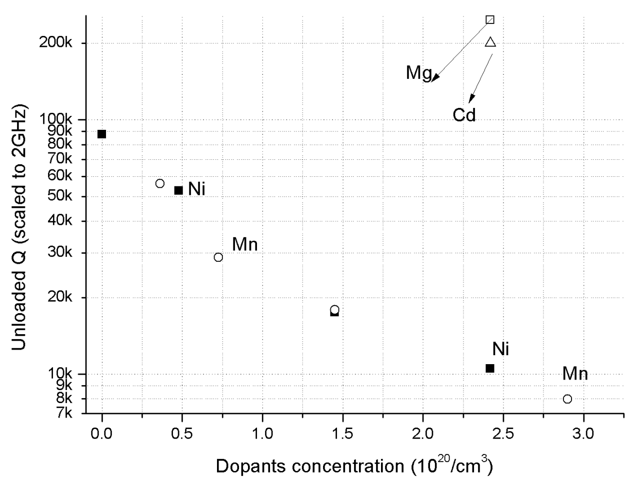

FIGURE 11

Microwave performance as a function of paramagnetic (Ni, Mn) and non-paramagnetic (Cd, Zn) concentrations. Transition metal dopants with unpaired electrons (*e.g.*, Ni & Mn) degrade Q in direct proportion to concentration. However, impurity dopants such as Cd and Mg can actually enhance the quality factor to a record for high dielectric constant materials of 200,000 @ 2 GH.

C. Nano-detector Based On Thermoelectric Nanowires
Investigator: Professor Tito Huber, Howard University, HBCU Award
Recipient: ARL Sensors and Electron Devices Directorate (ARL-SEDD)

With original support from ARO, researchers at Howard University have investigated the thermoelectric properties of arrays of densely packed, highly oriented, crystalline Bi nanowire composites. These were prepared by injecting molten Bi under high-pressure into the cylindrical channels (20-200 nm) of anodized aluminum (porous alumina). It had been predicted that large quantum confinement effects might lead to large enhancements in the thermoelectric properties of the material that would further the development of high performance thermoelectric coolers for IR detectors. However, exhaustive transport studies on individual wires established that surface bands rather than bulk states dominated the transport properties at lower temperatures and wire dimensions and that the anticipated gains in bulk thermoelectric performance were not to be realized. In fact, quantum confinement effects in the smallest wires (below 50 nm) actually drove the bulk semimetal-semiconductor transition resulting in an insulating state. However, these nanowires were found to have metallic surface states that showed topological insulator behavior, which resulted in extremely high surface electron mobility resulting from the limited scattering and time reversal properties associated with these surface states. In a rather surprising turn of events and with funding and technical support from Boeing, a team of researchers from Howard, Boeing and ARL-SEDD are now actively investigating whether these nanowire arrays might actually be used as the basis for a new IR nano-thermocouple detector which would have the attractive property of being able to scale down to very small pixel dimensions.

D. Microstructural Stability and Deformation Behavior in Tantalum Carbides
Investigator: Professor Gregory Thompson, University of Alabama - Tuscaloosa, Single Investigator Award
Recipients: Air Force Research Laboratory; Missile Defense Agency

One of the significant challenges of utilizing tantalum carbides (TaxC1-x) and other similar refractory compounds is their high melting points. Though advantageous for ultrahigh temperature applications, the difficulty in production of fully dense, near net shape structures limits the ability for easy manufacturing. This project investigates the γ-TaC phase, which has a melting temperature near 4,000 ^{o}C. The precipitation of substoichiometric Ta-rich phases, such as α/β-Ta2C and ξ-Ta4C3, with similar high melting points, provides ample opportunities to tailor the microstructure for improved thermomechanical behavior. Professor Thompson has collaborated and transitioned the ARO-sponsored research to the Air Force Research Laboratory - Materials Directorate, and the Missile Defense Agency for studies to further optimize (with high-resolution transmission electron microscopy analysis) and scale-up (via hot isostatic pressing) TaC components. An improved understanding of the thermomechanical behavior and scalability of tantalum carbides might lead to applications including rocket nozzle and other high operating temperature apparatus.

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. Fundamental Studies on Confinement Effects in Ionic conduction and Inversion Layers in 2D Single-crystal Free-standing Oxide Membranes

Professor Shriram Ramanathan, Harvard University, Single Investigator Award

The project aims to develop a fundamental understanding of conduction phenomena in quasi two-dimensional free standing functional oxide structures. Due to close proximity of free surfaces, 2D oxide materials are expected to have unusual conduction phenomena that include substantially altered electrolytic domain boundary, ionic-electronic conduction transitions not seen in bulk counterparts. Experimental techniques to fabricate such free standing membranes with single crystal oxides and test structures to probe conduction phenomena over a broad range of temperatures and environment will be pursued. Rapid modulation of conductivity will be explored in a custom-designed probe station by exposure to chemical and optical stimuli. Representative structures that will be explored include but not limited to rutile oxides such as TiO_2 that exhibit complex compositional phase diagrams and conductance transitions driven by defect ordering. It is anticipated that in FY12, first-of-a-kind information on variable temperature conduction in such space-charge dominated materials will be uncovered and potentially may lead to new class of materials for ultra-responsive chemical sensors operable at low power.

B. Charge Density Engineering

Professor Krishna Rajan, Iowa State University, Single Investigator Award

Professor Rajan at Iowa State University and co-investigator Professor Mark Eberhart at the Colorado School of Mines are seeking to explore and assess the feasibility of charge density engineering. More specifically, the research aims to uncover the relationships between a material's electronic structure, its local elastic properties, and its composition. These process-structure-property relationships will be discovered by seeking correlations between structural and phenomenological databases. The work builds on the quantum theory of atoms in molecules (QTAIM), which has demonstrated that the structure of the charge density may be compactly represented by a few parameters describing the density around specific points. This “local approximation” reduces the description of a 3D scalar field—the charge density—to that of identifying the locations of the specified points and computing the values of shape descriptors at these points. It is anticipated that in the coming year the researchers will create a data set giving the shape parameters at all bcc and fcc transition metal critical points, and perform a quantitative assessment of correlations between topological descriptors from critical points using data dimensionality reduction methods. It is expected this work will dramatically enhance the field of materials design, particularly in the areas of energetic and protective materials.

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

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

The goal of this project is to investigate the interaction of laser light with micron-sized barium titanate glass microspheres immersed in water solutions. These spheres have pronounced whispering gallery mode resonances with intrinsic quality factors in excess of 104. This results in a strong coupling to the laser light. Early experiments using a fiber-coupled semiconductor laser (50mW tunable from 1100 to 1300 nm) showed that select microspheres could be propelled at velocities approaching 10 μm/s. In the coming year new studies will commence that use a more powerful tunable light source to investigate the resonant nature of these propelling effects and to determine whether it might be feasibility to use resonant optical effects to perform ultra-precise size sorting of spheres to achieve an unprecedented uniformity on the order of ± 0.01%.

D. Transparent SiALON Armor

Professor Gary Messing, Pennsylvania State University, ARO and DARPA-funded Award

The objective of this project is to develop a basic understanding of how to produce high performance, lightweight SiAlON, having both optical transparency and high hardness/toughness. Thus far, precursors have been selected, powder processes which yield homogeneous green microstructures with high green densities have been developed and densification, and microstructure evolution of alpha-SiAlON as a function of doping and sintering conditions was analyzed. The researchers have determined appropriate compositions, processing and hot pressing conditions for the production of translucent alpha-SiAlON ceramics (see FIGURE 12).

It is anticipated that in the next phase of the project, the experience gained on processing translucent alpha-SiAlON will be used for the development of the appropriate processing conditions to produce transparent alpha-SiAlON. Compositions will be developed which yield finer microstructures and lower secondary phase concentration. The results of the hot pressing (HP) studies will be transferred to spark plasma sintering (SPS) where the kinetics can be more conveniently controlled. In addition to these studies, direct sintering of undoped alpha-SiAlON powders (developed in the first phase of the program) via SPS, which is designed to reduce secondary phases, will be studied. The ability to fabricate fully transparent SiALON with high hardness and toughness may result in a new class of transparent armor material, and represents a major breakthrough in security materials.

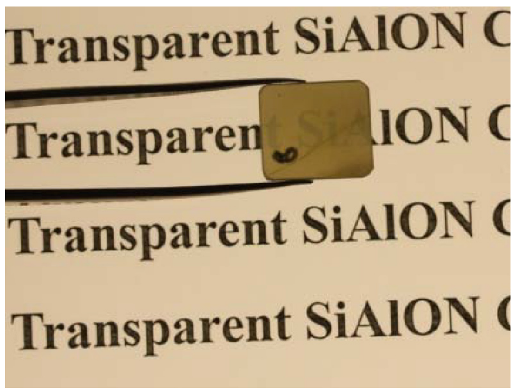

FIGURE 12

Image of translucent alpha-SiALON. An analysis of microstructure evolution of alpha-SiAlON as a function of doping and sintering enabled the investigators to determine the compositions, processing and hot pressing conditions for the production of translucent alpha-SiAlON ceramics. The sample is being held 5 cm above the letters.

VI. DIVISION STAFF

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Program Manager, Materials Design

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Dr. Suveen Mathaudhu
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Ms. Sandra Elizondo
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Mr. William Cheek
Administrative Support Assistant

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 2011* is to provide information on the programs and basic research efforts supported by ARO in FY11, 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 FY11.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mathematical Sciences Division supports research efforts to develop a foundational framework for the understanding and modeling of complex nonlinear systems, for stochastic networks and systems, for mechanistic models of adaptive biological systems and networks, and for a variety of partial differential equation (PDE) based phenomena in various media. These research areas focus on discovering nonlinear structures and metrics for modeling and studying complex systems, creating theory for the control of stochastic systems, spatial-temporal statistical inference, data classification and regression analysis, predicting and controlling biology through new hierarchical and adaptive models, enabling new capabilities through new bio-inspired techniques, creating new high-fidelity computational principles for sharp-interface flows, coefficient inverse problems, reduced-order methods, and computational linguistic models. The results of these research efforts will stimulate future studies and help to stay the U.S. at the forefront of research in the mathematical sciences.

2. Potential Applications. In addition to advancing worldwide knowledge and understanding of mathematical concepts, structures, and algorithms, the research efforts managed in the Mathematical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO research may provide 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. The results may provide full (*i.e.*, not only physical) situational awareness through multi-target recognition/tracking/monitoring of physical, informational, cognitive and social targets in asymmetric, often urban scenarios. It may enable faster/better analysis, design, prediction, real-time decision making, and failure autopsy. It may also provide enhanced levels of information assurance, improved awareness of and defense against terrorist threats, and may enable next generation communication networks along with improving weapon design, testing, and evaluation.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives and to maximize the impact of potential discoveries for the Army and the nation, the Mathematical Sciences Division frequently coordinates and leverages efforts within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), and the Air Force Office of Scientific Research (AFOSR). In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the ARO Computing Sciences Division include promoting research to investigate new architectures and algorithms for the future of heterogeneous computing and to pursue related interests in image recognition and information fusion. The Mathematical Sciences Division coordinates efforts with the Network Sciences Division to pursue common interests in cognitive modeling, bio-network modeling and design, and new concepts in computational optimization. The Mathematical Sciences Division also coordinates efforts with the Physics Division to pursue fundamental research on quantum control. Research efforts also complement initiatives in the Life Sciences

Division to model and understand the relationship between microbial growth conditions and composition, leading to advances in microbial forensics. The creation of new computational methods and models to better understand molecular structures and chemical reactions are an area of collaboration between the Chemical Sciences and Mathematical Sciences Divisions. Mathematical Sciences programs interface with the Engineering Sciences Directorate Program Areas on understanding the mechanics of fluids in flight and understanding combustion. These interactions promote synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

To meet the long-term program goals described in the previous section, the Mathematical Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY11, the Division managed research efforts within these four Program Areas: (i) Modeling of Complex Systems, (ii) Probability and Statistics, (iii) Biomathematics, and (iv) Numerical Analysis. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Modeling of Complex Systems. The goal of this Program Area is to develop quantitative models of complex, human-based or hybrid physics and human-based phenomena of interest to the Army by identifying unknown basic analytical principles and by using human goal-based metrics. Complete and consistent mathematical analytical frameworks for the modeling effort are the preferred context for the research, but research that does not take place in such frameworks is considered for support 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 three research Thrusts: (i) Information Fusion in Complex Physical, Informational and Social Networks, (ii) Geometric and Topological Modeling of Irregular Objects and Functions and (iii) Analytical Foundations for Human Cognitive, Behavioral and Social Modeling. However, in FY12, the Modeling of Complex Systems Program will include only legacy efforts in information fusion, and new efforts in information fusion will be part of the Information Processing and Fusion Program in the ARO Computing Sciences Division.

Research progress on improved information fusion in distributed sensor networks, including and especially hard/soft (all-source) fusion networks ("hard" refers to physics-based networks; "soft" refers to human-based networks), will ultimately fulfill Army C4ISR requirements for tractable/scalable methods for identification and tracking of hard and soft targets (*e.g.*, physical, informational, cognitive, social). Mathematical analysis for fully 3D (rather than 2.5D) geometric and topological modeling of large urban regions up to 100 km x 100 km is important for situational awareness, mission planning and training. In addition, mathematical analysis for human cognitive, behavioral and social modeling is important for identifying "soft targets" (*e.g.*, human beings, social networks, intentions) in asymmetric defense.

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 and stochastic fluid turbulence. 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 in 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.

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 approach 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 research Thrusts: (i) Modeling, Analysis, and Control of Biological Systems, (ii) Computational Biology, and (iii) Fundamental Laws of Biology. Within these Thrusts, basic, high-risk, high pay-off research efforts are identified and supported to achieve the program’s long-term goals. Research in the Modeling, Analysis, and Control of Biological Systems Thrust area focuses on finding realistic, yet mathematically tractable, mechanistic models for a variety of biological networks, both static and dynamic, along with methods for their control. Efforts in the Computational Biology Thrust area seek to elucidate and model the fundamental principles by which biological elements such as genes, proteins, and cells are integrated and function as systems. Research in the Fundamental Laws of Biology Thrust area is high-risk research in biomathematics at its most fundamental level, seeking to find and formulate in a mathematical way the basic, general principles underlying the field of biology, a feat that has been performed for other fields, such as physics, but is in its infancy with respect to biology.

While these research efforts focus on high-risk, high pay-off concepts, potential long-term applications for the Army include new and better treatments for biowarfare agent exposure, improved military policies on troop movements in the presence of infectious disease, optimized movements of groups of unmanned autonomous vehicles and communications systems, and improved understanding of cognition, pattern recognition, and artificial intelligence efforts. Research efforts in this Program Area could also lead to improved medical diagnoses, treatments for disease, limb regeneration, microbial forensics, detection of terrorist cells, and self-healing networks. Finally, efforts within this program may result in a revolutionized understanding of biology in general, which will at the very least allow future modeling efforts to be much more efficient and also undoubtedly have far-reaching effects for the Army in ways yet to be imagined.

4. Numerical Analysis. The goal of this Program Area is to develop a new mathematical understanding to ultimately enable faster and higher fidelity computational methods, and new methods that will enable modeling of future problems. The studies guided by 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 pay-off 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 FY11 were $17.7 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY11 ARO Core (BH57) program funding allotment for this Division was $5.0 million. The DoD Multidisciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engieers (PECASE) program provided $10.4 million to projects managed by the Division. The Small Business Innovative Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided $0.2 million for awards in FY11. Finally, $2.1 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

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

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). 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. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. Army Conference on Applied Statistics (SAS Institute, Cary, NC; 20-22 October 2010). The goal of this conference was to provide a forum for the presentation and discussion of theoretical and applied papers related to the use of probability and statistics in solving defense problems. The conference provided an invaluable opportunity for interaction among academic, industry, and defense scientists. It also served a nurturing role in the elevation of statistical competence among defense researchers in other disciplines who find themselves statistical practitioners because of the compelling benefits statistical science brings to defense research, development, and testing. The conference was structured to include general sessions that included invited presentations on emerging topics in statistics, and special sessions that focused attention on Army problem areas for which the role of statistical science should be more fully explored. Contributions to the conference sessions included papers ranging from new methodology to interesting statistical applications. In the clinical sessions, a distinct feature of the conference, presenters sought guidance from a panel of experts on problems that have not been completely or satisfactorily solved. Other noteworthy events included a tutorial that was presented on a statistical topic of interest for defense applications (presented prior to the conference). The Army Wilks award is periodically given at this conference to an individual who has made significant contributions to the practice of statistical science in the Army, through research in statistics and the application of statistics in the solution of Army problems.

C. Multidisciplinary University Research Initiative (MURI)

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

1. Designing and Validating Theories of Distributed Signal Processing. This MURI began in FY06 and was awarded to a team led by Professor Shankar Sastry of the University of California, Berkeley. The goals of this research are to: (i) develop new theories of distributed signal processing with random spatio-temporal sampling of complex scenes for recognition and tracking of object in heterogeneous sensor networks (HSNs), (i) develop theories for robust design principles for sensor networks with both low- and high-bandwidth sensors to automatically recognize and track targets in complex urban environments, (iii) develop theories for metrics for the design and deployment of sensor webs, and theoretical bounds on the performance of different kinds of sensor webs and (iv) develop theories for incorporation of mobility into sensor web models and into the algorithms for these webs.

The MURI team has developed a new approach to distributed fusion in graphical models that highlights the role of key nodes. This method makes use of the notion of a feedback vertex set (*i.e.*, a set of nodes that, if removed, render a graph cycle-free). With such a set identified, a new messaging algorithm results in which several message streams are created, culminating in fusion at the feedback vertex nodes and subsequent messaging to disseminate information throughout the graph. This algorithm provides exact answers for Gaussian inference but is computationally tractable only for graphs with modest-sized feedback vertex sets. The team has developed a method for choosing a set of most important vertices (*i.e.*, vertices that are the most significant information hubs for the graph) and then employing the same algorithm now using only these important hub vertices. The resulting algorithm yields approximate answers (since not all loops in the graph have been broken), but the results demonstrate that excellent and scalable performance is readily achieved using only modest-sized sets of hub vertices, including for graphical models for which previously developed algorithms fail to converge. The team has designed level-set methods for discrimination in both centralized and networked systems. These methods use available training data both to identify lower-dimensional projections of the data of most significance for the discrimination task and to determine decision boundaries in these reduced-dimension spaces via curve evolution. The team is currently upgrading the design of a wireless smart camera architecture that was designed in the first two years of this project. This research responds to the Army need for improved urban target recognition capabilities for military operations and for monitoring of military or terrorist activity.

2. Discovering Mathematical Theories in Spatial-temporal Nonlinear Filtering. This MURI began in FY06 and was awarded to a team led by Professor Boris Rozovsky at University of Southern California; however, Professor Rozovsky transferred to Brown University in FY07 and continued as the principal investigator (PI) of this project. The objective of this research is to invent new mathematical theory and techniques in spatial-temporal nonlinear filtering (NLF) and change-point detection (CPD) in order to develop a mathematical and systematic foundation and algorithms for spatial-temporal statistical inference and for fusion of heterogeneous information from multi-source, multi-sensor distributed sensor networks.

This research will explore three central scientific problems: (i) nonstationarity, (ii) integrating metric and symbolic information, and (iii) very high dimensionality. Current methods for pattern recognition in monitoring and surveillance, including network monitoring, are designed for stationary patterns, and cannot cope with new patterns in ever-changing environments. This project will develop new statistical methods for the nonstationarity problem, particularly spatial-temporal NLF, CPD, and advanced fusion methods. A distinctive feature of its approach is that the spaces in which estimation, classification and tracking are performed are both metric and symbolic. Just as a moving vehicle may be tracked in a metric coordinate space by conventional filters, so can an unfolding terrorist plan be tracked in plan space by a hybrid metric-symbolic nonlinear filter. To the extent that information in these spaces is dependent, each space can compensate for incomplete and ambiguous data in the other, improving fusion performance. The modern battlespace produces unmanageable amounts of data, as do the Maritime Domain Awareness and the Global War on Terror. Dimensionality, or the sheer number of objects about which information is available, grows faster than the human ability to track, fuse, interpret, and base decisions on the information. This project adapts and develops methods for quickly extracting *actionable* information, framing it for automated decision-making, and in this way helps to realize the potential of measurement and signature intelligence (MASINT), ground moving target indicator (GMTI) technology, video surveillance schemes and other massive and extremely expensive data collection programs.

3. Theories of Dynamic Modeling of 3D Urban Terrain. This MURI began in FY07 and was awarded to a team led by Professor Andrew Kurdila of the University of South Carolina. The goal of this research is to develop theory, algorithms, software, and experiments for the synthesis of urban terrain maps using dynamic point cloud sensor data. More specifically, the objective of this research is to develop theories (i) for capturing high-order topology through implicit representation of surfaces, (ii) for developing multiscale and adaptive algorithms that enable various resolutions of the rendered surface governed by the local density of the point clouds, (iii) for the fast computation of signed distances to the terrain surface thereby giving field of view from specified observation points, (iv) for the use of dynamic point cloud measurements for the navigation and control of autonomous vehicles in three dimensions, and (v) for change detection from point cloud observations taken at different times.

The MURI team has already developed a novel method called Wavelet Streaming Surface Reconstruction (WSSR) for reconstructing surfaces from point cloud data using wavelet decompositions. It combines the advantages of the implicit methods and the multiscale structure of the wavelets (subdivision) methods. This enables one to extract a polygonal model of the boundary by applying an octree contouring method to create a water-tight, adaptive contour, which is guaranteed to produce a topological and geometrical manifold. One of the great advantages of this approach is its locality. Each sample influences only a small number of coefficients in the representation. The method is very general in the sense that it can use any orthogonal or biorthogonal compactly supported wavelet basis. This research responds to the Army need for 3D urban terrain models for simulation, training, mission planning, operational situational awareness and vehicle navigation.

4. 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 functioning 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, named the Situation Understanding Bot Through Language and Environment (SUBTLE) project, is organized into nine synergistic tasks: 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.

5. 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.

6. Discovering New Theories for Modeling and Analysis of Multi-scale Networks. This MURI began in FY08 and was awarded to a team led by Professor Ness Shroff at the Ohio State University. The objective of this research is to invent new mathematical theory and techniques in order to enable modeling, analysis and control of complex multi-scale networks. In particular, the research will develop a mathematical theory and techniques for modeling, analysis, and control of complex multi-scale networks.

The research team is investigating multi-scale phenomenon and control of wireless systems including LRD in wireless systems, which is a consequence of the temporal and spatial complexity inherent in military networks. The research focuses on the impact of multi-scale phenomena on the control, performance, and security of these networks. This research will lead to a long-overdue union of stochastic control, statistics, queuing theory, complexity theory, and the distributed algorithms, which is necessary for the development of radically new strategies for controlling the increasingly complex military networks. In particular, the objective is to develop a unifying theory that is mathematically rigorous and leads to practically-implementable network control and distributed detection algorithms, thus providing an enormous tactical advantage for the U.S. military.

The research approach consists of three inter-related focus areas: (i) traffic modeling and analysis, (ii) network control, and (iii) information assurance. While the investigation covers both wired and wireless networks, it focuses heavily on the wireless portion of the overall networks, which is central to tactical communications and the Army's network centric operations, and is likely to have the most stringent resource constraints and greatest vulnerability to security breaches. The modeling approach takes into account the critical time scales in military networks, from user level applications (*e.g.*, time-critical data), to the time-scale required for the operations of various protocols and resource allocation schemes; this is significantly different from the state-of-the-art in traffic modeling, where the network is viewed as a physical entity whose laws are being passively observed through traffic studies. The team is formulating optimization and distributed control problems for providing network services and studies the impact of LRD traffic on network control, performance, and security. The project is also developing an integrative approach that combines the LRD modeling and network control to obtain non-parametric or semi-parametric techniques for the distributed detection of information flow and flow changes needed for preventing security attacks. The research is characterizing the ability of flow to be detected as a function of flow rate, delay and memory constraints, and develops distributed detection schemes that guarantee vanishingly low detection error probabilities. The outcomes of this project will result in distributed, low-complexity, and robust control mechanisms for achieving high network performance, intrusion detection, and security. These outcomes will provide high performance, reliability, and information assurance in support of the Army's future Network-Centric Operations and Network Centric Warfare (NCW). Further, the rigorous and conceptually unifying mathematical techniques developed in the course of this work will enable a deeper understanding of the dynamics and control of large and complex networks.

7. Network-based Hard/soft Information Fusion. This MURI began in FY09 and was awarded to a team led by Professor James Llinas of the University at Buffalo. The goals of this research are to develop a generalized framework, mathematical techniques, and test and evaluation methods for fusion of hard and soft information in a distributed (networked) Level 1 and Level 2 data fusion environment.

The MURI team is investigating source characterization of soft data input streams (human observation direct and indirect, open source inputs, linguistic framing, and text processing), common referencing and alignment of hard and soft data, generalized data association strategies and algorithms, robust estimation, dynamic network-based effects on fusion architectures, and test and evaluation. The team has already made progress in the following areas: creation of an overall system concept for human-centered information fusion and information processing architecture; development of an evolutionary test and evaluation approach that proceeds from "truthed" synthetic hard and soft data to human-in-the-loop experiments; creation of a counter-insurgency-inspired synthetic data set involving both hard and soft data; development of initial hard sensor processing algorithms for level 0-1 processing; development of a taxonomy for characterizing the human as observer (source characterization); selection of a tool for processing text messages, including semantics; development of an overall architecture and framework for soft data association that extends the traditional hypothesis generation-hypothesis evaluation-hypothesis selection paradigm for fusion of soft data and utilizes a data graph association process; development of a new method for data representation of image and acoustic data; and development of methods for representing uncertainty in soft data. This research responds to the Army need for hard/soft fusion models for operations, mission planning, training and simulation.

8. Theories of Tomography of Social Networks. This MURI began in FY10 and was awarded to a team led by Professor Patrick Wolfe of Harvard University. The goal of this MURI is to investigate theories for automatically analyzing heterogeneous, noisy, and incomplete multi-source data, and to infer information about individuals of interest and covert groups.

The MURI team will develop these theories using passive network observation and inference from traditional sources, as well as active sensing in a way that does not perturb the network as it evolves dynamically over time. In contrast to much prior work, this research places particular emphasis on the elicitation of metrics and models embedded in applicable sociological theory rather than simply on inference of latent structure in social networks. The effort has three focus areas, the first of which is metrics linking social structure to observable behavior. Two basic questions under consideration are (i) how is latent network structure manifested in observable data and (ii) how is observable data predictive of network structure. The second focus area is the interplay between individuals and groups as drivers of network dynamics. The third focus area is actionable intelligence from network models. In this area, the primary question is that of determining when is it possible to actively encourage (or disrupt) the formation of social structure. This effort responds to the Army need for time-sensitive and dynamic targeting of networks of hostile adversaries.

9. Modeling Approach 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 would 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.

10. Modeling the Effects of Training on Performance. This MURI began in FY10 and was awarded to a team led by Professor Alice Healy of the University of Colorado - Boulder. The goal of this research is to develop an empirically-based theoretical framework that can account for and make accurate predictions about the effectiveness of different training methods for militarily relevant tasks.

The research is proceeding in three directions (i) the development and testing of training principles, (ii) the development of principles on the acquisition and retention of basic components of skill, and (iii) the theoretical and computational modelling of training effects associated with levels of automation, individual differences, and team performance. To render the study of training effects tractable and to guide research, the MURI team has developed a multi-dimensional taxonomy that provides a framework by which training effects can be assessed and predicted for any task. The taxonomy involves a four-dimensional decomposition of the training space, including separate dimensions of classification for task description, training procedure, and the context and assessment of task performance. The training principles are considered the fourth dimension. The component of the project devoted to models consists of four parts: a data entry task, a more complex radar tracking task, an information fusion task, and stimulus-response compatibility effects. The research on model assessment is focused on model optimization. The Army has a significant need for research in training and training management, and this MURI team will make contributions to meet this need by providing performance-shaping functions (*i.e.*, quantitative versions of training principles that can be incorporated into computer models) and training principles.

11. 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 project 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.

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

No new starts were initiated in FY11.

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

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Error-Controlled Simulations of Electromagnetic Phenomena for High-performance Computing. Two Phase I STTR contracts were awarded to HyperComp, Inc. and Computational Sciences, LLC, to investigate numerical methods for predictably-accurate treatment of boundary conditions in electromagnetic and other wave-dominated phenomena, and to develop algorithms and computer software that can be implemented for military and commercial simulation applications. High-fidelity modeling of electromagnetic phenomena has become increasingly important in the design and virtual prototyping of navigation, detection, tracking, and communications systems, helping simulation become widely recognized as the third major component of scientific discovery and development, co-equal with experimentation and theory. However, the simulation of electromagnetic phenomena in the time-domain poses unique computational challenges; these systems are hyperbolic with propagation length scales that are many orders of magnitude greater than the wavelength. Although new algorithmic developments have greatly improved the reliability and efficiency of approximations to Maxwell's equations within the computational domain, a major obstacle to accurate long-time solutions is the presence of spurious reflections which occur at the computational boundaries and back-propagate to degrade the solution over the interior. The research team is attempting to overcome this barrier using an *a priori* error-bounded algorithm that can be encoded within standard high-performance computing libraries or computational electrodynamics packages for simulation on parallel, distributed, and grid-based computing platforms.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) – 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). The FY11 new starts within these programs are described here, while the missions of each of these programs were described *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Core HBCU/MI: A Study of Prediction Theory of Periodically-correlated Stochastic Processes. A new Core HBCU/MI award was granted to Professor A. Miamee at Hampton University to investigate the prediction problem for periodically correlated stochastic processes. The research team plans to pursue the recent developments in prediction theory of these processes and try to obtain an algorithm for determining the predictor of a future member of such a process based on its past. In the existing literature the prediction problem has been resolved by restating it in terms of a multivariate stationary process obtained from consecutive blocks of the original process and then invoking the available predicting algorithm for the multivariate stationary processes. However, this technique works primarily in the full-rank case. The investigators are investigating the prediction question directly, utilizing intrinsic properties of periodically correlated processes. This approach may allow researchers to construct effective prediction algorithms for both non-full rank processes as well as processes with large period.

2. PIRT: Extracting Social Meaning From Linguistic Structures in African Languages. This five-year PIRT project was awarded in FY11 to a team led by Professor Mohamed Chouikha of Howard University. The goal of this project is to develop quantitative procedures to identify social meaning from a variety of open-source texts in African languages.

This project focuses on codeswitching (*i.e.*, the alternation between two or more languages). Codeswitching is one of the primary mechanisms for conveying social meaning in interactions in multilingual African communities, especially among educated African urban dwellers who tend to alternate between African languages and former colonial languages. This study will investigate codeswitching involving English or French with selected African languages, with a focus first on Swahili and Zulu and then Lingala and Ciluba. Although these African languages are *lingua francas* in their respective regions, they remain low-resource languages compared with European languages. Prior research demonstrates that codeswitching can index power imbalance, affiliation/disaffiliation, change in footing, identity claims and other important issues in interaction. This project is the first of its kind that aims to automate codeswitching and related discourse features. This research may ultimately advance language technology and make it possible to predict specific kinds of interpretations of social meaning using computational tools. This research will also aid DoD and the Army in many humanitarian, peace-keeping and other operations.

3. PIRT: Multiscale Modeling of Cementitious Materials. This PIRT project was awarded in FY11 to a team led by Professor Ram Mohan at North Carolina Agricultural and Technical State University. The goal of this research is to create a multi-scale modeling methodology for cement-based materials that links and transcends across the different length scales from the nanoscale material constituents to the macroscopic deformation and failure behavior. This work may ultimately enable new design capabilities for these materials.

Advanced cementitious materials such as mortar and concrete both in original construction and as protective retrofitted quick-pour concrete panels combine traditional cementitious mortar or concrete with additional functional materials (*e.g.*, nanomaterial fillers and fibers). These materials have the potential to provide effective protection against attacks that include direct projectile impact and shock from blast waves. Further enhancement of the design, development and understanding of the shock and impact resistant properties of cementitious materials requires "materials by design" techniques and concepts instead of a trail-and-error approach in material processing. This project is pursuing the development of advanced computational algorithms and appropriate physics-based simulations 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 levels for the macroscopic structural configurations which are desperately needed. This research effort is being guided by an advisory team from ERDC and ARO with expertise in the cementitious materials and multi-scale computational modeling approaches. The multi-scale modeling approaches envisioned in this research will lead to a better scientific understanding of the performance of the cementitious-based force-protection material in a materials-by-design framework and characterize the effect of micro-structural design changes and nano-engineered material inclusions on their performance. This research may ultimately lead to the design and development of improved cementitious-concrete panels and retrofits for soldier protection, and safety and efficient designs for load-bearing and potentially light-weight concrete spans for military and civilian applications.

4. DoD REP Awards. As described in more detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, REP awards aim to enhance or increase the programs, capabilities, and graduates in scientific and engineering disciplines in universities serving underrepresented minorities. In FY11, the Mathematical Sciences

Division managed one new REP project, totaling $0.4 million. The equipment purchased with this award is promoting research in areas of interest to ARO, such as the dynamics of algebraic models as a potential model for molecular networks.

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

No new starts were initiated in FY11.

H. Defense University Research Instrumentation Program (DURIP)

As detailed 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 FY11, the Mathematical Sciences Division managed four 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 to explore a priori estimate methods for nonreflecting boundary conditions in electrodynamics and the ability of globally convergent methods for coefficient inverse problems to determine target constitution.

I. 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. The framework will provide 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 synonomous. Traditional theories of value do not incorporate the complex dynamics of social systems. This program will generalize physical models of interacting systems (interdependence, order and disorder, symmetry breaking, pattern formation, phase transitions) to socio-economic systems in order to create a theory of value. Developing the more general theoretical framework will include analyzing large amounts of data for validation and correctly identifying the universality class of complex economic systems. Both the perspective of the physics of complex systems and that of economics will be applied. The theory will be validated on historical commodity data (see FIGURE 1). The techniques developed in this work are important for defining value in many contexts, for example, value of information in the context of distributed information fusion. This work will provide a greater understanding of complex networks (physical, informational, cognitive, and social) and systems which is important because of the impact of these networks and systems on defense. A new economics-based theoretical framework for the relationship of "value" and "price" will be an important component in network analysis.

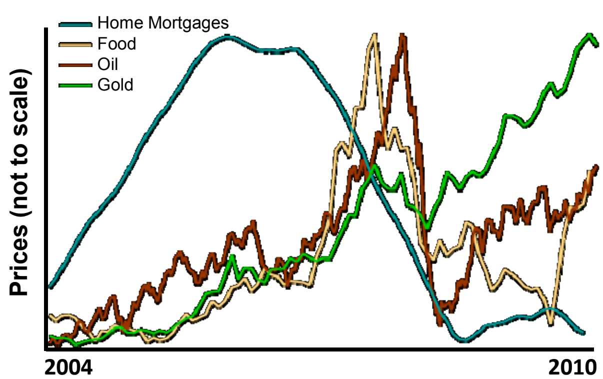

FIGURE 1

Historical commodity data. This commodity time series (2004-2010) plots relative changes in the prices of home mortgages (blue), food (yellow), oil (red), and gold (green), which are examples of the type of data used to text and validate theories developed by the research program.

J. DARPA Geometric Representation Integrated Dataspace (GRID) Program

The vision of the GRID program is 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 accurately encode the 3D geometry and surface properties of objects at various spatial scales and would provide 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 seeks 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 Mathematical Sciences Division has identified and initiated three pilot projects using DARPA funds to support the GRID program. In addition, many of this program's goals are complementary to the research directions pursued by Division's Theories of Dynamic Modeling of 3D Urban Terrain MURI.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. Representations and Metrics for Time-Varying Terrain Surfaces

Professor Zachery Wartell, University of North Carolina - Charlotte, Single Investigator Award

The objective of this project is to determine terrain metrics and efficient computational procedures that can provide real-time terrain analyses such as line-of-sight queries, trafficability, penetrability and feature-change detection.. In FY11, the investigator developed a probabilistic, volumetric terrain model and an interactive 3D visualization tool for terrain change detection over multiple time-steps along with scripts and a workflow to acquire, clean and organize laser RADAR (LIDAR) terrain data. Extracting surfaces from a surface probability field requires modifications of the marching triangles (MT) algorithm. This project used the MT algorithm with adjustments to switch between iso-surface and ridge surface extraction. Professor Wartell has integrated this algorithm with an octree gridding algorithm for representing the terrain surface (see FIGURE 2, red rectangles). He also developed an interactive 3D visualization tool that visualizes terrain changes between any pair of time-steps in a multi-time-step scenario. With this tool, the investigator explored various natural and urban terrain changes in a LIDAR data set from the North Carolina coast. He developed data structures that link change features to their raw LIDAR data, the time interval over which the change occurred and user annotation. To allow for parallelization, the interactive tool uses a simple, fast terrain change detection method. These items have been integrated into an interactive system.

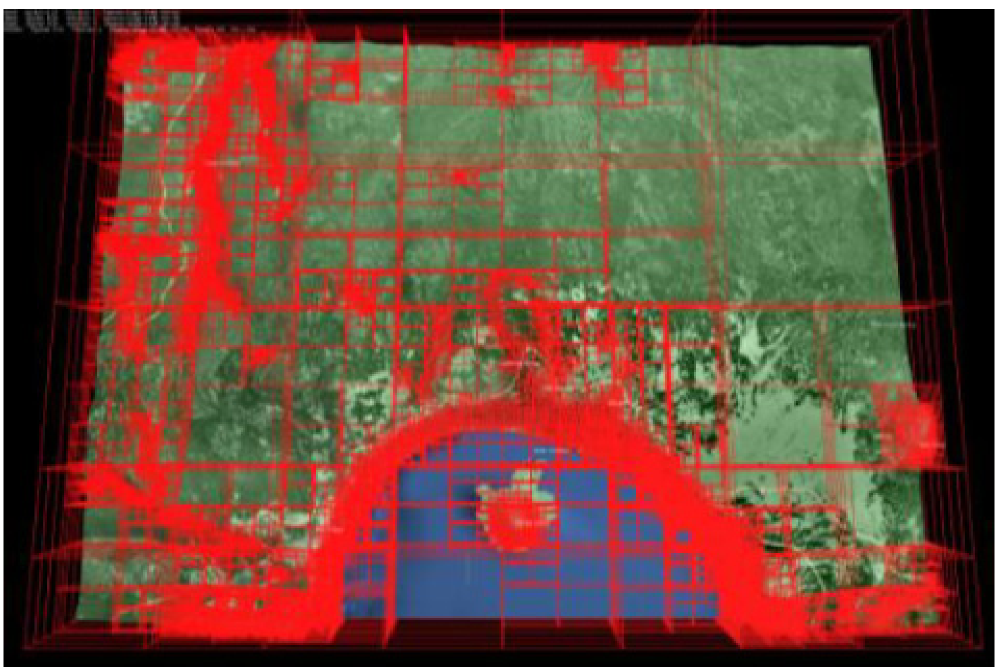

FIGURE 2

Octree gridding algorithm for representation of LIDAR terrain data. The data displayed is the output of the octree surface representation algorithm (input for marching-triangles algorithm). The output of this octree gridding algorithm (red rectangles) is the input for the marching-triangles algorithm that actually constructs the surface. This transition from discrete to continuous representation is a crucial step of the overall procedure.

B. 3D Object Recognition and Identification from Partial Information

Professor Guillermo Sapiro, University of Minnesota, Single Investigator Award

This project has further developed techniques for dictionary learning, including on-line learning, finalized a topologically robust framework for non-rigid 3D shape recognition based on the combination of diffusion distances with Gromov-Hausdorff distances and completed a framework for the extraction of 3D shapes and scenes from a single image. To reconstruct a 3D object from a single image, Professor Sapiro partitioned 3D space into voxels and estimates the voxel states that maximize a likelihood integrating two components: (i) the object fidelity, that is, the probability that an object occupies the given voxels, encoded as a 3D shape prior learned from 3D samples of objects in a class, and (ii) the image fidelity, meaning the probability that the given voxels would produce the input image when properly projected to the image plane. He has derived a loop-less graphical model for this likelihood and proposed a computationally efficient optimization algorithm that is guaranteed to produce the global likelihood maximum. The 3D object recognition procedure is a major step in 3D scene analysis from a single view (see FIGURE 3). Finally, he has derived a multi-resolution implementation of this algorithm that permits trading reconstruction and estimation accuracy for computational speed. This research responds to the Army need for rapid recognition of 3D objects from minimal information.

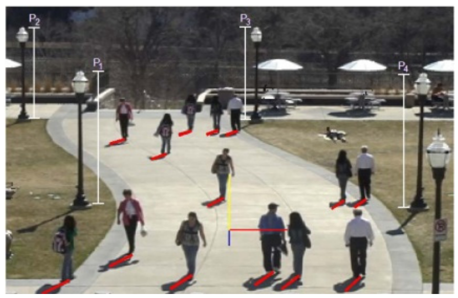

FIGURE 3

3D scene analysis from a single view. Professor Sapiro's research has led to this 3D object recognition procedure that is a major step in 3D scene analysis from a single view.

C. Multimodal Signal Processing for Indoor Personnel Detection and Activity Classification

Professor Pramod Varshney, Syracuse University, Single Investigator Award

The goal of this project is to develop novel schemes for the fusion of heterogeneous information for the detection and classification of personnel activity in an indoor environment. The term "heterogeneous information" refers to the information obtained from heterogeneous or multimodal sensors (networked and non-networked) as well as information obtained from the use of different models. This project has been exploring the problem of fusion for detection using dependent observations, a type that is particularly difficult to handle (see FIGURE 4).

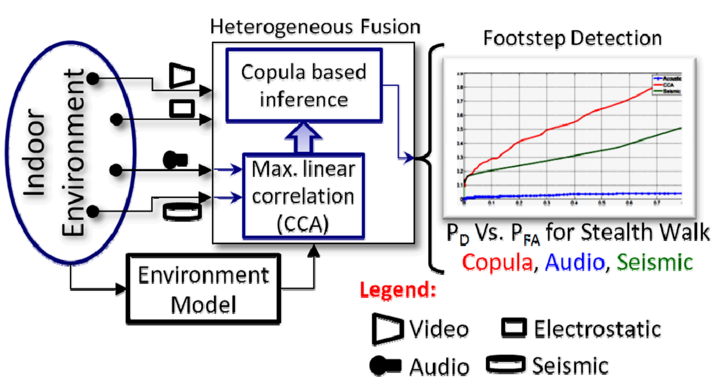

FIGURE 4

System structure for indoor personnel detection and activity classification. The term "heterogeneous information" refers to the information obtained from heterogeneous or multimodal sensors (networked and non-networked) as well as information obtained from the use of different models. This research has been exploring the problem of fusion for detection using dependent observations, a type of observation that is particularly difficult to handle.

Copulas are used to characterize the dependence and joint distribution between different sensor observations. The cumulative distribution function of dependent random variables can be expressed as a marginal distribution functions times a copula, and the marginal distribution function describes each component of the random variable and the copula describes the dependence structure between the components. The copula function is an explicit functional relationship between the joint distribution and its corresponding marginal distributions.

The investigator has recently solved a portion of the copula selection issue for the detection problem, using approaches based on area under the ROC and average loss of detection power. Asymptotic performance loss due to misspecification of the copula function in terms of error exponents was also quantified. When applied to a classification problem with heavy-tailed signals, copula-based features gave a classification accuracy of up to 85% on test data. An information theoretic bound is derived for detector performance, and performance loss due to misspecification of copulas is quantified. Detection performance is evaluated using footstep signals obtained using an array of geophones deployed indoors. The geophone data can also be used to classify the occupancy (one vs. more than one occupant) of a region under surveillance with up to 95% classification accuracy. A widely applicable theoretical result of this research is the Conditional Posterior Cramér-Rao Lower Bound (CPCRLB), a new bound for use in online tracking.

D. Adaptive Networks Foundations: Modeling, Dynamics, and Applications

Professor Leah Shaw, William and Mary University, Young Investigator Program (YIP) Award

The goal of this project is to study adaptive social networks, focusing on the spread of infectious disease as the primary example, with individuals as nodes. While the structure of static networks has been well-studied, when node states and links between nodes change over time, the feedback relationship between the node dynamics in the network and the changing pattern of interactions between nodes is often ignored. The goals of the project include incorporating more realistic network structure, studying the extinction of diseases, developing control strategies for epidemics on adaptive networks, and developing tools to quantify adaptive network properties. The theoretical approach is based on a compartmental differential equation model for individuals in which compartments represent disease status, with each individual in either the susceptible (S), infected (I), or recovered (R) compartment, and individuals linked to create a social network (see FIGURE 5). In an adaptive network, individuals change their social connections in response to the spread of an epidemic and these changes in network topology affect the subsequent spreading of the disease. Thus, as opposed to a standard epidemiological model, an individual avoids contact with an infected individual by disconnecting from the infected individual at a certain "rewire" rate and connecting to either a susceptible or recovered individual.

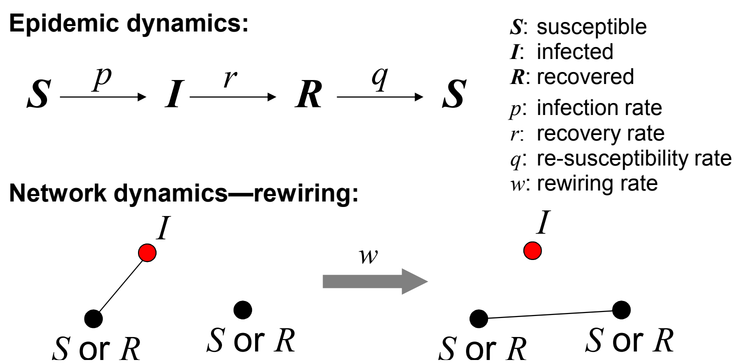

FIGURE 5

Epidemic and network dynamics model of disease spreading. The basic compartmental model (assuming re-infection is possible) is shown at the top, and the network dynamics model is illustrated at the bottom.

In FY11 the investigator attempted to build increased realism into network structure and disease avoidance. Previous models for epidemics in adaptive networks did not account for the local community structures that occur in real social networks. As a first attempt to address the role of community structure, a model for an adaptive network containing two (possibly heterogeneous) communities was constructed, with the link rewiring rules adjusted so that the two communities were maintained throughout the evolution process. Community structure was observed to have an equalizing effect on the connectivity of the communities as well as on infection levels in the communities. In addition, most adaptive models of disease spread assume that individuals are well-informed about their neighbors' disease status and their need to protect themselves from disease. This project considered the more realistic simultaneous spread of both the epidemic and information *about* the epidemic and found qualitative changes in the dynamics such as periodic oscillations in information and infection levels. Moreover, when only part of the population is informed, limits exist to the efficacy of avoidance rewiring in preventing disease spread. In particular, the epidemic threshold (transmission rate when spreading begins to occur) saturates at some rewiring rate, and increased efforts to avoid infection by rewiring do not further prevent an outbreak (see FIGURE 6). Finally, as a non-epidemic example of adaptive social networks, the research team began modeling recruitment to a cause, such as terrorist recruitment, in adaptive networks. Models that include both terrorism recruitment dynamics and networks structure are extremely rare, and no previous model considered adaptive change in the social network structure. The investigator developed a model for the time evolution of a social network as terrorists recruit individuals from a pool that is susceptible to radical ideas; members were classified as non-susceptible, susceptible, or terrorist. Radical ideas were treated as something that can spread from person to person through social contacts, with terrorist nodes adapting by rewiring their connections away from non-susceptible nodes and toward susceptible nodes to maximize their recruiting efforts. This type of rewiring is the opposite of the avoidance rewiring used in epidemic models and thus represents a new type of adaptation. The chief finding of the study was that when susceptible and terrorists both exist at low levels, adaptation is necessary for successful recruiting.

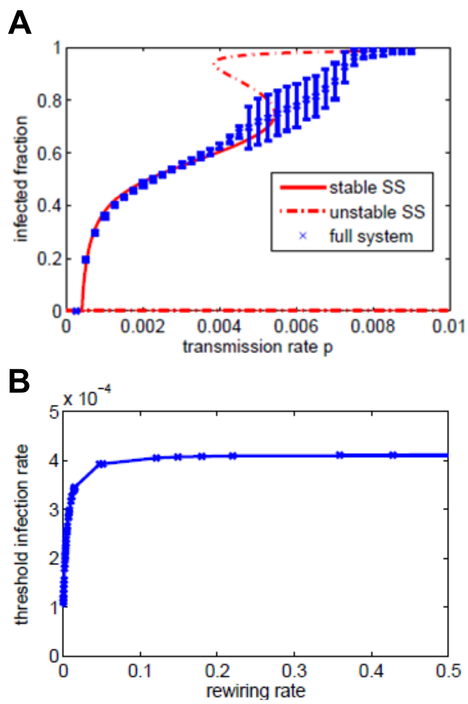

FIGURE 6

Epidemic in an adaptive network with partial information from media. (A) Bifurcation diagram for infected fraction versus transmission rate. Curves are mean field steady states; symbols are simulations of the full system. Bars indicate standard deviations of time series. Large bars are associated with regions of periodic oscillations. (B) Threshold infection rate versus rewiring rate. With partial information, avoidance rewiring effect is limited.

As adaptive social networks are ubiquitous in both the Army and society, these accomplishments will have wide-ranging long-term applications and benefits. With respect to social networks specifically considered in this project, likely results are improved policies on military troop movement in the presence of infectious disease, improvements in general public health policies, and a better understand of terrorist network recruitment. More generally, the mathematical tools developed for use with adaptive social networks may be applied to other types of adaptive networks such as communications systems and groups of unmanned autonomous vehicles.

E. Robust Modeling of Complex Systems with Heavy Tails and Long Memory
Professor Sidney Resnick, Cornel University, Single Investigator Award

The goal of this research is to improve the accuracy of risk calculations and predictions in complex systems subject to effects of extreme behavior, by properly accounting for the large movements and dependencies in system behavior. More specifically, Professor Resnick and colleague Professor Gennady Samorodnitsky will develop non-standard stochastic models whose critical features are determined by rare but influential extreme behavior as well as long-term dependencies. The models are developed in conjunction with associated statistical detection techniques that allow for fitting and prediction. Emphasis will be placed on structural and distributional properties that explain important relationships and consequences, and realistic fitting of non-Gaussian models to data will be promoted. Potential application areas for the fundamental techniques include complex networks including data networks, supply chains, reliability estimation, financial, operational, environmental and catastrophic risk analysis, and earthquake analysis.

The researchers made several noteworthy accomplishments in FY11, as listed below.

- Extreme excursions in random fields: Random fields are often used to describe phenomena dependent on location and are an important tool in analysis of image data. For a broad class of non-Gaussian infinitely divisible random fields, methods have been developed for describing the probabilistic behavior of the extreme exceedance sets, that is, the set of locations of extremes. This has potential applications in climatology, medicine, image analysis, and anomaly detection.
- Random walk: One way of broadening the random walk model to overcome reliance on the assumption of independent jumps is to introduce a random environment which serves as a latent, driving mechanism. It was shown that heavy tailed random walks in random environments behave markedly differently from their light tailed counterparts. Whereas the latter satisfy quenched weak theorems for almost every environment, the former do not, and quenched weak theorems only hold weakly in the environment. This leads to a class of weak limits in which the limiting distribution itself is random. Provided the latent environment is not deterministic as would typically be the case in reality, the randomness of a limit approximation must be accounted for when constructing statistical procedures; how to do this accounting is an ongoing open issue.
- Justification of visualization techniques: In risk analysis, a commonly used exploratory visual goodness of fit for identifying extreme behavior is the mean excess plot. A study was completed that showed precisely when such plots will appear eventually linear thus increasing reliability of such techniques.
- Engineers consistently report that traffic at a heavily loaded node subject to a high degree of aggregation should look Gaussian. Yet, theory predicts such traffic should either be Gaussian or heavy tailed, depending on how arrival rates and tails of durations compare. A superposition theory was developed that explains the prevalence of Gaussian traffic and found a data driven explanation originating in http traffic.

Hidden risks with non-zero probabilities are difficult to detect but there has been progress in detecting and estimating such risks in low dimensional cases and where sufficient data is available. The research team is pursuing more general methods allowing more flexibility in how such risks are estimated

F. Stochastic Semi-definite Programming
Professor K. A. Ariyawansa, Washington State University, Single Investigator Award

The goal of this project is to characterize and understand stochastic semidefinite programs (SSDPs), a class of new optimization problems proposed by Professor Ariyawansa (Ariyawansa and Zhu, 2006). There are a variety of optimization programs suited to specific data and problems (see FIGURE 7). Deterministic linear programs (DLPs) use deterministic data and have nonnegative vector variables. DLPs have been a very useful modeling tool in optimization. However, data in real applications are typically not known with certainty. To address this, stochastic linear programs (SLPs) with recourse were developed. SLPs thus extend the applicability of DLPs. They have random data and nonnegative vector variables. Random data refers to data that are random variables with known probability distributions. Deterministic semidefinite programs (DSDPs), have been the subject of intense research during the past 15 years. They extend DLPs and have deterministic data and positive semidefinite matrix variables, and this extension remarkably extends the applicability of DLPs. Given the extension of DLPs to DSDPs, it is then natural to seek an extension of DLPs that combine SLPs and DSDPs. SSDPs, as previously defined by the investigator, are such an extension.

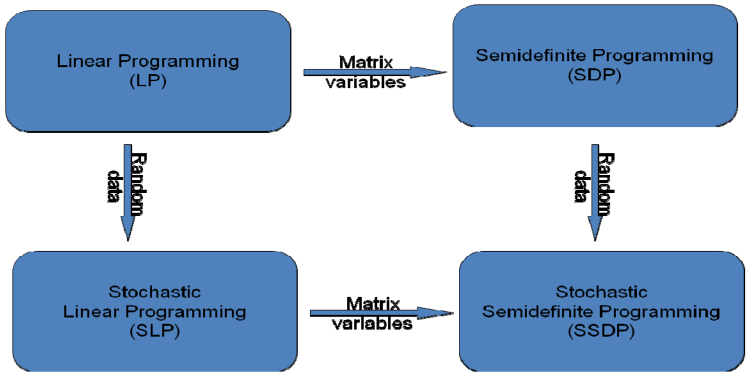

FIGURE 7

Comparison of optimization programs. The flow chart illustrates the relationships among the new class of Stochastic Semidefinite programming (SSDP) problems and previously-studied classes of related problems.

Applications and algorithms for the existing classes of DLPs, SLP, and DSDP have been well-studied. This research applied knowledge of interior point decomposition algorithms for SLP, and combines them with generalizations of nonnegative vector variables to positive semidefinite matrix variables. This research has demonstrated that models of important applications are special instances of the generic SSDP problem, and also constructed new algorithms (with convergence proofs and computational complexity estimates) for the generic SSDP. An example of the significance of these discoveries comes from targeting. For example, suppose that fixed ellipses represent targets that need to be destroyed and fighter aircraft take off from an origin with a planned disk of coverage that contains the fixed ellipses (see FIGURE 8). Suppose also that there are random ellipses that represent moving targets that also need to be destroyed. In order to be accurate, only the latest information about the realizations of random ellipses is used; this may require one to increase the radius of the planned disk of coverage after the latest information about the realizations of random ellipses become available, which may occur after the fighter aircrafts have taken off. This increase, dependent on the initial disk of coverage and the latest available information about the moving targets, may result in additional random costs. The SSDP model determines the initial disk of coverage so that the expected total cost (including the expectation of the random costs for any necessary corrective action) is minimized.

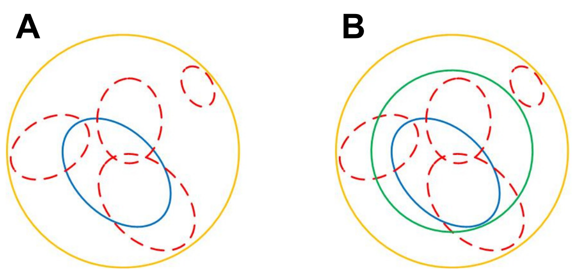

FIGURE 8

Example application of DLP, SLP, and DSDP. The (A) worst-case solution (yellow) and (B) optimal solution (green) for target coverage of one deterministically-located target (blue) and one stochastically-located target (four realizations as red dashed ellipses). The SSDP algorithm developed in this project determines the initial disk of coverage that rigorously minimizes the expected total cost (including the expectation of the random costs for any necessary corrective action).

This research team's specific FY11 accomplishments are listed below.

- Developed a new class of optimization problems termed *chance-constrained semidefinite programs* (CCSDP's) for handling uncertainty in DSDP's. CCSDP is an alternative to SSDP for handling uncertainty in data defining DSDP's. Applications where SSDP and CCSDP models can be developed to deal with uncertainty that cannot be adequately captured by existing approaches were identified.

Specifically, SSDP and CCSDP models were developed for random minimum-volume covering ellipsoid problem (which includes the problem of optimally tracking randomly moving targets described in the Significance section), for determining routing strategies in mobile ad-hoc networks, for designing RC circuits, for structural optimization, and for portfolio optimization under risk constraints.

- Derived and analyzed a new class of interior point decomposition algorithms for SSDP. Specific highlights were algorithms to decompose the problem into smaller independent subproblems making them suitable for implementation on parallel processors, and demonstration of convergence and polynomial complexity of certain members of the class.
- Derived two new interior point algorithms (homogeneous self-dual and infeasible) to decompose the problem into smaller, independent subproblems, more suitable for implementation on parallel processors, and demonstrated that complexity of the algorithms is the same order as decomposition algorithms.

G. Extensions of Signature Theory

Professor Frank Samaniego, University of California - Davis, Single Investigator Award

This project is investigating the joint behavior of systems with shared components using the structural, stochastic, and statistical reliability theory for systems and networks. The results of this study enable extensions of the concept of "system signature" to bi-variate situations in which pairs of systems share some components and thus have dependent lifetimes. The problem explored here is motivated by examples of the sharing of components in the design of selected computer networks. In order to study the performance characteristics of pairs of systems with shared components, one needs to have analytical entrée into the joint distribution of their lifetimes. While some progress of such problems has been made in selected parametric settings (*e.g.*, the Marshall-Olkin multivariate exponential model), the investigator's approach to the problem is fully general and removes parametric assumptions. The primary barrier to the envisioned work in this area is the absence of precedents in dimensions greater than one for representations of the type sought. The potential for generalizing signature representations to higher dimensions was quite difficult to predict. Even with such representations in hand, the possibility of identifying conditions under which a bi-variate ordering exists between two pairs of systems, each with shared components, was seen as an uncertain exercise.

In FY11, representations were prepared for the joint distribution (and joint reliability function) of pairs of coherent systems with shared components under the assumption that all components have i.i.d. lifetimes. The expression derived for the joint distribution G, for example, depends on a pair of matrices S and S*, each of which has total mass (the sum of all its elements) equal to 1. The pair (S, S*) is referred to as the joint signature, and under the assumption of i.i.d. component lifetimes, it is shown to be independent of the underlying component distribution. In the problem of making stochastic comparisons between two pairs of such joint systems, the project provides in two separate and quite different settings, sufficient conditions on the joint signatures to ensure that the two joint lifetimes satisfy a specific bi-variate stochastic ordering. Similar results were obtained from studying the ordering of two joint reliability functions. Although the occurrence of systems with shared components is quite common (a simple example being two computers dependent on a common server), a general and flexible theory for assessing the joint stochastic behavior of these systems has not previously been available. The representations expected from this research will break new ground in this area, providing a tool for describing the performance of pairs of systems whose components have i.i.d. lifetimes with some components in common. The utility of these representations is demonstrated through the stochastic ordering results that follow and shed light on the relative behavior of two such joint systems.

The abundance of circumstances in which pairs of engineered systems have components in common suggests that a general theory for the joint stochastic behavior of such systems is needed. The application of joint signatures to comparisons between such systems will contribute toward this need in existing reliability analysis. The research results will have significant impact on the design of weapon systems for the Army and DoD.

H. Problems in Classification and Regression and Bootstrap Hypothesis Testing

Professor Wei-Yin Loh, University of Wisconsin, Single Investigator Award

Generalized, Unbiased, Interaction Detection and Estimation (GUIDE) is a multi-purpose machine learning algorithm for constructing classification and regression trees. It was previously designed and is maintained by

Professor Wei-Yin Loh at the University of Wisconsin, in part through ARO funding. The objectives of the current research project are three-fold: (i) to make GUIDE the best classification and regression tree algorithm available, in terms of capability, power, and ease of use, (ii) to understand the operating characteristics of GUIDE through mathematical analysis and empirical evaluation, and (iii) to study the theoretical performance of the bootstrap method of hypothesis testing.

The GUIDE algorithm first constructs an importance score for each variable from its statistical significance at each intermediate node of a decision tree and then estimates a null distribution for the scores to determine a threshold for inclusion and exclusion. In drug discovery, "tailored therapeutics" is the term used for identifying segments of the population that are unusually responsive to a treatment. For example, people in a certain age group having specific symptoms or genetic traits may benefit much more from a treatment than other types of people. If this information is known, then a drug can be targeted to this subpopulation. Because of the large number of variables to be considered, it is typically very hard to accurately identify the target subpopulation. A major barrier in using existing approaches to extend decision tree algorithms to longitudinal data is the difficulty of estimating covariance matrices within the nodes of the tree. This is worsened when some data is missing; however, the investigator has recently demonstrated that this problem can be solved by treating each data trajectory as a curve and classifying shapes into a small number of categories. The GUIDE classification tree method is then used to model the data with or without missing values. Version 10 of the GUIDE algorithm was released in FY11, which addresses a fast method of scoring the importance of variables, a method to rank the variables in terms of their differential treatment effects (a key step to solving the tailored therapeutics problem), and an option to construct decision tree models for multi-response and longitudinal data. According to the results from an extensive head-to-head comparison using many real data sets, the GUIDE classification tree algorithm gives the most accurate and compact models, on average, relative to several well-known competitors.

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. Computer-Aided Design of Drugs on Emerging Hybrid High Performance Computers

Investigator: Professor Michela Taufer, University of Delaware, Single Investigator Award
Recipients: ARL Computational and Information Sciences Directorate (ARL-CISD), ARL Weapons and Materials Research Directorate (ARL-WMRD), U.S. Army Medical Research and Materiel Command (MRMC)

Molecular dynamics (MD) simulations are important in chemical research as they can provide an atomistic view of chemical systems and processes not available from experiments, while the Coarse-Grained Monte Carlo (CGMC) method is a multi-scale stochastic mathematical and simulation framework for spatially distributed systems important for studying catalysis, surface diffusion, and cell membrane receptor dynamics. The goal of this project is to validate computational methods and to design and implement computational tools incorporating Graphics Processing Units (GPUs), to be used for biomedical problems such as drug design.

Using GPUs, this project has provided a MD computer code having increased computational power enabling explicit simulation of solvents, as well as a parallel CGMC code for studying scalability and scheduling issues related to domain decomposition of molecular simulations using multiple GPUs. In addition, large-scale numerical simulations performed on parallel systems tend to be very sensitive to cumulative rounding errors and can result in different answers depending on platform and number of parallel units used. Thus, this project also provided new composite precision floating point arithmetic libraries and associated algorithms for GPUs that combine double precision accuracy with single precision performance by defining addition, multiplication, and division in terms of multiple single precision additions, subtractions, and multiplications as well as a single precision floating point reciprocal, at the same time keeping track of inherent error as the simulation evolves.

A combination of parallelism and composite precision arithmetic on GPUs has been predicted to improve performance and reliability for large-scale simulations in general and for drug design in particular (see FIGURE 9). In FY11, the code (FENZI) was shown to be faster than traditionally used codes such as CHARMM on high-end multi-core workstations and also scalable.

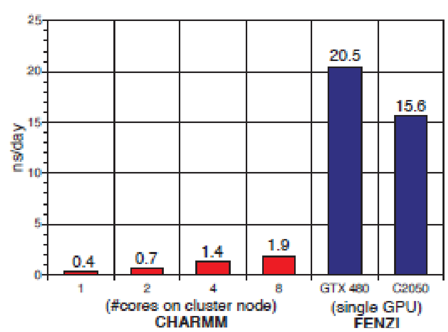

FIGURE 9

FENZI performance versus older CHARMM code. The bar graph compares the performance (ns/day) of (red bars) CHARMM code, optimized for 1, 2, 4, and 8 CPU cores, versus (blue bars) FENZI code on a single GPU. The performance values presented are the average values computed over three repeated simulations.

The researchers also found that membrane properties obtained with faster MD simulations on GPUs match experimental properties. Thus, these methods can significantly reduce the time required to find cures and vaccines for viruses and bacteria used as bio-weapons, lower the cost of new vaccines, and increase the effectiveness of existing cures. These algorithms were transferred to ARL-CISD, ARL-WMRD, and MRMC.

Researchers at these locations are in the process of evaluating the algorithms resulting from this project for use in solving reproducibility and stability issues, as well as domain decomposition of simulations across multiple GPUs for a variety of applications and are looking into computational drug design of small molecular therapeutics against bacteria and viruses. However, the methodologies resulting from this project are transferable across applications and thus provide Army scientists in general with important insights on how to migrate large-scale simulations on GPU clusters in order to provide benefits in additional areas of interest to the Army such as electromagnetic modeling, computational fluid dynamics, structural mechanics, and radiation transport.

B. Portable 3D Mapping of Building Interiors

Investigator: Avideh Zakhor, University of California, Berkeley, Single Investigator Award
Recipient: ARL Vehicle Technology Directorate (ARL-VTD)

Mapping and modeling of indoor environments in 3D has many applications both in the military and in the civilian sector. In this project, the researchers aim to develop techniques for fast, automated 3D modeling techniques which result in photo-realistic, high resolution, 3D graphics database for the interior of buildings. Having prior access to such a model is important to soldiers entering unknown interior structures. The approach is to use a human operated backpack system equipped with laser scanners, IMUs and cameras in order to capture geometry and texture of the building interiors. There are three main challenges to this problem: system architecture, localization algorithms, and 3D model construction algorithms. In year 1, the project addressed system architecture issues, even though there were a number of refinements during the last year. In year 2, the project worked on localization algorithms; specifically, localization algorithms that combine lasers, cameras and IMUs were developed and their performance was characterized. During the last year, the project applied the scan matching based algorithms to localize the backpack in complex indoor environments such as a T-shaped corridor intersection, a staircase, and two indoor hallways from two separate floors connected by a staircase. When building 3D textured models, the localization resulting from scan matching is not pixel-accurate, resulting in misalignment between successive images used for texturing. To address this, Professor Zakhor developed an image-based pose estimation algorithm to refine the results from the scan-matching-based localization. Finally, the localization results within an image-based renderer are used to enable virtual walkthroughs of indoor environments using imagery from cameras on the same backpack (see FIGURE 10).

FIGURE 10

3D Image Rendered from Backpack-mounted Cameras. This model of two hallways and connecting staircase was produced by the backpack system developed by Professor Zakhor's laboratory. the localization results within an image-based renderer were used to create virtual walkthroughs of indoor environments using imagery from cameras on the same backpack.

This renderer uses a three-step process to determine which image to display and a RANSAC framework to determine homographies to mosaic neighboring images with common SIFT features. In addition, the renderer uses plane-fitted models of the 3D point cloud resulting from the laser scans to detect occlusions. The performance of the image-based renderer was successfully tested on an unstructured set of 2,709 images obtained during a five-minute backpack data acquisition for a T-shaped corridor intersection. The transfer of the backpack technology to ARL-VTD began in FY11, for research and development as part of a robotic system.

C. Computational Modeling of Free-surface Fluid-object Interface Interaction

Investigator: Professor Yuri Bazilevs, University of California - San Diego, STIR Award
Recipient: Engineer Research and Development Center - Coastal Hydraulics Laboratory (ERDC-CHL)

The objective of this project is to investigate the feasibility of new scalable numerical methodology for simulating air-water free-surface flow, fluid-object interaction (FOI), and fluid-structure interaction (FSI) phenomena for complex geometries, and with no limitations on the motion of the free surface. In FY11, mixed Interface-Tracking/Interface-Capturing Technique (MITICT) was developed and investigated to track the ship-fluid interface and capture the air-water interface. This computational methodology was implemented in the investigator's software. The more successful versions of the formulation have been implemented in the ERDC-CHL software called Proteus, which directly enhances the computational capabilities of the U.S. Army Corps of Engineers (USACE). This work is directly relevant to the mission of the USACE in the areas of Coastal Hydraulics and Navigation. Prediction of ship squat, sloshing of liquids (e.g. fuel) in tanks, marine transportation of cargo, evaluation of unsteady loads on levies and embankments arising due to vessel motion in open channels are of great interest to the USACE.

This research team's specific FY11 accomplishments are listed below.

- Developed free-surface flow formulation suitable for discretization by finite elements and isogeometric analysis
- Developed a six degree-of-freedom rigid object formulation and coupled with free-surface flow
- Validated free-surface flow for linear FEM and isogeometric analysis discretizations (see FIGURE 11)
- Developed geometry modeling and meshing capabilities for ship hulls
- Simulated a free-surface fluid-object interaction for a ship hull at lab scale in high-amplitude head waves
- Implemented in ERDC-CHL code Proteus: (i) A new discrete formulation of free surface flow, (ii) new meshing capabilities for ship hulls, (iii) modified data structures and memory management to enable running simulations at a significantly larger scale than done previously, and (iv) validated Proteus on several complex free-surface problems

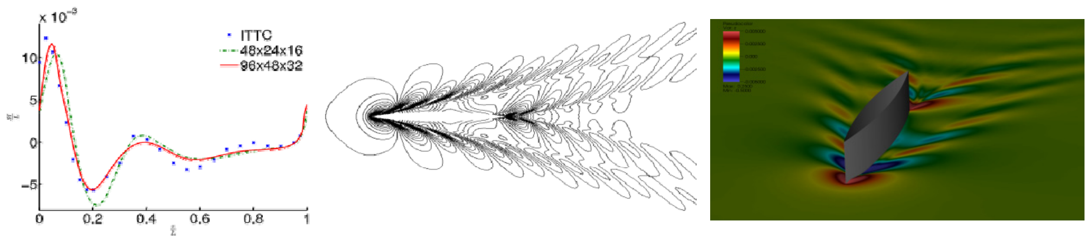

FIGURE 11

Validation of free-surface flow for linear FEM and isogeometric analysis discretizations. Verification and validation of the developed computational methodology for free-surface flow. Results for Wigley hull simulation using isogeometric analysis are shown, obtained from both finite element and isogeometric discretizations.

This technology was transferred to ERDC-CHL through visits by Professor Bazilevs to ERDC-CHL in Vicksburg, MS, where he interacted with Dr. Christopher Kees and Dr. Matthew Farthing on methods development and implementation, research planning, and definition of research deliverables. Dr. Akkerman, a postdoc co-supervised by Professor Bazilevs and Dr. Kees, visited ERDC-CHL in Vicksburg, MS, where he worked with Drs. Kees and Farthing on the development ERDC-CHL general-purpose FEM code Proteus. Dr. Akkerman spent the majority of his time at UC, San Diego implementing the developed technology in Proteus. Dr. Akkerman also participated in weekly tele- and video-conferencing with ERDC-CHL researchers, and delivered weekly progress reports to Dr. Kees. This project was successful enough to result in awarding a new start Single Investigator grant to continue the work, collaboration, and transition.

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. Algorithmic and Software Infrastructure for Extension of Indoor Portable 3D Mapping System

Professor Avideh Zakhor, University of California - Berkeley, Single Investigator Award

The objective of this project is to further develop the architecture and algorithms for GPS-denied navigation and photo-realistic rendering for integration in studies using a wheeled, mobile robot at ARL-VTD. The investigators existing laser-based navigation algorithms will be used for localization. The required hardware items include a yaw scanner, pitch scanner, two roll scanners, two side-looking modeling scanners, Intersense IMU, high-end Applanix IMU and three cameras (see FIGURE 12). The software is being prepared for on-line and off-line localization and algorithms for six DOF pose recovery, recognition of planes and features, loop closure, backward correction in time, merger, fusion and registration of multiple sub-models.

As was predicted in *ARO in Review 2010*, this research project has progressed in FY11 as anticipated, which included (i) successful 3D localization by a "2xICP+IMU" algorithm based on two applications of an iterated closest point (ICP) scan matching algorithm for *x*, *y* and yaw ("2xICP") and on an inertial measurement unit (IMU) for *z*, pitch and roll, (ii) design and implementation of the image capture pipeline, and (iii) the texture mapping of the detected planes. However, the full assembly of the operational system and the testing of the system have not yet been completed. It is anticipated that in FY12, the full system with algorithms and software for three degrees of freedom for navigation and localization will be assembled, tested, and verified in fully 3D environments with non-horizontal floors and no assumption of planarity of the floors.

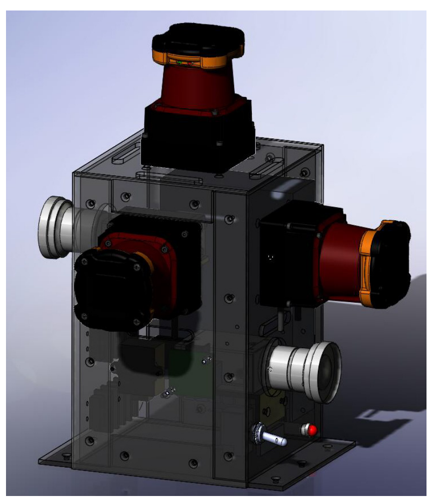

FIGURE 12

Compact hardware for 3D indoor mapping system (15 cm x 15 cm x 30 cm). It is anticipated that in FY12, the full system with algorithms and software for three degrees of freedom for navigation and localization will be assembled, tested, and verified in fully 3D environments with non-horizontal floors and no assumption of planarity of the floors.

B. Achieving a Systems Level Understanding of Changing Cell shape

Professor Tim Elston, University of North Carolina - Chapel Hill, Single Investigator Award

The goal of this project is to characterize and understand large-scale changes in cell morphology. An important property of all cells is their ability to sense and respond to their environment. For example, signaling molecules, such as hormones or growth factors, can lead to cell differentiation, proliferation, or migration. Understanding how the cytoskeleton and associated regulatory proteins function as an integrated system to generate changes in shape is a central challenge in cell biology. The morphological oscillations that occur in rounded cells constitute a mechanochemical prototype for studying regulation of the cytoskeleton by biochemical signaling networks as well as the biochemical properties of the cell that feed back to influence signaling. Computational approaches are required to fully understand the self-emergent properties of the cytoskeletal system. Fortunately, the oscillating cell system has several features which lend themselves to computational approaches. First, modern technology such as probes and microscopes allow the spatiotemporal dynamics of the cortex and signaling molecules to be visualized and manipulated with unprecedented resolution. Second, the mechanical properties of the cortex can be interrogated and perturbed in the oscillating cell. Third, oscillating cells have a well-defined period and shape history that are easily measured and can be directly compared with mathematical models.

Using high resolution confocal imaging, the investigator and his team have shown that during morphological oscillations, the actin cortex is reshaped and spontaneously polarizes toward alternate sides of the cell and that sites of high actin density correlate with active myosin, the protein that generates contractile forces (see FIGURE 13). In addition, they have shown, using biochemical methods, that the biochemical processes that regulate the oscillations are coupled to the biophysical mechanism generating the active forces required for the oscillations.

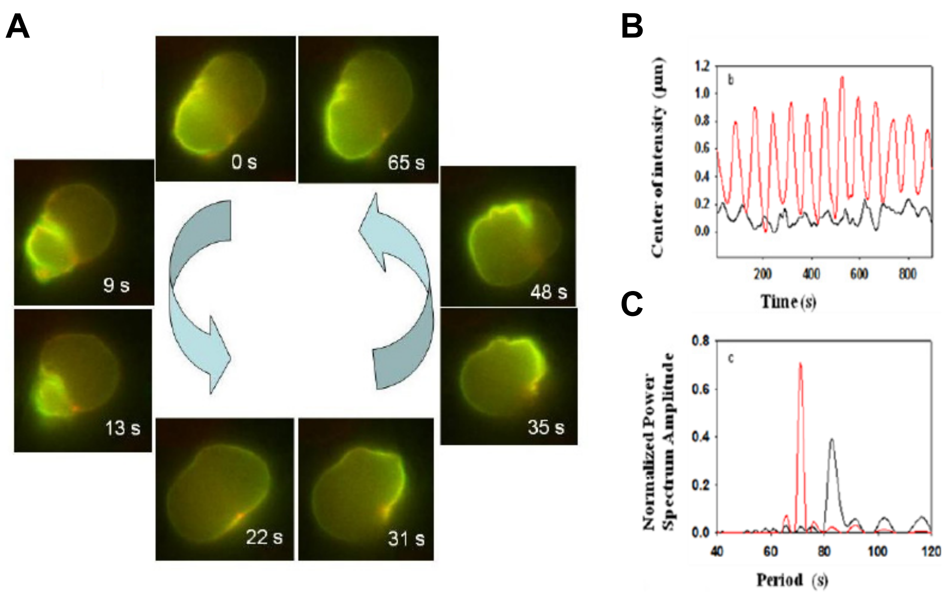

FIGURE 13

Cell changes during morphological oscillations. (A) Cytoskeletal dynamics during cell oscillations. Fluorescence image of f-actin (Lifeact, green) and myosin (red) during one cycle of oscillation. (B) The movement of the center (first moment) of phase contrast image intensity as a function of time for a single oscillating cell before (black) and after (red) depolymerization of microtubules. (C) Corresponding power spectra from the Fourier Transform of the wavesforms in (B).

To further investigate the actin-dependent morphological oscillations, this project will use an approach that combines experimental methods, including biochemical assays, novel biosensors, genetic techniques, biophysical measurements and high resolution imaging, with modeling and computational approaches to quantify, analyze and interpret the data. By tightly integrating modeling and computational approaches with quantitative experimental measurements in live cells, this project will produce novel mechanochemical models for understanding global shape changes.

It is anticipated that in FY12, the research team will develop multiphase models in order to investigate potential mechanisms for generating sustained oscillations in cell shape. Experiments involving novel reagents, live cell microscopy and local mechanical measurements will be designed to inform and test the multiphase model in order to test two hypotheses regarding these sustained oscillations; the first is that the oscillations are driven by a traveling wave of RhoA activity, independent of the cortex, and the second is that the cortical actomyosin cytoskeleton plays an active role in the oscillations. In addition, image analysis techniques based on level-set methods and needed for comparing experimental results with model predictions will be developed and used to generate and analyze high-resolution 4D image reconstructions of the oscillatory cycle.

Developing a mechanistic understanding of this system will yield insights into the design principles that regulate the dynamic properties of the cell cytoskeleton that are key to cell division, motility and differentiation and the alterations that occur in pathological processes. The research results will have significant impact on the understanding of wound healing and possibly, in the long term, on limb regeneration, among other areas related to soldier health of interest to the Army and DoD.

D. Stochastic Analysis & Control of Transonic Helicopter Aerodynamics and Supersonic Projectiles

Professor S. Sritharan, Naval Postgraduate School, Single Investigator Award

The objective of this project is to develop a systematic mathematical theory for the robust real time feedback control and stochastic analysis of unsteady transonic aerodynamics of helicopter rotor blades, supersonic ballistic projectiles and propagation of blast waves in the presents of adverse external disturbances. Modern tools in stochastic analysis of discontinuous processes and control theory of nonlinear partial differential equations are combined to develop a penetrating theoretical foundation for the agile management of unsteady, highly vortical aerodynamics with shocks. In this research, the state space variables of the control system are physical quantities of fluid dynamics such as velocity field, vorticity field and pressure distribution. The state equations for control and stochastic analysis are the Euler equations for compressible rotational gas dynamics and the quasilinear unsteady potential equations of irrotational flows. These nonlinear hyperbolic and elliptic-hyperbolic type mixed equations are subjected to additive and multiplicative external disturbances modeled as Gaussian, Poisson and Levy type noise forces. Point vortex and turbulent shell models also give useful insight in the understanding of highly vertical structures associated with the helicopter blade tip aerodynamics. With H. Kunita's theory of stochastic characteristics for nonlinear hyperbolic systems, control and estimation problems were formulated. Main research directions are mathematical characterization of entropy solutions for stochastic hyperbolic systems of conservation laws, state estimation and feedback control analysis as well as assessment of the impact of noise in controlled and uncontrolled aerodynamic flows of the above type. Necessary conditions for optimal controls are worked out using a stochastic counterpart of the Pontryagin maximum principle while feedback analysis utilizes infinite dimensional Hamilton-Jacobi theory.

The scope of this basic research is critical for the Army's command and control and C4ISR at large as it seeks to develop a fundamental capability to enhance understanding as well as strategic and dynamic management of aerodynamic flows over helicopter rotor blades and ballistic projectiles subjected to adverse uncertainties. Breakthroughs in this research will impact the transonic aerodynamics of helicopter rotor dynamics as well as Army technologies such as combustion control, multiphase flows, and possibly to crumpling of surfaces in armored vehicles subjected to shell attack. A Directed Energy Weapon (DEW) such as a CO-2 Laser, Free Electron Laser or microwave directed energy weapons such as the Russian RANETS-E attacking a helicopter or a missile may be modeled as an abrupt noise forcing of Levy type addressed in this paper and the estimation, control and mitigation techniques that were developed can give insight in to counter measures to such adversarial situations. Army's unmanned systems roadmap highlights the need for enhanced autonomy and this will in turn increase the importance of real time management of turbulence in aerodynamic configurations subject to uncertainties. This research program is at the heart of this paradigm.

It is anticipated that in FY12, the investigator will demonstrate the following.

- Solvability of strong path-wise solutions to Navier-Stokes equations with Levy noise
- Solvability theorems for nonlinear filtering equations of infinite dimensional Fujisaki-Kallianpur-Kunita and Zakai equations that correspond to nonlinear estimation of stochastic Navier-Stokes equation with Levy noise
- Stochastic Lagrangian particle method for Euler flows with jump noise and their solvability theorems
- Stochastic particle method for nonlinear filtering equations for N-point vortex models with noise and convergence theorems

VI. DIVISION STAFF

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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 2011* is to provide information on the programs and basic research efforts supported by ARO in FY11, 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 FY11.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mechanical Sciences Division supports research efforts to advance the Army and Nation's knowledge and understanding of the fundamental properties, principles, and processes involved in fluid flow, solid mechanics, chemical reacting flows, explosives and propellants, and dynamics of complex systems of relevance to the Army and the DoD. More specifically, the goal of the Division is to promote basic research studies to uncover the relationships to: (i) contribute to and exploit recent developments in kinetics and reaction modeling, spray development and burning, (ii) gain an understanding of extraction and conversion of stored chemical energy, (iii) develop a fundamental understanding that spans from a material's configuration to a systems response to create revolutionary improvements through significant expansion of the design landscape used to optimizing systems, (iv) advance knowledge and understanding governing the influence of inertial, thermal, electrical, magnetic, impact, damping, and aerodynamic forces on the dynamic response of complex systems as well as improving the inherent feature set of the components (*i.e.*, mechanisms and sensing) that comprise them, (v) provide the basis for novel systems that are able to adapt to their environment for optimal performance or new functionality, and (vi) develop 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, the research efforts 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 allowing implementation of renewable fuel sources and new understanding of energetic materials with improved methods for ignition, detonation, and control.

3. Coordination with Other Divisions and Agencies. The primary laboratory interactions of this Division are with the ARL Weapons and Materials Research Directorate (ARL-WMRD), ARL Vehicle Technology Directorate (ARL-VTD), ARL Sensors and Electron Devices Directorate (ARL-SEDD), the Joint IED Defeat Organization (JIEDDO), the U.S. Army Corps of Engineers (USACE), and various Army Research Development and Engineering Centers (RDECs), including the Aviation and Missile RDEC (AMRDEC), Natick

Soldier RDEC (NSRDEC), and the Tank-Automotive RDEC (TARDEC). The Division also facilitates the development of joint workshops and projects with Program Executive Office (PEO) Soldier and the Army Medical Research and Materiel Command (MRMC). In addition, the Division often jointly manages research efforts with ARO programs in the ARO Chemical Sciences, Materials Science, Mathematical Sciences, Computer Sciences, and Life Sciences Divisions, through co-funded efforts, projects, workshops, and committees. Strong coordination is also maintained with other Government agencies, such as the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the National Science Foundation (NSF), the National Aeronautics and Space Administration (NASA), the National Institute of Standards and Technology (NIST), and the Department of Energy (DoE). Several international efforts are also coordinated through the International Science and Technology office in London (ITC-London) and the Pacific (ITC-Pacific).

B. Program Areas

To meet the long-term program goals described in the previous section, the Mechanical Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of projects. In FY11, the Division managed research efforts within these four Program Areas: (i) Solid Mechanics, (ii) Complex Dynamics and Systems, (iii) Propulsion and Energetics, and (iv) Fluid Dynamics. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Solid Mechanics. The goal of the Solid Mechanics Program Area is to develop physically-based mechanics tools (theory, experiments, computations) 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 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 efforts in the Multiscale Mechanics of Heterogeneous Solids Thrust is to extend the design envelope of current and future Army structures is predictive continuum damage and cohesive models with physical basis that are supported by *ab initio* and molecular dynamics 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 efforts in this Program Area are focused on long-term, high risk goals that strive to develop the underpinnings for revolutionary advances in our military systems. It is developing the methods needed to take advantage of recent advances in new materials technology, including nanotubes, nanocrystaline solids, and bio-inspired and hierarchical polymeric- and nano- composites. As a result of the long-term vision of the program, some future applications are yet unimagined while others will lead to the creation of ultra-lightweight, high strength materials for applications such as lightweight armor, unmanned aerial vehicles (UAVs), unmanned ground vehicles (UGVs), and munitions.

2. Complex Dynamics and Systems. The goal of the Complex Dynamics and Systems Program Area is to exploit trans-disciplinary nonlinear science while vigorously pursuing new mathematical frameworks for the intelligent synthesis and exploitation of multi-dimensional flows in high-dimensional dynamical systems. This Program Area encompasses a significant shift away from traditional investment areas in legacy dynamics programs at ARO in order to capitalize on remarkable advances in scientific understanding of *dynamical systems theory* (the study of the temporal evolution of abstract vector flows that are not necessarily mechanical in nature) and *non-equilibrium physics*. Programmatic strategy is to foster mathematically sophisticated, interdisciplinary, and hypothesis-driven research to elucidate the classical physics and analytical methods pertinent to the foundations of a broad spectrum of ARL Major Laboratory Programs to include: mobility, power and energy, sensors, lethality, and trans-disciplinary network science.

This Program Area is divided into two research Thrusts: (i) Mathematics and Control of Complex Dynamical Systems and (ii) Force Generation. The thrusts are comprised of Army-relevant problems in both low- and high-dimensional dynamical systems, and the exploitation of nonlinear and stochastic dynamic interactions at the nanoscale. New efforts in geometric biomechanics, neuromechanics, and granular dynamics have been introduced in respective thrust areas in low and high dimensional dynamical systems to inspire deep intuition for decentralized control, terramechanical interaction physics, and mathematical formalisms to enable solutions to agile robotic mobility problems. Provided the ubiquity of coupled oscillators and interdependent dynamic systems with underlying graph structure in a wide range of Army-relevant research programs from neuroscience to NEMS/MEMS frequency sources to networks, there is a resounding need for the establishment of a high-dimensional dynamical systems theory for which coherent structures, new understanding of attractors and bifurcations in high-dimensional phase space, state-estimation and control, heavy-tail distributions, and multiscale phenomena can be understood with an emphasis on implications for engineering design. Complicated multiphysics interactions as well as the inescapable manifestation of noise and nonlinearity at the nanoscale demands complete understanding to push the boundaries of our ability to analyze and engineer infinitesimal systems. Accordingly, the Complex Dynamics and Systems program balances theoretical and experimental investigations and emphasizes interdisciplinary approaches in order to lay the foundations for the analysis of dynamic phenomena extensible to a wide range of more focused Army research programs.

3. Propulsion and Energetics. The goal of this Program Area is explore and exploit recent developments in kinetics and reaction modeling, spray development and burning, and our understanding of extraction and conversion of stored chemical energy to ultimately enable higher performance propulsion systems, improved combustion models for engine design, and higher energy density materials, insensitive materials, and tailored energy release rate. Research in propulsion and energetics supports the Army's need for higher performance propulsion systems. These systems must also provide reduced logistics burden (lower fuel/propellant usage) and longer life than today's systems. Fundamental to this area are 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 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 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, continues. 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 FY11 were $20.6 million. These funds were provided by multiple sources and applied to a variety of Program Areas, as described here.

The FY11 ARO core (BH57) program funding allotment for this Division was $5.8 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 $4.2 million to projects managed by the Division. The Division managed $5.9 million provided by the Defense Advanced Research projects Agency (DARPA), and $1.8 million provided by other agencies. The Small Business Innovative Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided $0.9 million for projects managed by the Division in FY11. 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 identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY11 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). 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. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. Multi-Agency Coordinating Committed for Combustion Research (MACCCR) Turbulent Combustion Workshop (Atlanta, GA; 20 March 2011). The goal of this workshop to discuss research needs relating to turbulent combustion modeling and areas of research that are needed to be able to better validate models and predictive codes. The workshop discussion considered specific regimes of combustion as needed for various combustion applications, such as gas turbine engines, diesel engines and rocket propulsion. This workshop was held in conjunction with the US Combustion Meeting in Atlanta, GA. Participants were comprised of DoD and other government researchers, as well as academic and industry researchers and representatives.

2. Workshop on Revolutionary Energy Harvesting (Austin, TX; 7 April 2011). The goal of this workshop was discuss new approaches to the extraction of useful energy from ambient mechanical excitation. The focus of the workshop concerned exploitation of nonlinear mechanical design. The participants were comprised of researchers from academia, industry and DoD.

C. Multidisciplinary University Research Initiative (MURI)

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

1. Enabling Science for Future Force Insensitive Munitions. This MURI began in FY05 and was granted to a team led by Professor Don Thompson at the University of Missouri, Columbia. The objective of this MURI is to understand and predict the sensitivity of energetic materials to externally-impressed mechanical and thermal loadings. The specific goals include developing understanding of the chemistry and physics that determine the onset of chemical reaction in crystalline energetic materials and their formulations.

This project is a coordinated effort by several research groups. The first group, headed by Professor Thompson, is developing a unified, multiscale model to predict energetic material sensitivity. The second group, headed by Professor Michael Pravica of the University of Nevada, Las Vegas, is investigating the effect of defects in energetic crystals upon mechanisms of initiation and energy release. Co-investigators in this effort include Professor W. Goddard III at the California Institute of Technology, who is investigating the fundamental chemistry and physics of energetic materials under extreme conditions. Efforts at developing multi-scale models of the phenomena are by Professor M. Ortiz, also at the California Institute of Technology. Research from this project is closely monitored by, and coordinated with investigators from DoD and DoE laboratories.

2. Ultrafast Laser Interaction Processes for LIBS and Other Sensing Technologies. This MURI began in FY06 and was awarded to a team led by Professor Martin Richardson at the University of Central Florida. The objective of this research is to develop a theoretical understanding of femtosecond laser/materials interaction that is expressed in combined physical and chemical models, rigorously grounded by experimental characterization and detailed physical and chemical observations. These models will then be extended to the irradiation of complex sample matrices characteristic of chem/bio threat scenarios, and the use of advanced laser beam modalities, including femtosecond laser self-channeling (FLSC), with an ultimate goal to develop laser induced breakdown spectroscopy (LIBS) stand-off technologies to the kilometer range. This understanding is expressed in combined physical and chemical models, rigorously grounded by experimental characterization and detailed physical and chemical observations relevant to LIBS and other spectroscopic sensing techniques. The techniques include fluorescence an dRaman scattering and resonance enhanced multiphoton ionization. The models will then be extended to irradiation of complex material samples characteristic of chemical and biological threat scenarios, and energetic materials such as those found in improvised explosive devices (IEDs).

3. 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 focusing 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 both 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 combustion physics of gelled hypergols.

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

No new starts were initiated in FY11.

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

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Hierarchically Assembled Self-Healing Material. A Phase I STTR contract was awarded to AstroTerra Corp. to establish the feasibility of fabricating a multilayer composite through the Hierarchical Combinatorial Technique and characterize the response of the material under fatigue and high-rate loading conditions. The piezoelectric PDMS and PDMS-based polyionenes will be fabricated and integrated by Virginia Commonwealth University (VCU) into a single step manufacturing process. A multiphysics model will be developed for the interactions in the composite as a function of its microstructure and compared with characterization studies. The multiphysics model will be expanded to predict the multi-scale behavior for a scaled up material. The model will be developed using ANSYS by VCU and the code delivered to AstroTerra Corp (ATC) for development beyond Phase-I. The procedure developed by VCU and Virginia Tech to prototype this material will be used by ATC in Phase-II and beyond for optimization and commercialization.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) – 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). The FY11 new starts within these programs are described here, while the missions of each of these programs were described *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. DoD REP Awards. As described in more detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, REP awards aim to enhance or increase the programs, capabilities, and graduates in scientific and engineering disciplines in universities serving underrepresented minorities. In FY11, the Mechanical Sciences Division managed four new REP projects, totaling $1.9 million. The equipment purchased with this award is promoting research in areas of interest to ARO, such as the study of laminar to turbulence transition in boundary layers that are typically developed in low hypersonic flow regimes, and to measure fracture parameters in a bi-material interface under high-strain-rate loading.

2. DoD TCU Instrumentation Awards. As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the TCU program aims to enhance science, mathematics, and/or engineering education programs and/or research capabilities through the acquisition of equipment and/or instrumentation that will augment existing facilities, enhance curricula, or help develop new laboratories, programs, and capabilities in these areas. In FY11, the Mechanical Sciences Division managed one new TCU project. The equipment purchased with these awards is promoting education and research in areas of interest to ARO, including instruction in theoretical modeling, mechanics, and research in bio-medical applications.

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

No new starts were initiated in FY11.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY11, the Mechanical Sciences Division initiated six new DURIP projects, totaling $1 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies to explore aerosol shock tube experiments up to 60 atm, dynamic triaxial strain experiments with a novel pressure chamber, and imaging unsteady flows with a high framing rate imaging system.

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 late in FY08 with an objective of developing and demonstrating materials/material systems that can serve as reactive high strength structural materials (*i.e.*, be able to withstand high stresses and can also be controllably stimulated to produce substantial blast energy). Research is investigating innovative approaches that enable revolutionary advances in science, technology, and materials system performance. These approaches touch on several Mechanical Sciences Division research areas, including: rapid fracture and pulverization of the material, dispersion of the particles, and material ignition and burning, all while achieving strength, density and energy content metrics. The vision of the RMS program is to be able to replace the inert structural materials currently used in munition cases with reactive material structures that provide both structural integrity and energy within the same material system along with the ability to rapidly release the energy upon demand.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. Multiscale Meshless and Finite Element Methods

Professor Ted Belytschko, Northwestern University, Single Investigator Award

The goal of this research project is to develop hierarchical and concurrent methods for determining material constitutive models for finite element computations, and the incorporation of particle methods such as molecular dynamics into multiscale frameworks for investigating material failure phenomena such as cracks and dislocations. The improvement of accuracy in multiscale methods can reduce the need for testing and prototyping of armored vehicles and protective gear by providing reliable numerical estimates of performance. The work enables an atomistic level insight of the behavior and failure of materials through micro-crack propagation, which will facilitate the design of improved armor and other structural components.

The researchers have developed a new method for modeling the evolution of defects and material failure with coupled discrete particle and continuum mechanics simulations. In this method, a domain is decomposed into discrete particle and continuum regions, where an energy weighting function partitions the energy between the two models where they are overlapping. The particle domain tracks defects as they propagate, and features such as crack faces or dislocation glide planes are coarsened and represented by enrichments to the finite element basis. These features allow for computationally more expensive particle methods such as molecular dynamics (MD) to model defects only in the parts of the domain where they are necessary (see FIGURE 1).

The investigators have also developed a new coupled quantum/continuum mechanics method, which links extended finite element method (XFEM) and density functional theory (DFT) to investigate fracture at the bond-breaking level. The three main features of this method are: the DFT-based material model from the hierarchical framework, the electron density criterion for fracture and adaptivity of the DFT domain during crack growth.

The dislocation analysis method has been improved for more complicated materials and coupling to fine scale (atomic) models. Dislocations play a large role in dissipating energy during a failure process in ductile materials. Dislocations are caused by inter-atomic surfaces slipping relative to each other, but can be characterized as discontinuities at the macro level. The capabilities of the recently-developed XFEM have been expanded for dislocation analysis to model anisotropic materials and use higher-order elements.

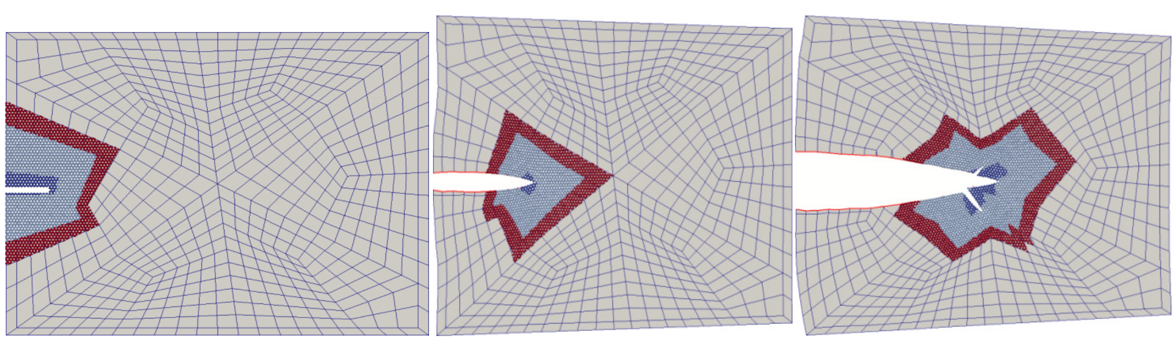

FIGURE 1

The panels illustrate the propagation of zigzag edge cracks in an adaptive, coupled atomistic-to-continuum calculation. The grey regions are modeled as a continuum with the extended finite element method, and the remaining regions are modeled by molecular dynamics. The colors of atomic regions indicate whether the regions is (dark blue) a region containing a defect, (light blue) a buffer region around defects, or (red) the coupling region.

B. Characterization and Failure Theories for 3D Textile Composites under High Strain Rate Loading
Professor B. Sankar, University of Florida, Single Investigator Award

The objective of this research is to develop a fundamental understanding of high-strain rate behavior and high-velocity impact-induced damage in 3D textile composites. Professor Sankar, and co-investigator Professor Subhash, are characterizing the effectiveness of through-the-thickness yarns to impact loads, considering impact loads that are both concentrated (due to a sharp projectile) and distributed (due to a blunt projectile). The progression of damage during impact will be investigated and the residual strength of the composite estimated.

The researchers have developed micromechanical models for damage development in 3D textile composites in order to predict experimental observations. Ten different composite designs have been evaluated including a 2D baseline composite and nine different 3D woven composites using short beam bend tests. These tests were performed at several different rates of loading. Static tests were performed with rates of 0.1 mm/s, 1.0 mm/s and 10 mm/s (see FIGURE 2). Using the split Hopkinson bar apparatus, high rate loading bend tests were performed at a rate of 10 m/s. A high-speed camera was used to record both dynamic and static bend tests. From these images it is possible to observe the progression of damage during testing. Specimens subjected to dynamic testing were subsequently retested to determine the residual stiffness. The residual stiffness after impact can be used as an indicator of damage tolerance. Tests indicate that the 2D woven specimens achieved the maximum load before the initiation of damage at all loading rates. However these specimens also showed a large loss in stiffness during reloading. High speed images of 2D woven specimens during impact show cracks propagating to the edge of the specimens often concentrated on one side of the indenter. These large delaminations reduce the stiffness and strength during subsequent reloading. 3D woven composites with large volumes of z-fibers show much smaller delamination cracks distributed throughout the specimen. These smaller cracks do not reduce the strength of the specimen as greatly as those in the 2D woven specimens. Further tests are to be conducted at higher rates of loading. In addition to bend tests, small coupons will be tested using a "blunt" spherical indenter. The coupons will be sectioned into bend specimens and tested to evaluate the damage caused during impact. A new hybrid 3D woven design will also be tested. This hybrid design includes Twaron® z-fibers and will include IM-7 carbon fiber in the top and bottom layers of the composite along with S-2 glass fibers.

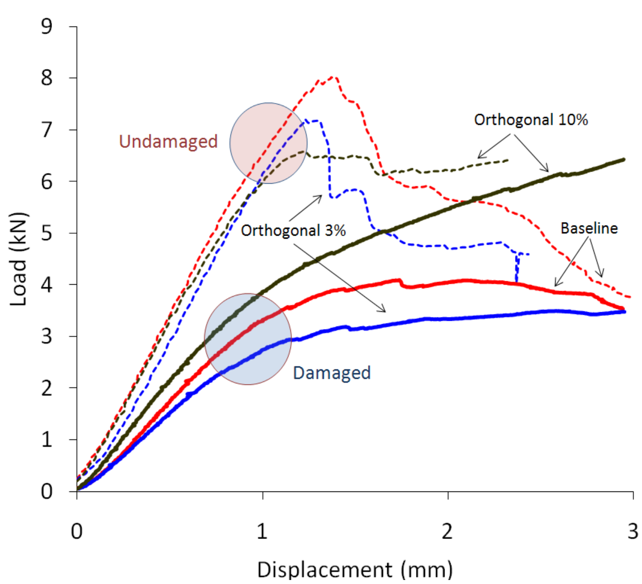

FIGURE 2

High-rate loading bend tests to assess dynamic and static bend. Static tests were performed with rates of 0.1 mm/s, 1.0 mm/s and 10 mm/s. Preliminary results from split-hopkinson pressure bar to perform blunt impacts indicate that the baseline and 3% orthogonally woven specimens show a higher loss in strength and stiffness than the 10% orthogonal. Test indicates a higher damage tolerance in 3D woven specimens with 10% z-yarn

The researchers have also completed an analytical non-dimensional model to analyze crack propagation in a z-pinned double cantilever beam specimen (DCB) under Mode I loading. Effect of various design parameters on the crack bridging length and apparent fracture toughness are investigated using this model. The efficacy of the analytical model is evaluated by comparing the same with 3D finite element (FE) simulations of the DCB. In the FE model the z-pins are modeled as discrete non-linear elements. Bi-linear cohesive elements are used ahead of the crack tip to account for the inherent fracture toughness of the composite material. The results for load-deflection and crack length obtained from the analytical model and the FE model are compared and found to be in good agreement. Proposed non-dimensional analytical model will be useful in the design of z-yarns and translaminar reinforcements for composite structures.

C. Exploring Passive and Active Mechanisms of Massively Separated High-Speed Flow Control

Professor J. Dutton, University of Illinois - Urbana-Champaign, Single Investigator Award

Professor Dutton and co-investigator Professor Elliot are studying the effects of passive splitter plates placed in the recirculation region behind a blunt-based axisymmetric body aligned in supersonic Mach 2.49 flow. The goals of this research project are to obtain a better understanding of the physical phenomena that govern these massively-separated high-speed flows and to determine the flow-control authority of this passive device. Triangular splitter plates dividing the near wake into 1/2, 1/3, and 1/4 cylindrical regions were designed to exploit specific stability characteristics of this flow, to affect the near-wake flow, to alter the base pressure, and ultimately to affect base drag. Mean and high-frequency static pressure measurements were acquired on the base to assess the influence of these plates (see FIGURE 3). Schlieren imaging, surface flow visualization, and pressure-sensitive paint measurements were also employed to document the near-wake flowfield, surface flow structure, and surface pressure, respectively. The time-averaged base pressure distribution, time-series pressure fluctuations, and presumably the stability characteristics were altered by the spatial division of the near wake. The area-integrated pressure was only slightly affected. Normalized rms levels indicate pressure fluctuations were significantly reduced (as much as 39%) with the addition of the splitter plates. Power-spectral-density estimates revealed a spectral broadening of fluctuating energy for the 1/2 cylinder configuration compared to no control and a bimodal distribution for the 1/3 and 1/4 cylinder configurations.

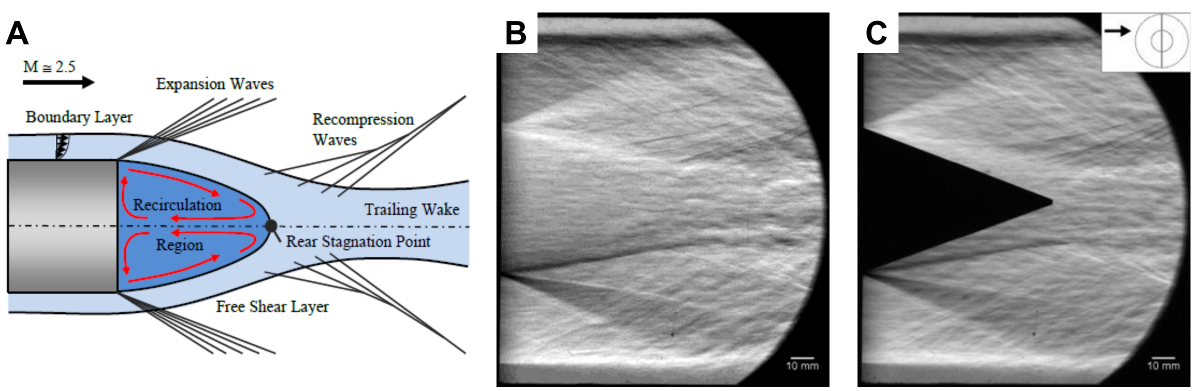

FIGURE 3

Flow control approaches. (A) Schematic of mean near-wake flow field for blunt cylindrical afterbody and instantaneous schlieren images: (B) base flow with no control and (C) 1/3 cylinder splitter-plate control.

Based on these studies, the investigators found that (i) insertion of the solid plates into the separated region affected the near-wake flow structure such that the time-averaged radial base pressure distribution was altered, (ii) normalized rms ressure levels were substantially decreased with increasing number of near-wake divisions, and for all configurations, the normalized rms magnitudes of the inner radial location were observed to be higher than for the outer location. In addition, (iii) the power-spectral-density estimates revealed the differences in base pressure fluctuations at two radial locations for the no-control and splitter plate cases. For the 1/2 cylinder splitter-plate configuration, the fluctuating pressure peak is broadened to higher frequencies compared to the no-control case. For the 1/3 and 1/4 cylinder splitter-plate configurations, two distinct peaks in the power-spectral-density were observed, which suggested that more than one mechanism is accountable for the pressure fluctuations on the base.

D. Effect of Stroke Deviation on Forward Flapping Flight

Professor Danesh Tafti, Virginia Polytechnic Institute and State University, Single Investigator Award

The goal of this project is to understand the physics of flapping wings. Understanding the unsteady aerodynamics of flapping wings is critical to the design of efficient micro air vehicles (MAVs). The kinematics of wing motion is often a complex combination of translation and rotation in the stroke plane with significant morphological changes for optimal flow control. A number of aerodynamic mechanisms, such as, clap and fling, delayed stall, wake capturing, and rotational circulation have been proposed to explain the generation of lift in birds and insects. However, the Leading Edge Vortex (LEV) dynamics concept (or delayed stall) still remains one of the most influential factors affecting overall production of lift by a flapping wing. The study builds on the LEV concept by focusing on the role of the out-of-stroke-plane displacement of the wing (stroke deviation). The stroke deviation concept can explain some of the common wing trajectories seen in nature, as mapped by a point near the wing tip (see FIGURE 4).

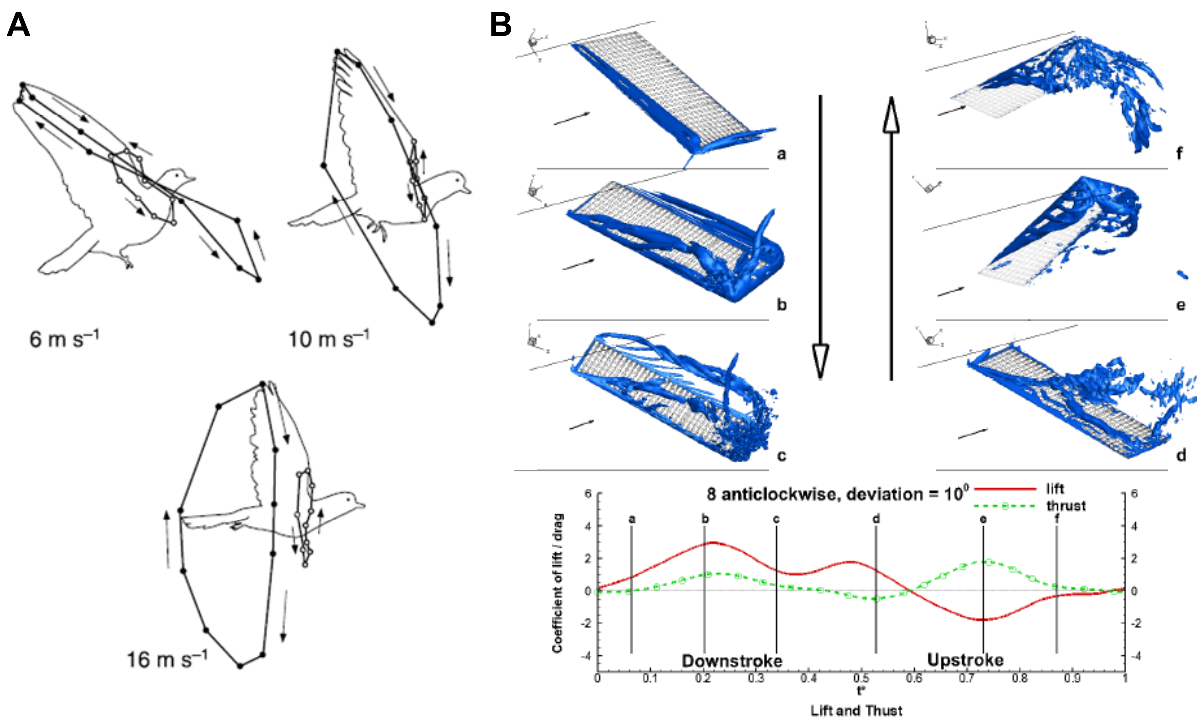

FIGURE 4

Flapping Wing Stroke Deviation and Time history of vortex formation. (**A**) Birds with pointed, high-aspect ratio wings such as the pigeon, Columba livia, transition from tip-reversal upstrokes, figure-of-8, during slow flight to feathered upstrokes at intermediate speeds and a swept-wing upstroke, O-cycle, during fast flight, (**B**) The wing surface is shaded dark for top view (a, b, c) and shaded light for bottom view (d, e, f). Bottom plot shows lift and thrust coefficient variation for a flapping cycle over normalized time.

In this study, the performance of a rigid flapping wing in forward flight was investigated at Re = 10,000, using a number of different stroke deviation trajectories. The instantaneous lift and thrust profiles were observed to be influenced by a combination of the Leading Edge Vortex (LEV) and the Trailing Edge Vortex (TEV) structures existing in the flow at any given time. Unlike regular no-deviation flapping cycles, the TEV is shown to be significant for out-of-plane trajectories. The clockwise O-cycle trajectories seem to hold potential as a viable stroke deviation flapping trajectory with better performance for similar power input and a uniform force output while the other trajectories make available various choices in lift and thrust capabilities at the cost of higher power over the no-deviation base case.

E. Bio-inspired Flexible Cellular Actuating Systems

Professor Soon-Jo Chung, University of Illinois - Urbana-Champaign, Single Investigator Award

The objective of this project is to utilize a model-guided and neurobiologically inspired approach to design and control bio-inspired flexible actuating systems for compliant and lightweight robotic arms and grippers for tightly constrained environments, and energy-efficient muscle actuators for biomimetic locomotion (see FIGURE 5). In particular, compliant robotic actuators provide the ability to interact with dynamically varying external conditions. The realization of the proposed actuation and sensory framework will assist in exploration of currently forbidden terrains, monitoring of critical assets, as well as mitigation of environmental hazards. The effort is unique in that it will develop neurobiologically inspired sensory and control strategies to hyper-redundant cellular flexible arms that form bundles of braided and intertwined laminated layers, assembled with different bundle orientations. The network of braided actuators will provide the many degrees of freedom that mimic an octopus arm's functionality. This project leverages multidisciplinary expertise of Professor Chung (nonlinear control theory and robotics) and co-investigator, Professor Ashraf Bastawros at Iowa State University (composite mechanics/materials).

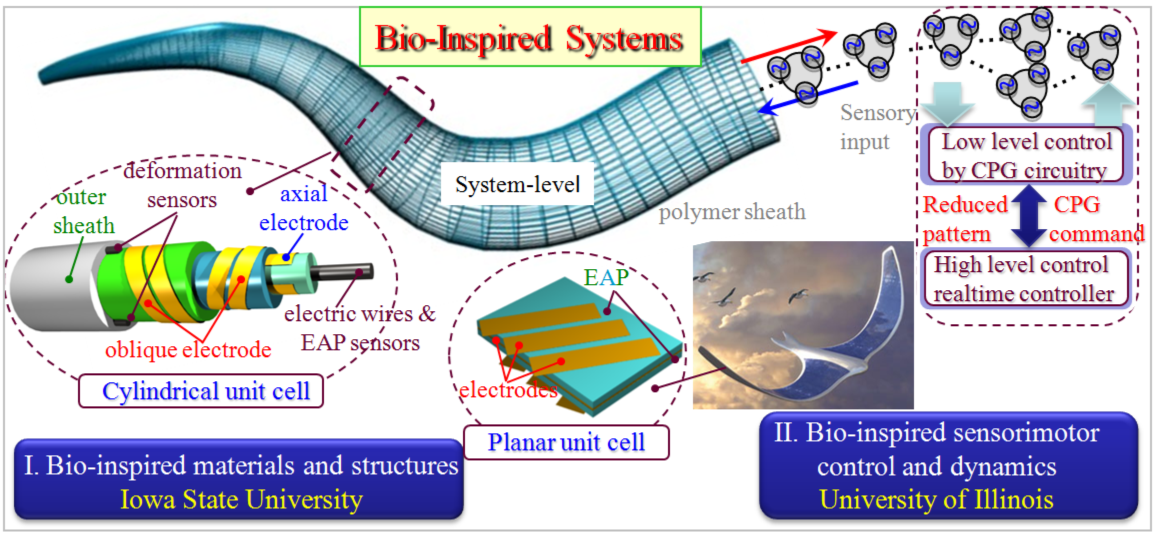

FIGURE 5

Multidisciplinary research approaches to explore bio-inspired systems. The figure highlights the two approaches being pursued by the investigators to understand and control bio-inspired systems.

Thus far, research in this field has (i) established control-theoretic framework for engineered sensorimotor control, and (ii) developed boundary control of partial differential models of flexible structures. For sensorimotor control, various sensing schemes have been integrated with biomimetic actuation systems, such as artificial arms. Most of them measure strain and bending only at discrete joints in the actuators. There have been, however, few reports on integrated sensing schemes for soft and flexible actuators without distinct joints with a notable exception. Inspired by the hierarchical control structure found in both vertebrates and invertebrates, we are deriving the mathematical framework for control theories based on physical models that can mimic the neurobiological control structure of flexible octopus arms by means of central pattern generators (CPGs). An engineered CPG network, which ensures the stability and robust adaptation of motion, can significantly reduce the complexity associated with numerous degrees of freedom. Concerning flexible structure boundary control, Professor Chung has derived control strategies for coupled PDEs of beam bending and twist with a system output given by a spatial integral of weighted functions of the state.

This formulation is directly applicable to the control of an aerial robot with articulated flexible wings or flexible robotic arms, in which case the output of interest is a net aerodynamic/hydrodynamic force or moment. Flexible arms can be controlled via actuation at the root or the tip, and this is by far more efficient than distributed actuator schemes in terms of reducing the number of actuators and implementation complexity. The problem of beam twist was analyzed in detail to illustrate the formulation, and the investigators demonstrated that the control law ensures that the error between the desired output signal and the actual output signal decreases exponentially to a uniform ultimate bound (see FIGURE 6). Rigorous stability analysis of the closed loop system is proved by Lyapunov techniques applied to infinite dimensional PDEs.

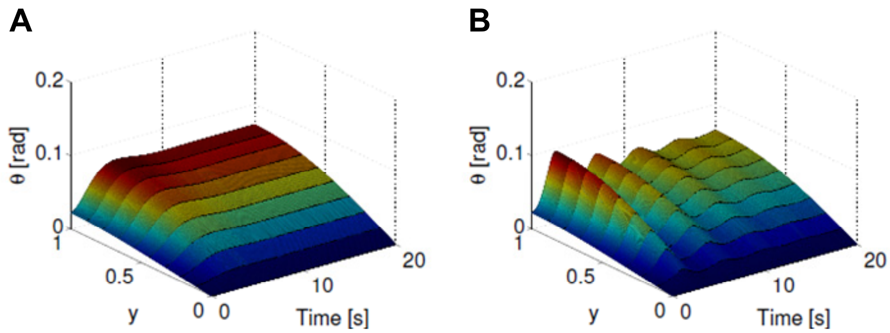

FIGURE 6

PDE boundary control of hyperbolic PDEs. A twist profile of flexible wings as a function of time, (A) assuming known system dynamics, and (B) assuming aerodynamics to be linear but otherwise unknown.

F. Development of Fully-integrated Micromagnetic Actuator Technologies
Professor David Arnold, University of Florida, PECASE Award

The goal of this research project, led by Professor Arnold at the University of Florida, is to develop the foundational principles of microscale electromagnetic mechanical actuation for use in advanced Army systems such micro-air-vehicles, insect-sized robots, directed munitions, communication devices, or man-portable combat systems. These microelectromechanical systems (MEMS) are built in large quantities at low cost via semiconductor chip-like manufacturing. The significance of this research is the development of mass-manufacturable, ultra-miniature electromechanical actuators at size scales not possible with conventional manufacturing. A key enabling technology is the ability to integrate high-performance permanent magnet materials into wafer-level microfabrication processes.

Over the past year, tremendous progress has been made in the manufacture, modeling, and characterization of first-generation experimental proof-of-concept testbeds. Simple out-of-plane microactuators have been microfabricated and tested to showcase the technology. These experimental devices operate using the magnetic forces between a coil and a tiny permanent magnet attached on flexible polymer membrane (see FIGURE 7). In operation, electrical current is supplied to the coil, resulting in piston-like motion of the diaphragm.

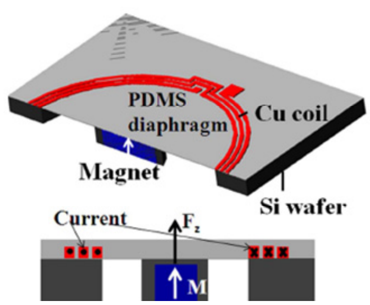

FIGURE 7

Cutaway and cross-sectional diagrams of out-of-plane magnetic microactuator. Simple out-of-plane microactuators have been microfabricated and tested to showcase first-generation experimental proof-of-concept testbeds. These experimental devices operate using the magnetic forces between a coil and a tiny permanent magnet attached on flexible polymer membrane

Reduced-order (lumped) parametric models are used to model the device behavior. These models are validated via extensive electromechanical characterization. The research team has measured velocity and compared the results to model predictions for a 5-mm-diameter device, with and without a mass load on the piston (see FIGURE 8). In the unloaded case, at the resonant frequency of 240 Hz, the microactuator exhibits 150 mm/s velocity per ampere of excitation current. Ongoing efforts aim to continuously improve the device performance via design optimization and fabrication enhancements. Future device designs will also be tailored for specific applications, such as microscale flow control.

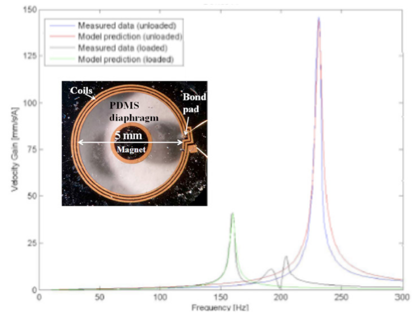

FIGURE 8

Comparison of experimental microactuator data vs reduced-order parametric model predictions. The electromechanical response (velocity per ampere) of a 5-mm-diameter microactuator is shown in the plot, revealing excellent agreement between experimental measurements and parametric models.

G. Rational Engineering of Reactive Nano-Laminates for Tunable Ignition and Power

Professor Jon-Paul Maria, North Carolina State University, Single Investigator Award

The objective of this research, led by Professor Maria, with co-investigators Donald Brenner and Douglas Irving, is to conduct a collaborative experimental/computational investigation of reactive nanocomposite structures identified as attractive new energetic materials with the potential for tunable power via engineered ignition. The material combinations being studied belong to a family of metal/metal oxide nanolaminates that are thermodynamically predisposed to the rapid release of chemical energy via oxygen exchange. The energy densities are up to four times larger than values accessible to conventional organics (*e.g.*, RDX) and there are electrical ignition possibilities that span local to volumetric geometries. Consequently a new generation of energetic composite is foreseen that, in conjunction with conventional materials, creates a new capability to design and fabricate munitions with tunable lethality.

The researchers initially evaluated reactive multilayer systems including CuO-Al, CuO-Zr, and CuO-Mg. These were chosen as they represent systems with terminal oxides that are good diffusion barriers (Al_2O_3), fast ion conductors (ZrO_2), and exhibit a large volume change upon oxidation from the parent metal (MgO). In all cases, self-propagating reactions could be initiated by low temperature anneals. X-ray diffraction studies were conducted on multilayer stacks that exhibited systematically varied layer thicknesses, after annealing to increasingly high temperatures. The post-annealing diffraction studies are used to estimate the temperature onset of oxygen exchange reactions. In all cases, decreasing the layer thicknesses reduces the temperature at which the reactions initiate. For CuO-Al, CuO-Zr, and CuO-Mg, the initiation reactions occurred in the range of 500 °C, 300 °C, and 400 °C. These values are consistent with the expectation that CuO-Al will be the slowest because of the diffusion barrier effect, CuO-Zr be the fastest due to anion conductivity, and CuO-Mg be intermediate.

At this initial stage, a number of experiments were conducted to evaluate the effect of layer thickness variation for the three systems investigated. It was observed that in all cases, thinner layers produced greater reactivity, and a lower temperature onset of oxygen exchange. Though at this point the data remains qualitative (given the challenge of knowing exactly when fast reactions begin), it was found that reducing the CuO thickness in CuO-Zr can reduce the reaction onset by 200 °C. Similar effects were seen for the other systems. In addition, during this optimization stage the impact of total number of metal/oxide layers was explored. A total of five cycles (ten total layers) produces a "bulk-like" response (*i.e.*, adding more layers does not change the experimental observations). An interesting, but yet not understood observation is that the lowering of reaction temperatures by thickness required much lower thicknesses for the case of CuO-Mg as compared to the other systems.

Also in FY11, the investigators used calorimetry to evaluate multilayer reactions. To address concerns regarding quantitative measurements of interface reactions, techniques were developed that use a commercially available calorimeter. The investigators assessed calorimetry results collected in inert (Ar) atmospheres (see FIGURE 9). These data were the group's first attempt at quantitative analysis of oxygen exchange reactions, and demonstrated the ability to change/overcome kinetic factors by layer geometry. As shown in FIGURE 9A, the arrows labeled 1 and 2 correspond thermal events that are believed to be (2) the low temperature initial reaction/oxygen exchange between the metal and CuO that is stopped by the simultaneously forming alumina barrier layer, and (1) the higher temperature reaction where the barrier layer is overcome by higher temperatures and the reaction continues. The arrows labeled (3) and (4) are believed to correspond to the same initial reaction/exchange, but the reaction goes to completion because the individual layers are so much thinner. Although a full explanation of the calorimetry data for CuO-Zr has not yet been fully explained (see FIGURE 9B), some important phenomena have already been observed: the first exothermic reaction becomes monotonically lower as the number of interfaces increases. This suggests that increasing the number of interfaces reduces the kinetic barrier to oxygen exchange. It is interesting to note that in comparison to the CuO-Al case, the reaction onset temperature changes.

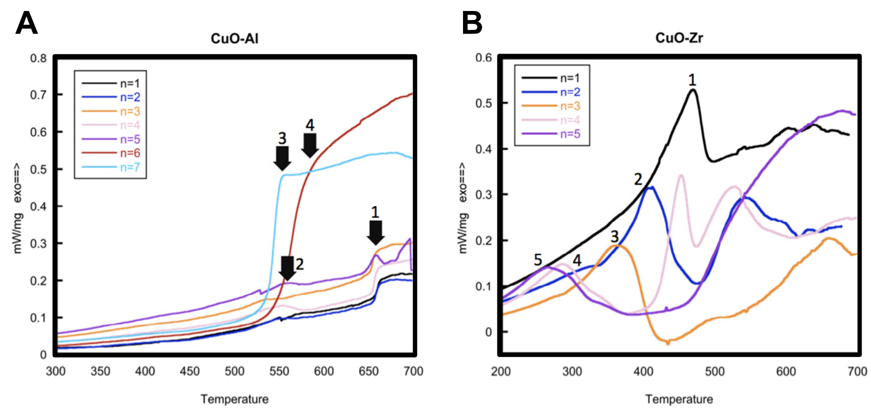

FIGURE 9

Calorimetry results collected in inert (Ar) atmospheres. The plots display (**A**) calorimetry data for a series of CuO-Al multilayers where the total thickness is constant (~ 1000 Å), but the number of internal interfaces increases from n=7 (100 nm CuO – 53 nm Al) to n=1 (700 nm CuO – 369 nm Al), and (**B**) calorimetry data for an identical series of CuO-Zr mulitlayers with the same total thickness, but a range of internal interfaces from n=5 (700 nm CuO – 389 nm Zr) to n=1 (140 nm CuO – 78 nm Zr).

Currently, the computational effort is exploring new model nano-laminate systems that are computationally feasible for our first principles methods. Forty-five elements and their oxides were screened to identify two candidate systems, Zr/ZnO and Ca/BaO. Materials were down selected based on the criteria of having similar symmetry, similar lattice parameter, and an exothermic exchange reaction. Currently it is using these systems to explore exchange reactions across a variety of interfaces. Insights from these model systems will also aid in the interpretation of experimentally studied systems.

H. Shock Tube/Laser Absorption Studies of Jet Fuels at Low Temperatures (600-1200 K)

Professor Ronald Hanson, Stanford University, Single Investigator and DURIP Awards

The objective of this research is to study ignition (especially at low temperature) and burning of Army and DoD-relevant fuels and fuel-surrogates using shock-tube and laser diagnostics. To achieve this, experimental studies include ignition delay time, multispecies concentration time-history measurements, and reaction rate measurements; theoretical and modeling studies will include the development, validation and refinement of reaction mechanisms. The investigator is focusing on studying the uncertainties in ignition chemistry models at low temperatures. The fuels studied will initially include jet fuel and its archetypal surrogate components and will evolve, during the grant period, to include bio-derived and synthetic jet fuels and their surrogates.

Shock tube measurements of ignition delay times with high activation energies are strongly sensitive to variations in reflected shock temperatures. At longer shock tube test times (needed at low reaction temperatures), small gradual increases in pressure (and simultaneous increases in temperature) that result from incident shock wave attenuation and boundary layer growth can significantly shorten measured ignition delay times. To obviate this pressure increase, the researchers made use of a recently developed driver-insert method of Hong *et al.* that allows generation of near-constant-volume test conditions for reflected shock measurements. Using this method, they have measured propane ignition delay times in a lean mixture (0.8% C_3H_8 / 8% O_2/Ar) over temperatures between 980 and 1400 K and nominal pressures of 6, 24 and 60 atm, under both conventional shock tube operation and near-constant-volume operation (with dP5/dt = 0%/ms). The near-constant-volume ignition delay times provide a database for low-temperature propane model development that is independent of non-ideal fluid flow and heat transfer effects. Comparisons of these near-constant-volume measurements with predictions using the JetSurF v1.0 mechanism of Sirjean *et al.* and the Curran *et al.* mechanism of NUI Galway were performed. The ignition delay times measured with dP5/dt = 1–7 %/ms were found to be significantly shorter (about 1/3 of the near-constant-volume values) at the lowest temperatures and highest pressures studied. However, these ignition times are successfully simulated using the JetSurF v1.0 mechanism when an appropriate gasdynamic model was used, which accounts for changes in pressure and temperature.

The first simultaneous multi-species laser absorption time-history measurements for OH and C_2H_4 were acquired during the oxidation of n-hexadecane and commercial diesel fuel (DF-2). The experiments were performed behind reflected shock waves in a new second-generation aerosol shock tube over a temperature range of 1120 K to 1373 K and a pressure range of 4–7 atm. Initial fuel concentrations varied between 150 and 1800 ppm with equivalence ratios between 0.4 and 2, and were determined using 3.39 lm He–Ne laser absorption. OH concentration time-histories were measured using absorption of frequency-doubled ringdye laser radiation near 306.7 nm. Ethylene time-histories were measured using absorption of CO_2 gaslaser radiation near 10.5 micron. Comparisons are given of these species concentration time-histories with two current large n-alkane mechanisms: the LLNL-C-16 mechanism of Westbrook *et al.* and the Jet-SurF C-12 mechanism of Sirjean *et al.* (see FIGURE 10). Fair agreement between model and experiment is seen in the peak ethylene yields for both fuels; however, modeled early time-histories of OH, an important chain-branching species, differ significantly from current measurements.

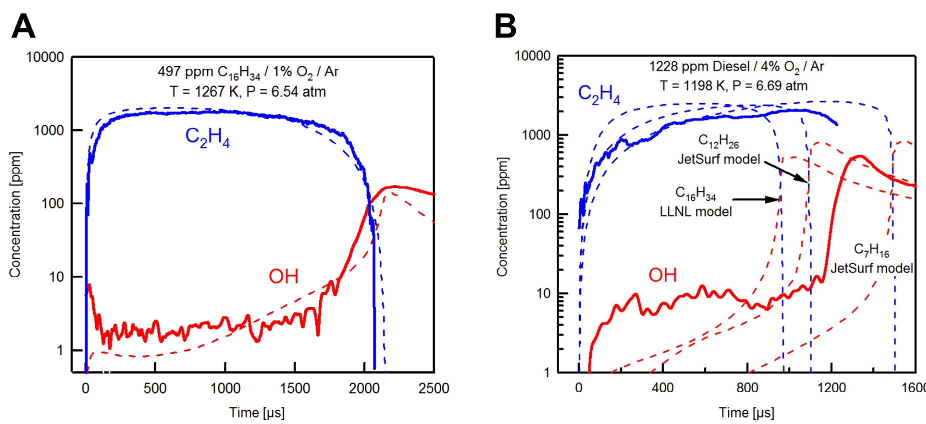

FIGURE 10

OH and C_2H_4 species time-histories and simulations during n-hexadecane and diesel/DF-2 oxidation. (A) OH and C_2H_4 species time-histories during n-hexadecane oxidation, with initial reflected shock wave conditions ϕ = 1.2, 1267 K, 6.54 atm; initial test gas mixture: 497 ppm $C_{16}H_{34}$, 1% O_2/argon. (B) OH and C_2H_4 species time-histories during diesel oxidation, with initial reflected shock wave conditions: ϕ= 0.5, 1198 K, 6.69 atm; initial test gas mixture: 1228 ppm diesel, 4% O_2/argon. Simulations shown for single-component surrogate models were: n-heptane and n-dodecane use the JetSurf mechanism; n-hexadecane used the LLNL mechanism.

A novel, mid-IR scanned-wavelength laser absorption diagnostic was developed for time-resolved, interference-free, absorption measurement of methane concentration. A differential absorption (peak minus valley) scheme was used that takes advantage of the structural differences of the absorption spectrum of methane and other hydrocarbons. A peak and valley wavelength pair was selected to maximize the differential cross-section (peak minus valley) of methane for the maximum signal-to-noise ratio, and to minimize that of the interfering absorbers. Methane cross-sections at the peak and valley wavelengths were measured over a range of temperatures, 1000 to 2000 K, and pressures 1.3 to 5.4 atm. The cross-sections of the interfering absorbers were assumed constant over the small wavelength interval between the methane peak and valley features. Using this diagnostic, methane concentration time histories during n-heptane pyrolysis were measured behind reflected shock waves in a shock tube. The differential absorption scheme efficiently rejected the absorption interference and successfully recovered the vapor-phase methane concentration. These measurements allowed comparison with methane concentration time-history simulations derived from a current n-heptane reaction mechanism.

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. Turbulent Dispersion of Film Coolant and Hot Streaks in a Turbine Vane Cascade

Investigator: Professor John Eaton, Stanford University, Single Investigator Award
Recipients: NASA, GE Aerospace

Turbulent mixing of fluid streams is an important process for applications ranging from mixing of fuel in a combustor to the dispersion of contaminants in the atmosphere. In general, turbulence mixing rates are orders of magnitude greater than molecular diffusion rates. Unfortunately, the turbulence mixing process is neither well understood by fluid dynamics researchers nor well characterized in available computational models. A major problem in developing turbulent models is the lack of availability of data on the mixing of two fluids in complex three-dimensional flow fields. In efforts to provide the much needed data, new measuring techniques based on the use of modern medical magnetic resonance imaging (MRI) scanners have been developed.

Magnetic resonance velocimetry (MRV) measures the three component mean velocity everywhere in a 3D turbulent field. The magnetic resonance concentration (MRC) method measures the 3D concentration of one fluid which is mixing into another.[1] Both concentration and velocity are measured on a regular Cartesian grid with spatial sampling volumes as small as 0.2 mm^3. The total volume of the flow apparatus may be thousands of cubic centimeters, so the MRI techniques provide highly detailed data that can be used to understand turbulent mixing both qualitatively and quantitatively. A significant advantage of these techniques is the rapid turnaround time. A full-field MRV scan can be completed in a few hours, and an MRC scan requires about 12 hours. This can be compared to months of work that would be required to collect similar data using laser-based techniques. The research team is currently examining the spread of coolant in gas turbine engines (see FIGURE 11). These studies revealed that changes to the slot geometry can reduce the strength of the vortices and improve the distribution of coolant.

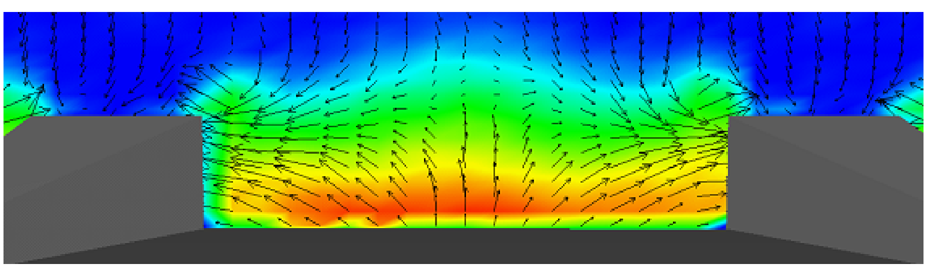

FIGURE 11

Vectors and concentration contours of coolant flow downstream of the slot of a turbine blade. 3D Velocity and scalar field diagnostics were completed using magnetic resonance imaging with applications in film-cooling, showing a cross-section of the coolant flow emerging from a slot in the trailing edge of the turbine blade. The colors show the concentration of the coolant while the vectors show the velocity field which is advecting the coolant.

Fuel consumption by gas turbine engines is a major area of concern for the Army and the other DoD services. Advanced gas turbines operate at very high temperatures and improvement of the effectiveness of the cooling systems offers the most leverage for increasing efficiency. Propulsion gas turbines such as those used in advanced helicopters use compressor bypass air to cool the high temperature turbine blades. Excess coolant is used to ensure that all parts of the turbine are adequately cooled. If the turbulent dispersion of cooling air was

[1] Benson et al., *Exp. Fluids* (2010) 49:43-55.

better understood, the total coolant flow could be reduced and the engine efficiency would be markedly improved. A more effective cooling scheme would provide both improved fuel economy and longer engine life. The results of this project have been transitioned to NASA, GE Aerospace, and other jet engine manufacturers.

B. Space-Time Multi-Scale Analysis of Fracture and Fatigue in Composite Structures
Investigator: Professor Somnath Ghosh, The Ohio State University, Single Investigator Award
Recipient: ARL-WMRD

This project is developing an integrated system of multi-scale computational models as predictive tools for enhancing performance and reliability of composite structures and materials used in military applications. This research has the overall objective of developing a robust multi-scale framework for computational modeling of these three tasks: (i) ductile failure in metallic materials containing discrete heterogeneities using an integrated multi-scale characterization/analysis framework, (ii) homogenized damage in 3D fiber reinforced composites under monotonic and cyclic loading conditions, and (iii) high strain rate loading (*e.g.*, blast) induced damage in composite plates. Spatial scales in the multi-scale framework include: (a) the macroscopic scale of components, and (b) scale of microstructural constituent phases, like fibers and micro-cracks. Such models will find application in various metallic components undergoing failure by particle fragmentation and ductile matrix cracking or for the design of composite impactors and novel protective armors and that undergo damage and failure when subjected to impact loading. The models can be extended to the design of protective covers for IED or mine blasts that are threats to light armored vehicles. This basic research led to the development of the accurate and computationally efficient Continuum Damage model (HCDM), which was developed in close collaboration with ARL, and has transitioned to ARL-WMRD for use in subsequent studies.

C. Combustion and Ignition Studies of Nanocomposite Energetic Materials
Researcher: Professor Michelle Pantoya, Texas Technical University, PECASE Award
Recipients: ARL-WMRD

The goal of this research project is to understanding combustion behaviors of energetic composite materials (*i.e.*, reactive materials and thermites) through understanding the processes controlling extraction and conversion of stored chemical energy. New diagnostic techniques are also being developed to quantify energy storage and transport under multiple spatial and temporal resolutions. An energetic material heat flux sensor was engineered by Professor Pantoya, and has been transferred to the super igniter and enhanced blast programs at ARL-WMRD. This new sensor captures energy transfer measurements in extremely high temperature, highly corrosive environments generated from the igniter formulations under investigation for existing and future small arms primers. These measurements are enabling characterization of many different formulations for optimal tailoring and tuneability of the munitions. This new diagnostic has impacted how formulations are compared for optimal performance.

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. Cyclical Dynamics and Control of a Neuromechanical System

Professor Eric Tytell, Johns Hopkins University, STIR Award

Since their inception, neuroscience and biomechanics have often been studied in isolation. Only recently has their coupled interaction begun to be fully appreciated. The goal of this project is to develop general principles for understanding cyclical dynamics in neuromechanical systems and how the dynamics lead to task-level maneuverability. Specifically, the investigator is addressing the question of how the stability and maneuverability of a whole animal are linked to the stability and adaptability of its underlying cyclic neuromechanical system. During the next year, the investigator will determine whether or not feedback allows a coupled neuromechanical system to reject perturbations more quickly than either the isolated neural central pattern generator (CPG) or the isolated mechanical system could.

The technical approach consists of two components: (ii) Characterization of the cyclical dynamics of open- and closed-loop neuromechanical systems and (ii) development of numerical and mathematical tools that can be applied to experimental data and more complex numerical models. Floquet modes will be estimated numerically from a simulated CPG and of the mechanical system as open-loop components, determining the modes that have dynamics that persist over a significant length of time. The mode structure in the coupled system will be examined by gradually increasing feedback strength and observing any changes in the number and structure of slowly-decaying Floquet modes as the system changes from open-loop dynamics to increasingly strongly-coupled closed-loop dynamics. The second aim will be accomplished by generating simulation data, generated using the models described below, will be crucial for the development of techniques that can accurately characterize dynamical behavior from empirical data.

The principles uncovered in this work will be useful in understanding animal locomotion in general, and will also have implications for the improvement of prosthetic devices for humans, therapies for victims of spinal cord injury or stroke, and controllers and actuators for robotics autonomous vehicles.

B. Dynamics of Systems of Systems with Applications to Net-zero Energy Facilities

Professor Igor Mezic, University of California - Santa Barbara, Single Investigator Award

This project is testing the hypothesis that multiscale expansions, such as wavelet expansions, provide reduced representation of the continuous spectrum in the way similar to the Fourier expansion in the context of point spectrum of the Koopman operator. The investigator is analyzing the continuous part of the spectrum of the Koopman operator for the classical standard map (kicked pendulum) problem using multiscale (wavelet-based) expansion. This approach allows for a physical understanding of the associated Koopman Eigen distributions which, in turn, will allow for understanding the general structure of continuous spectrum and its decomposition in complex systems. The continuous spectrum issue is the outstanding open problem of Koopman operator theory and its resolution will enable the development of a complete model reduction theory.

The investigator proposes to develop a theory capable of delineating structural properties and architectures of engineered system of systems based on spectral properties of the underlying directed graph. This will enable mathematical connection to Koopman operator spectral properties. In fact, this connection is another major open issue in the theory of large-scale interconnected dynamical systems. A class of systems that oftentimes arises in engineering will be focused on--that is, a system where structural properties of the graph are closely related to functional properties of the system. Specifically, investigators will determine the Koopman operator spectrum for skew product systems that have horizontal-vertical graph representation. These have numerous applications in engineering practice. The basic hypothesis is that the horizontal-vertical structure of the system graph leads to

Koopman spectrum and eigenvalues that are structured in a horizontal-vertical way. This research is expected to substantially simplify analysis and computation of the Koopman spectrum of hierarchical systems.

C. Dynamic Mobility via Cellular Decompositions of Coordination Spaces
Professor Anthony Stentz, Carnegie Mellon University, STIR Award

The goal of this research project, led Professor Stenz with collaboration by co-investigator Professor Clark Haynes, is to develop a new formalism for dynamic mobility and animal/robot gait selection through symmetry, algebraic topology, and classical group theory to replace traditional, computationally expensive methods of combinatorial search and optimization.

To accomplish feats of rapid, nimble locomotion through challenging terrains, the ground mobile robots of tomorrow must exhibit great dexterity and dynamic mobility. As complexity increases for such systems, however, the need for principled approaches to coordinating a robot's multitude of actuators becomes apparent. It is anticipated that in FY12, the investigators will develop foundations for a new mathematical formalism for solving such problems. The theory will use algebraic topology and classical group theory to replace traditional methods of combinatorial search and optimization with a computationally easier and conceptually more straightforward approach that seeks to identify and exploit symmetries and other simplifying structure. Through studying this variety of representations and the cellular decompositions that arise from them (exhibiting symmetries and reducing overall complexity), the investigator will develop a novel approach to the fundamental control problems necessary for achieving dynamic robotic locomotion.

The technical approach is comprised of decomposing the space of coordination for a system into cells that index various symmetric configurations of control. In the case of a multi-legged robot running through a rubble-strewn terrain, the robot must choose between a vast number of alternative ways to move its legs through the terrain, and then to recover or switch amongst these options as it negotiates the inevitably unanticipated perturbations encountered along the way. The proposed theoretical formalism reduces this problem to changes on a much simpler combinatorial space of possible gait timings by discretizing the space into gait cells while also providing a simple roadmap to facilitate transitions between them. Incorporating aspects of changing terrains, body morphology, actuator limitations, and dynamic constraints will also be studied—thus allowing for a more general theory. By studying cross products of various cellular decompositions, the researchers plan to produce new decompositions of higher-dimensional spaces, testing both the descriptiveness of the abstractions as well as the algebraic foundations of the approach.

Example applications would include studies of the ability of a robotic system to run through a terrain and jump, dynamically, over an obstacle. Computation of allowable gaits, for running, for jump preparation, and the jump itself, give rise to necessary transitions. The investigator plans to identify equivalence classes describing the constraints necessary for the machine to succeed (identifying the minimum speed and torque, and allowable starting gaits, for instance). While focused directly on the study of gaits for legged robots, the combinatorial simplification methods can also be applicable to other forms of robotic mobility as well as to robotic manipulation.

D. Investigation of the Microstructural Parameters to Improve Dynamic Response in Al-Cu Alloys
Professor Murat Vural, Illinois Institute of Technology, Single Investigator Award

This research involves conducting comprehensive parametric experiments on single crystal Al, polycrystal Al, and several Al-Cu alloys by using fully instrumented state-of-the-art experimental tools such as cryogenic and high-temperature split Hopkinson pressure bar (SHPB) setups. Thermal-mechanical processing techniques are being used to systematically modify the microstructural configurations of these materials to investigate the effects of grain texture, bimodal distribution of grain size, precipitate density and distribution on high-strain-rate response as well as evolution of dynamic deformation substructure. It is anticipated that in FY12, extensive microstructural characterization work by using SEM, TEM, X-ray diffraction and orientation imaging microscopy (OIM) will be used to investigate initial microstructure and evolution of deformation substructure in specimens subjected to controlled dynamic loading histories. In addition, the investigator will complete the experimental measurement of dynamic energy storage rate in these microstructures via high-speed IR radiometry integrated to SHPB setup. The major objective of the proposed research is to isolate microstructural configurations that have the maximum potential in suppressing the localized shear deformation and improving the dynamic response of Al-Cu alloys. Recognizing the fact that ballistic performance is significantly improved by delaying the onset of ASB in dynamically deforming Al alloys, the approach has the potential of providing unique guidelines for developing thermal-mechanical processing techniques to obtain high performance Al alloys applicable to army mission.

E. Three-dimensional Flow Visualization of a Turbulent Boundary Layer

Professor Brian Thurow, Auburn University, STIR Award

The goal of this project is to utilize a recently-developed plenoptic camera, to study the 3D characteristics of large-scale structures contained in a turbulent boundary layer under the influence of an adverse pressure gradient. The Advanced Laser Diagnostics Laboratory (ALDL) at Auburn University specializes in the development and application of laser diagnostics for measurements in fluid dynamics. Using a custom-built pulse burst laser system, the present research focuses on seeking an improved understanding of the three-dimensional structures in a turbulent boundary layer. The understanding of the organized motion in a turbulent boundary layer and its dynamics are very important as researchers seek to accurately model, predict, and control wall bounded flows. In this study, three-dimensional flow visualization is accomplished by scanning a high-repetition rate laser light sheet through the desired flow field and acquiring 2D images of the flow throughout the scan. The resulting sequence of 2D images is reconstructed to form a 3D image of the flow field (see FIGURE 12). The unique aspect of this 3D technique is its high-speed capabilities which are made possible using a home-built third generation pulse burst laser system with a galvanometric scanning mirror and a high framing rate CCD camera.

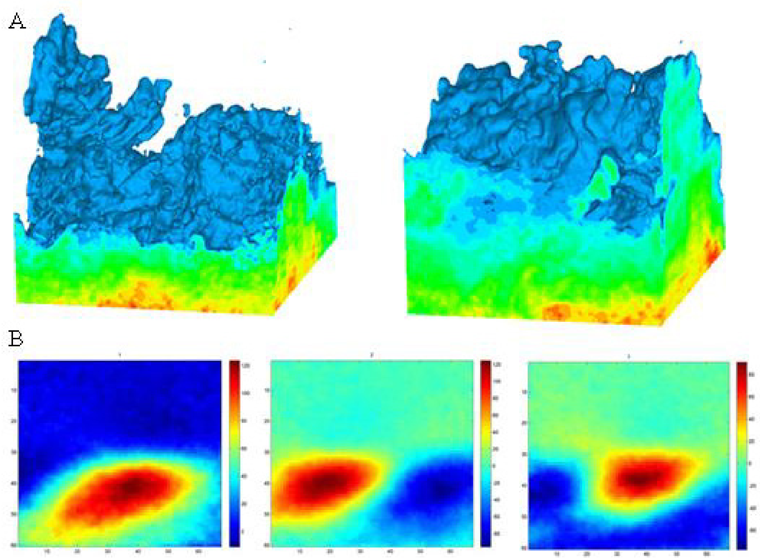

FIGURE 12

Flow Visualization of a Turbulent Boundary Layer. (**A**) 3-D flow visualization images at 2 different instances, (**B**) First 3 velocity POD modes of the u –velocity component.

Many observations can be made by studying individual snapshots of the flow. There are, however, efficient ways to decrease the data into more manageable sets, while still being able to make observations about the structures in the flow. Proper orthogonal decomposition (POD) has been used extensively in fluid dynamics, and extracts a basis for modal decomposition from a set of images. The modes represent the most common structures in the flow. The POD provides an objective technique to study the images and can be used to compare a set of trials with different parameters (*e.g.*, velocity vs. smoke intensity, zero pressure gradient vs. adverse pressure gradient).

It is anticipated that in FY12, the investigators will complement this 3D flow visualization with simultaneous 2D particle image velocimetry (PIV) to correlate the flow visualization POD modes with velocity POD modes. This correlation will be used with linear stochastic estimation (LSE) with the goal of approximating the velocity field given a known flow visualization field.

F. Nonlinear Corrections to Temperature in Computer Simulations of Complex Systems

Professor Ralph Chamberlin, Arizona State University, Single Investigator Award

Finite-size thermal effects are found to significantly influence the fluctuations and reaction rates of many systems. This research will complete a detailed investigation of the nonlinear corrections to temperature that come from finite-size thermodynamics. The work will investigate the fundamental ways that these corrections influence the behavior of generic models. The basic knowledge that is gained from understanding these models will improve the accuracy and efficiency of molecular-dynamics simulations of realistic materials.

This research will be validated/implemented via close collaboration with scientists at the University of Missouri, Columbia, with integration proceeding through the following four approaches.

(i) run a test simulation of nitromethane molecules in a crystal to establish the relevance of nonlinear corrections for MD simulations of energetic materials (see FIGURE 13)

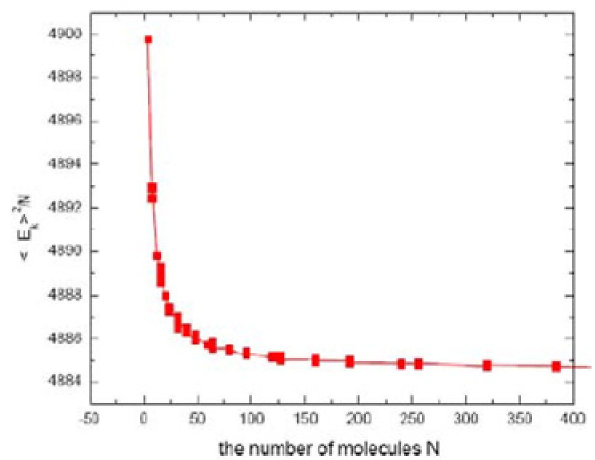

FIGURE 13

Fluctuations in kinetic energy per molecule from an MD simulation of nitromethane. <(ΔEK)2 >/N comes from the motion of molecules (primarily their rotation) in the low-temperature, crystalline phase. Each value of <(ΔEK)2 >/N is obtained from the same simulation, by averaging over different numbers of molecules in a local region. Note the decrease in <(ΔEK)2 >/N for large regions, corresponding to nonextensive entropy, which violates the equipartition theorem. Thus, a nonlinear correction factor from the effective local temperature added to the dynamics of each region should improve the simulation.

(ii) investigate nonlinear corrections to MD simulations for mobile molecules, starting with simplified models such as the Lennard-Jones fluid, then transfer the ideas to more-detailed models (see FIGURE 14)

(iii) explore models that bridge the scale of complexity between the Ising model and models for energetic materials, such as the Potts model for multiple degrees of freedom on a lattice

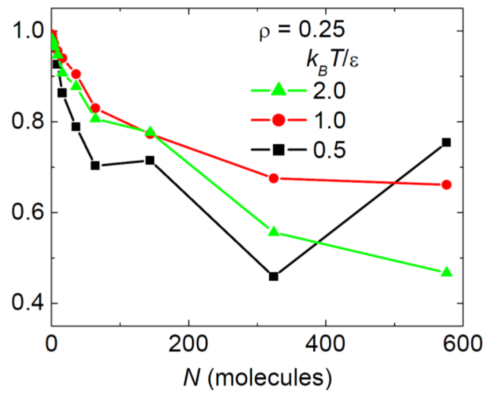

FIGURE 14

Preliminary results showing fluctuations in kinetic energy per particle as a function of region size from MD simulations of the two-dimensional (2D) Lennard-Jones fluid. Different symbols come from simulations at different average temperatures, given in the legend. The limit <(ΔKE/kBT)2 >/N◊1 is consistent with the equipartition theorem for this 2D system. These simulations show a decrease in <(ΔKE/kBT)2 >/N for large regions, similar to that shown for nitromethane (refer to FIGURE 13). However, here the decrease at large N is more conspicuous, perhaps because this system is in the fluid phase. The researchers will use the Lennard-Jones model as a simple system for studying finite-size effects in MD simulations.

(iv) evaluate various moments in the distribution of jump rates, focusing on outlier statistics (see FIGURE 15)

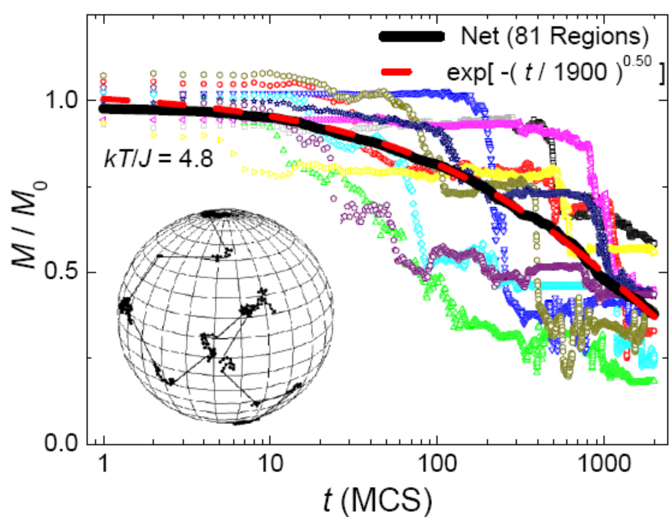

FIGURE 15

Non-exponential relaxation as a function of time after removing an applied field in a simulation of a supercooled liquid. The solid (black) curve shows the net alignment from 81 regions, each of size 16x16x16. The dashed (red) curve shows a fit to the net behavior using the stretched-exponential function. The symbols show the response of 10 individual regions, showing sharp jumps and steps in the local response. The relatively static periods come from entropic entrapment, when the region is in a state of low entropy. The large jumps arise when the region becomes activated by high entropy. The inset shows results from NMR measurements of the molecular rotation angles in a supercooled liquid, showing similar small-angle diffusion combined with occasional large-angle jumps.

VI. DIVISION STAFF

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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 2011* is to provide information on the programs and basic research efforts supported by ARO in FY11, 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 FY11.

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 promote basic research that will help create new mathematical principles and laws that hold true across networks of various kinds, and use them to create algorithms and autonomous systems that can be used to reason across data generated from disparate sources, be they from sensor networks, wireless networks, or adversarial human networks, with the resulting information used for prediction and control. Given that network science is a nascent field of study, the Network Sciences Division also supports basic research on metrics that are required to validate theories, principals and algorithms that are proposed.

2. Potential Applications. In addition to advancing worldwide knowledge and understanding of networks, the research efforts managed in the Network Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO through network science research may provide new and revolutionary tools for situational awareness for the Solider and new regimes for command, control and communication for the Army. Furthermore, work supported by ARO through the Network Sciences Division could lead to autonomous systems that work hand-in-glove with the Soldier.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Network Sciences Division frequently coordinates and leverages efforts within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). In addition, the Division frequently coordinates with other ARO Divisions to co-fund research efforts, identify multi-disciplinary research topics, and to evaluate the effectiveness of research approaches. For example, interactions with the ARO Computing Sciences Division include promoting research to investigate game-theoretic techniques that could lead to better cyber situational awareness and to address concerns about performance and resilience to cyber attacks in ad-hoc dynamic wireless networks in a uniform fashion. The Network Sciences Division also coordinates efforts with the Mathematics Division to pursue studies of game theory that address bounded rationality and human social characteristics in a fundamental way. The Network Sciences Division also coordinates with Life Sciences on studies at the neuronal level to understand human factors in how decisions are made under stress. Lastly, the Mechanical Sciences Division's Program Areas also interface with the Network Sciences Division to understand the interplay between learning and manipulation and locomotion in robotic systems. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

To meet the long-term program goals described in the previous section, the Network Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY11, the Division managed research efforts within these four Program Areas: (i) Multi-agent Network Control, (ii) Decision and Neuro Sciences, (iii) Communications and Human Networks, and (iv) Intelligent Networks. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Multi-agent Network Control. The objective of this Program Area is to develop the theory and tools, through appropriate application and creation of relevant mathematics, to ultimately model, analyze, design, and control complex real-time physical and information-based systems, including distributed and embedded, networked autonomous and semi-autonomous, non-linear, smart structures, and decentralized systems. This Program Area invests in fundamental systems and control theory and relevant mathematical foundations for areas of control science such as multi-variable control, non-linear control, stochastic and probabilistic control distributed and embedded control, and multi-agent control theory. Further, the Program also involves innovative research on emerging areas such as control of complex systems and theories for the design of large heterogeneous multi-agent teams with desired emergent behaviors. This Program Area is divided into two research Thrusts: (i) Intelligent Control and (ii) Multi-agent Systems. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. The Intelligent Control Thrust involves research topics focusing on non-traditional approaches to control with focus on the Army's interest in basic research on intelligence, embedded in a single agent operating in highly uncertain, clustering, and complex environments. The Multi-agent Systems Thrust involves research focused on extending the mathematical foundations of distributed system theory, with a focus on basic research in the massive-scale, low cost, highly distributed agents cooperating over networks in highly uncertain, clustering, and complex environments. In addition, research focuses on the design of emergent behavior for heterogeneous multi-agent systems, accommodative-cooperative-collaborative theory of multi-agent behavior and interaction, and multi-player/multi-objective game theory.

2. Decision and Neuro Sciences. The goal of this Program Area is to advance frontiers of mathematics and neuroscience to support timely, robust, near-optimal decision making in highly complex, dynamic systems operating in uncertain, resource-constrained environments. This Program Area involves two major research Thrusts: (i) Mathematical Modeling of Neural Processes and (ii) Stochastic Optimization and Modeling. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. The Mathematical Modeling of Neural Processes thrust addresses innovations to quantitatively model decision behaviors in neural-anatomical or other observable measures to explain how factors such as complexity, uncertainty, stressors, social and other dynamics affect decisions. The Stochastic optimization and modeling thrust addresses advances in mathematical algorithms to better address stochastic data properties common in highly dynamic, heterogeneous and complex operational environments and in environments with ill-conditioned and varying information such as in dynamic complex social contexts. Based on operations-research methodologies such as modeling, simulation and numerical optimization, this Program Area includes a significant multi-disciplinary emphasis, specifically with neuroscience, to address the complex, multi-dimensional decision frameworks in today's asymmetric warfare.

3. Communications and Human Networks. The goal of this Program Area is to better understand the fundamental scientific and mathematical underpinnings of wireless communications and human networking, their similarities, and the interactions between these two networks. This Program Area is divided into two research Thrusts: (i) Wireless Communications Networks and (ii) Human Networks. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. The Wireless Communications Networks Thrust supports research efforts to discover the fundamental network science principles as they apply to the wireless multi-hop communications systems, while the Human Networks Thrust identifies and supports research to better understand social network structures from heterogeneous data, the structures effect on decision making, and the interaction of communications and human networks. The research efforts promoted by this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications could include wireless tactical communications, improved command decision making, and determining the structure of adversarial human networks.

4. Intelligent Networks. The goal of this Program Area is to develop and investigate realizable (i.e., computable) mathematical theories, with attendant analysis of computational complexity, to capture common human activity exhibiting aspects of human intelligence. These studies may provide the foundation for helping augment human decision makers (both commanders and Soldiers) with enhanced-embedded battlefield intelligence that will provide them with the necessary situational awareness, reconnaissance, and decision making tools to decisively defeat any future adversarial threats. This Program Area is divided into two research Thrusts: (i) Integrated Intelligence and (ii) Adversarial Reasoning. These thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long term goal. The Integrated Intelligence Thrust supports research efforts to discover the mathematical structuring principles that allows integration of the sub-components of intelligent behavior (such as vision, knowledge representation, reasoning, and planning) in a synergistic fashion, while the Adversarial Reasoning Thrust area brings together elements of Game Theory, knowledge representation and social sciences to reason about groups/societies in a robust manner. The research efforts promoted by this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications could include robotic unmanned ground and air vehicles, reasoning tools for wild life management, and decision making tools in the context of command, control, communications, computers, intelligence, surveillance and reconnaissance (C4ISR).

C. Research Investment

The total funds managed by the ARO Network Sciences Division for FY11 were $19.5 million. These funds were provided by multiple sources and applied to a variety of Program Areas, as described here.

The FY11 ARO core (BH57) program funding allotment for this Division was $5.5 million. The DoD Multi-disciplinary University Research Initiative (MURI) Program, the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $2.8 million to projects managed by the Division. The Division also managed $10.9 million provided by the Defense Advanced Research Projects Agency (DARPA). The Small Business Innovation Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided $0.2 million for awards in FY11. Finally, $0.15 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

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

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). 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. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. Fourth Annual North American School of Information Theory (Austin, TX; 27-30 May 2011). The objective of this workshop was to bring top information theory researchers together to discuss new areas of information theory, including how the theory applies to wireless tactical networks and to familiarize information theory graduate students and post-docs with new research, including tactical networking. This workshop brought together experts in academia and the government as well as top graduate students to discuss emerging concepts in information theory.

2. Workshop on Reasoning in Adversarial and Non-cooperative Environments (Durham, NC; 18-19 November 2010). The goal of this workshop was to bring together leading researchers from different backgrounds that work in game theory, including psychologists, computer scientists, economists, logicians and control theorists. The outcome was a report identifying the current state of field, and problems of interest to the DoD in the near future.

3. Workshop on Geo-spatial Abduction (College Park, MD; 3-4 March 2011). The goal of this workshop was to bring together anthropologists, epidemiologists, mathematicians and computer scientists that have been working on the problem of reasoning about geographical and cultural information to understand the relationship between cause and effect of observed events, whether they spread of disease, occur of crime, or by explosion of IEDs. The workshop brought together people from disparate areas that were not even aware that they had similar goals. The outcome of the workshop was an increase in cross-fertilization of ideas, a report, and a catalogue of unclassified datasets that could be used by the research community.

4. Augmenting the Accuracy, Speed, and Efficiency of Human Choice – Improved Mathematical Models of Multi-Scale Neuronal Processes (Evanston, IL; 28-29 September 2011). The objective of this workshop was to develop a roadmap for research topic areas that should be addressed within the Decision and Neuro Sciences Program, Mathematical Modeling of Neural Processes in Decision Making Thrust. Fifteen neuroscience and quantitative scientists focused on multi-disciplinary approaches in decision neuroscience, including comparison of biological algorithms for choice with existing artificial algorithms with a focus on strengths of biological systems that should be emulated and weaknesses of biological systems that should be remediated, non-traditional input-output connections (EEG, eye movement monitoring, etc) research tools, and considerations for stochastic versus deterministic behaviors. This workshop resulted in a white paper identifying important topics areas of research.

C. Multidisciplinary University Research Initiative (MURI)

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

1. Determining the Mathematical Basis of Swarming. This MURI began in FY05 and was awarded to a team led by Professor Vijay Kumar at the University of Pennsylvania, with participation from researchers at the Massachusetts Institute of Technology (MIT), Yale University, and the University of California, Santa Barbara. The goal of this research is to understand the mathematical basis of swarming and its potential applications to cooperative control of tasks of all types, including the control of formations, the management of sensor networks, and the dynamics of achieving a consensus in a rapidly changing environment. This research effort will draw inspiration from biological paradigms and create a mathematical basis for modeling, analysis, and synthesis of swarming systems that are applicable to cooperative control tasks of all types, including the control of formations, the management of sensor networks, and the dynamics of achieving a consensus in a rapidly changing environment. The project consists of four research approaches: the modeling of group-behaviors in biology, the analysis of group behaviors, the synthesis of novel controllers for networked groups of vehicles, and experimental demonstrations and validation.

Future Army vehicle networks will perform a wide variety of coordinated sensing, motion and target prosecution. Coordination algorithms with the required scalability and correctness properties resulting from this project will enable future groups of robotic vehicles to be autonomous and adaptive in the face of communication constraints. The high levels of autonomy and robustness will allow future Army robotic teams or mixed human-robotic teams to carry out tasks with guaranteed performance. Specific applications are numerous. The tools from this project will enable new biologically-inspired control paradigms for swarms that will be usable in the context of adaptive tracking, surveillance, and navigation. The tools will also enable a solution to the problem of determining when an observed group exhibits normal behavior and when it exhibits atypical behavior - which has significant implications to homeland security and warfare. This technology will also enable monitoring and surveillance applications on geological and ecological scales previously prohibited by practical considerations and will provide tools for a host of security and surveillance applications.

2. 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.

3. 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.

4. Scalable, Stochastic and Spatiotemporal Game Theory for Adversarial Behavior. This MURI began in FY11and was awarded to a team lead by Professor Milind Tambe of the University of Southern California, with participation from researchers at UCLA, Duke University, Stanford University, UC Irvine and California State University at Northridge. The objective of this MURI is the development of game theory formalisms that account for bounded rationality, scalability of solutions, real-world adversaries, and socio-temporal issues. The technical approach to be followed by the team will involve a mix of behavioral experiments and development of theoretical formalisms to characterize individual human behavior and that of adversarial groups; it is expected that psychological theories such as prospect theory and stochastic theories for coalitional games will play equal part in the technical development. The results of this MURI may have significant impact on diverse applications of the Army such as scheduling of resources for ISR and for monitoring of contracts while building nations or societies.

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

No new starts were initiated in FY11.

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

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*

1. Automatic Causality Determination and Narrative Extraction using the Semantic Inference and Filtering Tool (SIFT). A Phase I STTR contract was awarded to Intelligent Automation Inc., in partnership with Professor Dan Roth at the University of Illinois Urbana-Champaign (UIUC) to develop an intuitive web-based tool to search, filter, and collaboratively work on document chains. Mechanisms for understanding event chains is directly responsive to the future Army need to establish methods for dealing with the massive amount of information resulting from web publishing technologies. The Semantic Inference and Filtering Tool (SIFT) will incorporate Natural Language Processing (NLP) tools for automatic causality determination and narrative extraction from online resources for users to interactively narrow down the search space, locate key document chains, and create a personal workspace with document chains of interest. Analysts can share workspaces containing one or more document chains, and a document chain discovery feature will have a feedback mechanism by which search results can be interactively manipulated by modifying search and ranking parameters. The system is intended to help analysts, researchers, and law enforcement find causality that connects documents and extract relevant topics from vast quantities of unstructured information.

2. Story Creation and Inference through Bayesian Extraction (SCRIBE). This Phase I STTR contract was awarded to Decisive Analytics Corporation, in partnership with Professor Noah Smith at Carnegie Mellon University to develop a genre- and language-independent system with explanatory cause-and-effect models to simplify and expedite an analyst's task of discovering stories and sequences of events from large quantities of unstructured text in varied open sources to explain current events of interest. The process of event and entity discovery from unstructured text will be accomplished by using an innovative, unsupervised method that can operate on the spectrum of language genres and sources. Event linking, to explain the state of affairs from this data, will be achieved by exploiting statistical cues from available information about entity and topic storylines of real-world activity. Lastly, SCRIBE has a visualization component that will provide users with interactive visualizations of the cause and effect models to offer views of underlying event sequences at varying granularities to navigate a complex web of causally linked events. The system will allow more rapid and thorough analysis of reported information from large quantities of data to assist with integrating intelligence and forming effective courses of action.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) – 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). The FY11 new starts within these programs are described here, while the missions of each of these programs were described *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. DoD REP Awards. As described in more detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, REP awards aim to enhance or increase the programs, capabilities, and graduates in scientific and engineering disciplines in universities serving underrepresented minorities. In FY11, the Network Sciences Division managed three new REP projects, totaling $1.5 million. The equipment purchased with these awards is promoting research in areas of interest to ARO, including efforts to develop a gimbaled platform that can be driven by a computer model and to investigate wireless network capabilities of underwater sensors.

2. DoD TCU Instrumentation Awards. As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the TCU program aims to enhance science, mathematics, and/or engineering education programs and/or research capabilities through the acquisition of equipment and/or instrumentation that will augment existing facilities, enhance curricula, or help develop new laboratories, programs, and capabilities in these areas. In FY11, the Network Sciences Division managed two new TCU projects. The equipment purchased with these awards is promoting education and research in areas of interest to ARO, including efforts to improve library equipment and to upgrade media authoring software and hardware at Chief Dull Knife College.

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

No new starts were initiated in FY11.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY11, the Network Sciences Division managed three new DURIP projects, totaling $0.85 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies to explore full duplex wireless communications, Quality of Services (QoS) of multiple, simultaneously running instances of cognitive radios at realistic levels (thousands), methods for optimizing cognitive networks, and optimal methods for cooperating robots to carry out missions.

I. DARPA Anomaly Detection in Multiple Scales (ADAMS)

The ADAMS program is an effort to understand how insider threats to an organization (such as MAJ Nadal Hassan or Robert Hansen) can be predicted based on changes in behavior of individuals, or a small group of people within an organization. At a technical level this program involves mining incredibly large graphs (based on normal human activity) in a manner that is cognizant of human behavior, which reduces to computational challenges in managing and reasoning of large datasets, statistical reasoning techniques to find black swans, and efforts to manage uncertainty in both data and reasoning techniques. This program is managed on behalf of DARPA through the Network Sciences Division, Intelligent Networks Program.

J. 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.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. Geo-spatial Abduction

Professor V. Subrahmanian, University of Maryland, Single Investigator Award

Geo-spatial abduction is the problem of explaining the cause of a set of events that have been observed. The events could be occurrences of crime in a community, reports of incidents of flu contagion, or explosion of IEDs. Identification of the cause of the reported events, depending on the situation, could be a serial criminal, a farm where a disease jumps from animals to humans, or a warehouse containing bomb making material. The process of geo-spatial abduction involves identifying potential causes with reported incidents in a way that accounts for geographical and cultural constraints.

In FY11, Professor Subrahmanian demonstrated that the problem of geo-spatial abduction is NP-complete by reducing set covering, a well known NP-complete problem, to geo-spatial abduction. Furthermore, he has proposed approximation algorithms, based on greedy heuristics. Finally, he has shown how his algorithm can be adapted to predict the location of weapons caches based on IED explosion data and information about adversarial groups in a certain area and has applied the resulting system to data from Baghdad and Afghanistan (see FIGURE 1).

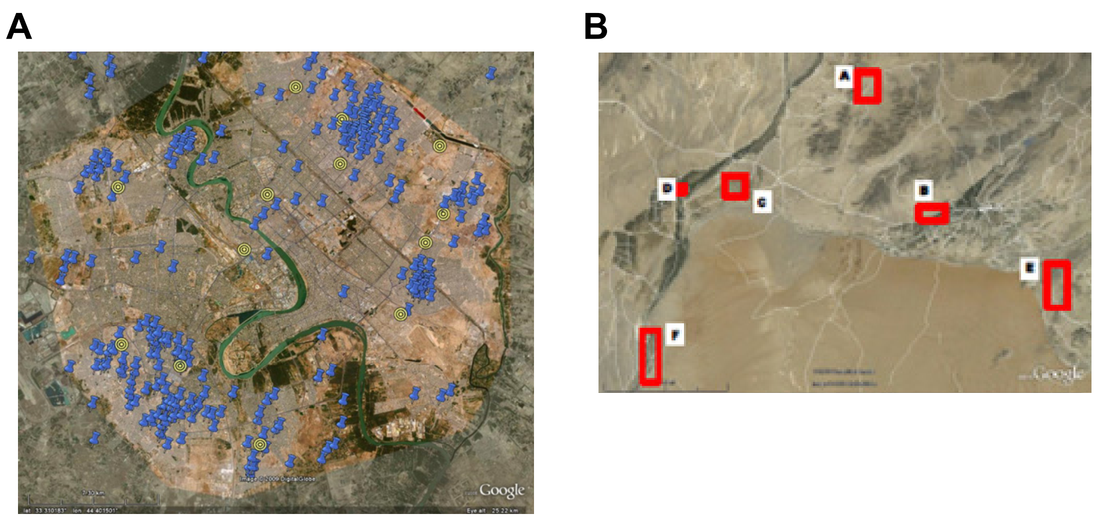

FIGURE 1

Utilizing reported events to generate approximation algorithims. The photographs are Good Earth maps of (**A**) Baghdad, with prediction of weapons cache sites, and (**B**) a region in Afghanistan, with prediction of villages containing high value targets.

B. High Throughput via Cross-Layer Interference Alignment

Professor Robert Heath, University of Texas - Austin, Single Investigator Award

In many wireless communications networks, the primary limiting factor to data throughput is interference from other transmitters. Techniques to mitigate interference usually assign each transmission to a different channel (time slot, frequency, or orthogonal code). Interference alignment is a technique in which the interference at the receiver from all of the undesired transmissions is in the same subspace and therefore can be nulled out or removed from the desired transmission. With interference alignment, each transmission has the capacity of half of the non-interference channel, whereas with different channels, the capacity is reduced by the inverse of the number of transmitters. However, there are several practical issues to overcome to efficiently implement interference alignment.

Professor Heath is currently investigating using multi-antenna on both the transmitter and receiver (multi-input multi-output; MIMO) to enable interference alignment. In FY11, he investigated adding secondary users to a set of communicating primary nodes while minimizing the interference, forviding for the determination of how many secondary users can be added without any impact on the primary users. In addition, the research further determines how to implement coder on the transmitter to align the new signal into the null space of the existing receivers. Since tactical battlefield communications is highly dynamic in nature, this can be also used to determine if a new node can start transmitting without causing interference incrementally and thus save on time and computation.

C. Learning in the Presence of Unawareness
Professor Joseph Halpern, Cornell University, Single Investigator Award

Representing knowledge and capabilities of agents can take on various forms of transitions systems with associated stochastic notions of rewards. The goal of this research project is to understand how an agent can learn new facts about its environment, and actions it can carry out to change that environment. In FY11, with colleagues Professors Nan Rong and Ashutosh Saxena, Professor Halpern introduced the notion of Markov Decision Processes with Unawareness (MDPUs). Traditional MDPs assume that agents know all states and actions. However, this may not be true in many situations of interest. MDPU's allow modeling of agents that may not be aware of all possible actions, but could learn them by using an "explore" action; when the agent plays "explore" then, with some probability, it will learn a new action (if there is one to be learned). The investigator has provided a complete characterization of when an agent could learn to play near-optimally in the setting of MDPU, and have designed an algorithm that allows the agent to learn to play near-optimally when it is possible to do so, and as efficiently as possible. Furthermore, Professor Halpern and his team have recently applied the MDPU framework to robotics, and in particular to robotic cars that could learn to turn tight corners by drifting.

D. Resource-Constrained Project Scheduling under Uncertainty: Models, Algorithms and Applications
Professor Haitao Li, University of Missouri - St. Louis, Single Investigator Award

The goal of this research project is to understand the challenging problem of scheduling projects with both resource constraints and uncertainties, known as the stochastic resource-constrained project scheduling problem (SRCPSP). The ultimate goal is to develop computationally tractable algorithms for obtaining near-optimal closed-loop policy. From the modeling perspective, it is desirable that the models are able to capture both the non-structural randomness such as stochastic task duration, and the structural randomness (*i.e.*, randomness in the nodes and arcs connections of the network). While the existing literature has focused on solution approaches for obtaining *a priori* task sequence with minimum expected "makespan," this research seeks to obtain a dynamic and adaptive closed-loop policy. Another objective of the research is to develop an algorithmic framework to embed constraint programming (CP) based techniques, which has proved to be both effective and efficient for handling complex scheduling problems.

In FY11, the investigators have (i) developed Markov decision process (MDP) model for SRCPSP, which is general and flexible enough to capture both non-structural randomness such as stochastic task duration and structural randomness, (ii) developed the first computationally tractable algorithm for obtaining dynamic and adaptive closed-loop policy to SRCPSP, and (iii) embedded constraint programming (CP) in the rollout framework to replace the priority-rule heuristic as the base policy.

Since the SRCPSP includes various machine scheduling problems as special cases, the model can be immediately adapted to deal with machine scheduling problems under uncertainty. The researchers show theoretically that a static priority-rule based scheduling heuristic is sequential consistent for SRCPSP. Using the methodology of approximate dynamic programming in the rollout framework, the rollout policy is able to sequentially improve the base policy offered by a priority-rule heuristic. Given constrain programming's advantage over a priority-rule heuristic in solution quality, the resulting augmented rollout algorithm is able to significantly improve over the basic rollout algorithm. This design is innovative in that it offers an effective way for integrating techniques from the artificial intelligence area with optimization, statistics and simulation to tackle the curses-of-dimensionality of high-dimensional stochastic scheduling problems.

E. Discrete Event Supervisory Control and Nonlinear Motion Control for DoD and Industry

Professor Frank Lewis, University of Texas - Arlington, Single Investigator Award

This objective of this research is the rigorous derivation of advanced control theory applicable to the constraints and dynamic environments to be encountered by future high-performance Army vehicles and Autonomous Unmanned Vehicles (UAV/UGV). In particular, investigations focus on the inherent complexity and design challenges of achieving significant performance in short time intervals through three goals to significantly improve performance precision and speed of Army systems with uncertain dynamics, disturbances, and control actuator limitations: (i) neural-network high-performance nearly-optimal control, (ii) neural-network H-infinity structured output feedback control, and (iii) decision and control for distributed heterogeneous teams of autonomous rotorcraft, ground vehicles, and humans.

During FY11, Professor Lewis' research culminated in a Best Paper Award for Autonomous/Unmanned Vehicles at the 2010 Army Science Conference. The award-winning paper defined a new class of continuous-time games where individual agent only plays a game with his local neighbors on a communication graph structure. The restrictions of the communication topology on the control decisions mean that standard definitions of Nash equilibrium are not useful and new definitions of game theoretic equilibria must be made. In military organizations and autonomous teams, each player typically interacts only with his neighbors, not all other agents. Therefore, this research developed a theory for differential games with local interactions between the systems. This allows the performance objectives of teams to change in real-time response to dynamically changing environments. The framework developed allows for both cooperative and adversarial objectives of teams and players.

F. Strategic State Estimation in Uncertain and Mixed Multi-agent Environments

Professor P. Doshi, University of Georgia, Single Investigator Award

The objective of this project is to take critical steps toward establishing field-valid probability assessment and update techniques using a realistically simulated UAV theater (see FIGURE 2). In FY11, several studies involving human subjects were conducted at the Georgia Decision Lab in order to test for the presence of cognitive biases in probability judgments in strategic settings.

FIGURE 2

Simulated environment for Unmanned Aerial Vehicles. The objective of this project is to take critical steps toward establishing field-valid probability assessment and update techniques using a realistically simulated UAV theater.

The first study, completed in FY11, tested for inaccuracies in verbal assessment using Mazur's adjusting delay procedure modified to deal with probabilities. Decision theorists such as Savage and DeFinetti were skeptical of the reliability of verbal expressions. On the other hand, psychologists such as Kahneman and Tversky were more trusting of verbal expressions. The first study investigated whether direct verbal reports of probabilities are consistent with degrees of uncertainty inferred from choice data. For example, if a subjective probability of 0.5

is attributed to an outcome A, is the participant indifferent between betting on A and betting on a coin flip resulting in heads? A total of 109 subjects were recruited with 96 from the general psychology research pool and 13 from the Army and Air Force ROTC. The results of this first study were statistically analyzed to identify the bias on average in the research pool and ROTC populations, if any, and differences between the two populations. Results were analyzed using classical stochastic models. The Hosmer-Lemeshow test shows a good fit of the model to the data. Because both intervals contain 1.0, no systematic inflationary or deflationary bias in the uncertainty expressions is currently inferred. However, the significantly smaller interval for ROTC participants despite the small sample indicates a much better behaved population and calibrated assessments in the context of this experiment, as compared to the general research pool.

The second study, also completed in FY11, tested for a lack of honesty in probability assessments using proper and non-proper scoring rules. In this study, 122 subjects from the general psychology research pool were recruited. Results did not indicate any systematic inflationary or deflationary bias although the ROTC pool was significantly better behaved. Positive effect of the non-proper scoring rule was observed when participants experienced predefined flight trajectories. These positive effects were not observed when participants were additionally burdened with decision making.

G. Insect-Inspired Visual Flight Control for Aerial Microsystems

Professor Sean Humbert, University of Maryland, Young Investigator Award

The objective of this research is to formalize the wide-field processing principles of the insect visuomotor system for an intended audience of microsystem roboticists, engineers, and designers. The scientific approach seeks to address this problem by developing a common state-space framework to investigate the interplay between visual sensing architectures and flight dynamics. In FY11, Professor Humbert and his research made significant advances concerning the analysis of information contained in spherical optic flow patterns for 6-DOF micro air vehicles maneuvering in 3D environments. In addition, optimal techniques for generating weighting functions to extract individual state estimates from instantaneous patterns of optic flow were developed.

The biological inspiration for this project was drawn by a mathematical interpretation of *tangential cells*. Tangential cells are large, motion-sensitive neurons that reside in the visuomotor systems of most flying insects. They are believed to pool the outputs of large numbers of local optic flow estimates and respond with graded membrane potentials whose magnitude is both spatially and directionally selective (see FIGURE 3). The integrated output is a comparison between the cell's spatial sensitivity pattern and that of the visual stimulus. An algebraic model of such optic flow was developed based on a parametrization of the family of expected 3D environments. Small perturbation techniques were then applied to link weighting patterns to functions of relative proximity and velocity with respect to the parametrized environments. It was found that the resulting output matrices were not sparse (*i.e.*, few direct linkages from weighting function shape to rigid body states). This motivated the concept of state extraction weighting functions, that when applied to instantaneous optic flow measurements on the sphere generated least squares optimal state estimates (see FIGURE 4).

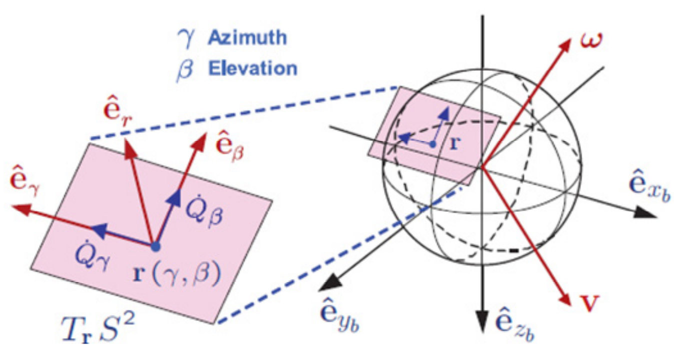

FIGURE 3

Geometry for spherical optic flow. Optic flow is the projected relative velocities of objects in the environment into the tangent space of the imaging surface: a sphere.

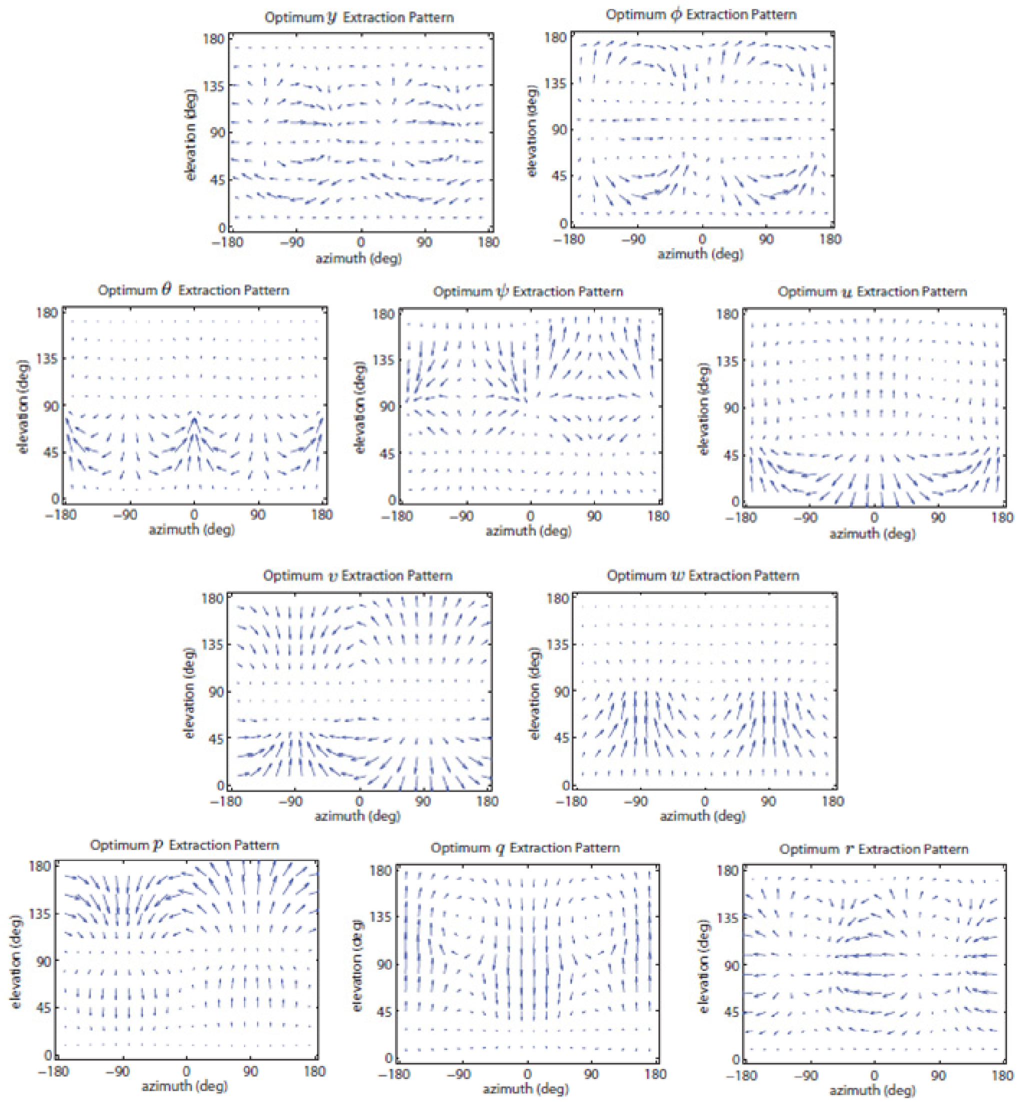

FIGURE 4

Least-squares optimal weighting patterns to recover environment-scaled states from the instantaneous optic flow field. When state extraction weighting functions were applied to instantaneous optic flow measurements on the sphere, least squares optimal state estimates were generated.

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. MIMO for Wireless LANs

Investigator: Professor Srikanth Krishnamurthy, University of California - Riverside, MURI Award
Recipient: Cisco Corp.

Judicious use of multiple antennas on both wireless transmitter and receiver, also known as MIMO (for multi-input multi-output), can significantly increase the data throughput on a wireless network. Through a recently-completed MURI, Professor Krishnamurthy performed analysis and experiments on MIMO performance and found that channel bonding can have an adverse impact on performance. Channel bonding is a technique used in on certain MIMO systems, including 802.11n, which combines two adjacent frequency bands to form a wider band to facilitate higher data rate transmissions. Under Cisco-funded follow-on research that was performed in collaboration with their engineers, Professor Krishnamurthy investigated why and under what circumstances channel bonding reduces performance. Based on the results of these Cisco-funded studies, an algorithm was developed that configures and performs channel allocation for 802.11n. These results were then transitioned to one of Cisco's product-development units.

B. Application of Geo-spatial Abduction to identifying High Value Targets

Investigator: Professor V. S. Subrahmanian, University of Maryland, Single Investigator Award
Recipient: ARL Computational and Information Sciences Directorate (ARL-CISD)

Working with ARL-CISD scientists, CPT Paulo Shakarian, a PhD student under Professor Subrahmanian, has applied geo-spatial abduction algorithms to identification of high value targets and weapons caches in two provinces of Afghanistan. Using data available from ARL-CISD, CPT Shakarian was able to show that it is possible to take into account tribal affiliations, geographical information, and the road network to reason about location of commanders who were directing flow of material and men, and the location of weapons caches, based on information about IED explosions that were being targeted against ISAF. The algorithms have been transitioned to ARL-CISD for further hardening before it can be included in DSGS-A, a common software platform used by the Army.

C. Reliability-Based Design Optimization (RBDO)

Investigator: Professor K.K. Choi, University of Iowa, Single Investigator Award
Recipient: Tank and Automotive Research and Development Center (TARDEC)

Professor Choi at the University of Iowa has developed a new Dynamic Kriging (DKG) method, designed to obtain accurate surrogate models. This method was developed by (i) using a pattern search algorithm to obtain the global optimum correlation parameters, and (ii) using basis functions that are selected by a genetic algorithm from the candidate basis functions based on a new accuracy criterion to obtain an optimal mean structure of the Kriging model. In addition, sequential sampling (SS) points selected based on the prediction interval of the surrogate model, were integrated to develop the SS-DKG method. Comparison studies to verify the accuracy of the DKG method were completed. The DKG method was compared with four other existing surrogate modeling methods, such as the universal Kriging (UKG), the polynomial regression (PRS), the radial basis function (RBF), and the blind Kriging (BKG). Each of the four surrogate modeling methods is carried out with the optimized parameter obtained by globally minimizing the cross-validation error. A mathematical benchmark problem and M1A1 Abram Tank Roadarm problem were used for the comparison study (see FIGURE 5). In these tests, the DKG method showed the highest frequency of being identified as the best among all candidate methods. The sequential sampling in the SS-DKG method improved the accuracy of the obtained surrogate models further.

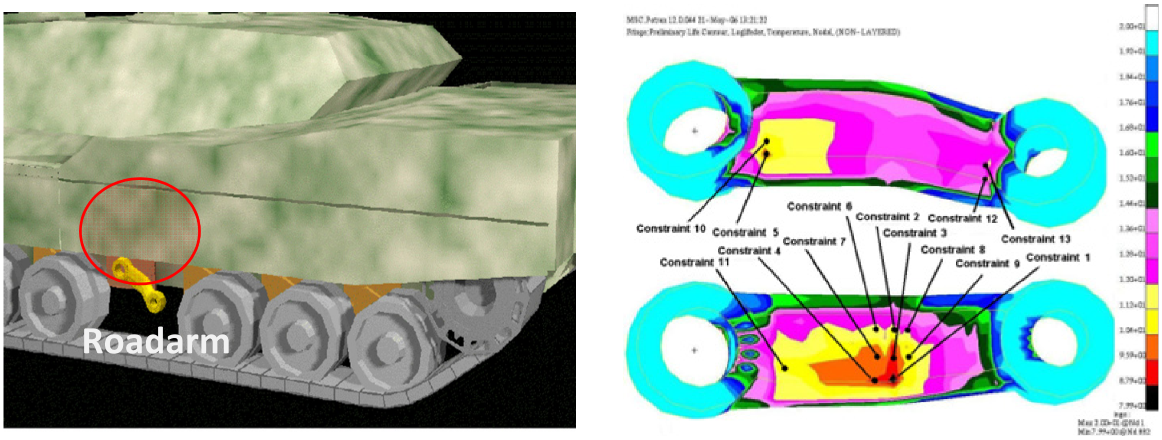

FIGURE 5

Abrams Tank Roadarm Component. A mathematical benchmark problem and M1A1 Abram Tank Roadarm problem were used for the comparison study of the four surrogate modeling methods. To reduce the effect of randomness from the sample profiles, 100 consecutive trials for each problem were carried out, and the performances of the total five surrogate modeling methods were compared. The ranks of the surrogate model were reported for each problem at different sample sizes when at least one of the five candidate methods achieves the acceptable accuracy (*i.e.*, when the coefficient of determination, R2, of the surrogate model were larger than 99%). In these tests, the DKG method showed the highest frequency of being identified as the best among all candidate methods. The sequential sampling in the SS-DKG method improved the accuracy of the obtained surrogate models further.

This newly-developed SS-DKG methodology recently received TARDEC support, and has been integrated with earlier Iowa-developed capabilities into a comprehensive system to support component and systems design. With this new toolbox, TARDEC scientists will carry out the RBDO and obtain the reliable optimum design for large-scale problems, without requiring sensitivity, for broader applications, including engine design, crashworthiness, robotics, blast-resistant structures for safety, design for human factors, and fluid-structure problems. These designs will benefit from the reliable optimum design obtained in reducing the maintenance and/or manufacturing costs in Army operation. The University of Iowa research team also provided a workshop at TARDEC for training TARDEC engineers with application-specific modeling and simulation emphasis through a modular approach. Three capabilities, SS-DKG (ARO funding), Copula (TARDEC funding), and sampling-based RBDO (TARDEC funding), are now integrated into a comprehensive software system that includes a very easy-to-use user interface.

D. Discrete Event Supervisory Control and Nonlinear Motion Control

Investigator: Professor Frank Lewis, University of Texas at Arlington, Single Investigator Award
Recipient: TARDEC

Professor Lewis, through an ARO-funded project, has developed a family of optimal adaptive control methods and a class of discrete-event decision controllers that has lead to numerous joint publications with TARDEC regarding trust-based control and supervisory decision for networked military teams. This ARO-funded technology has been transitioned to a SBIR Phase I contract from DARPA to pursue applications for UAV control. In addition, Dr. Grant Gerhart of TARDEC and Professor co-organized special sessions on Intelligent Behaviors at SPIE Defense Symposium, Orlando. These sessions brought together many internationally-known scientists in Intelligent Control and Autonomous Systems.

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. Information-Theoretic Model Selection with Applications to Social Networks

Professor Sriram Vishwanath, University of Texas - Austin, Single Investigator Award

Inferring the network structure of social networks from large databases of diverse data types is extremely time consuming. Professor Sriram Vishwanath is investigating the use of mathematical concepts from information theory to derive techniques for determining network topology from large datasets.

It is anticipated that in FY12, information theoretic techniques, such as divergence will be used to analyze the dependencies between variables in a given dataset. If successful, this framework will formalize and generalize existing techniques, and then simulate them to study loopy graphical models, with a special emphasis on graphs with short loops. The framework will then be applied to social networks datasets in order to learn its limitations and scope of applications within the social networking area. Since social networks have inherently short loops, including cliques, the results of the proposed research has a high likelihood of being applicable to analyzing them. The results of applying the techniques to social networks will be integrated into the ongoing research to progressively improve data accuracy.

B. Microbiorobots for Manipulation and Sensing

Professor Minjun Kim, Drexel University, Single Investigator Award

In FY12, a highly ambitious and challenging project will investigate a new paradigm for micro-assembly and manipulation incorporating state-of-the-art technology in control theory, fluid mechanics, microbiology, microfabrication, robotics, and systems biology. Although nano- and microfabrication techniques are rapidly advancing, it remains a challenge to fabricate separate individual microscale actuators and sensors en masse. A possible resource for such tiny elements exists within microorganisms. Specifically, the abilities of bacteria to move in a self-propelled manner and to detect and process sensory information represent enormous potential that can be harnessed and integrated into microscale robotics and biosensor systems.

The objective of this research is to develop a platform that integrates bacteria with enhanced motility and signaling behavior (through synthetic biology) into a microscale sensing and robotic system. The platform, termed microbiorobots (MBRs), consists of controllable, reconfigurable elements of a microscale sensing and transportation network in biofactory-on-a-chip systems. Multiple types of bacteria will be used, categorized as two functional types, propulsion/actuation and sensing/computation, to enhance the capabilities of existing microrobots through localized sensing and computation. The interdisciplinary research team will use synthetic biology to engineer microbes capable of sensing chemicals or other environmental cues and tuning their motility. In addition, intercellular communication will be exploited to further coordinate the microbial populations. The use of bacteria as bio-info-micro system represents a critical step toward both how microbiorobotics can be introduced as a tool in nano/microscale engineering work as well as how scientists and engineers can learn from nature using modern fabrication, genetic manipulation, and deterministic and stochastic modeling and control.

It is anticipated that in FY12, the investigators will demonstrate all the tools, including mathematical models that are necessary for characterizing and optimizing genetically-modified engineered bacteria as the engine of a microbiorobotic system. In particular, the design and synthesis of synthetic sensing and information processing modules will be emphasized. All of these elements will be demonstrated so that integrated systems can be assembled, modeled and utilized during subsequent years of the project.

C. Cultured Neural Network

Professor Thomas Shea, University of Massachusetts - Lowell, Single Investigator Award

A joint project between the ARO Network Sciences and Life Sciences Divisions has led to an innovative approach to study learning behavior in cultured neural networks. This new methodology allows tracking neural responses, including learning behaviors, in a highly controlled experimental setting. It is anticipated that in FY12, Professor Shea and his collaborator Professor Holly Yanko, will develop a self-contained system in which cultured neurons receive sensory input from the environment (see FIGURE 6), process this input, and generate motor functions. This goal will be accomplished by feeding a digitized camera signal (sensory input) to cortico-hippocampal neurons cultured on multi-electrode arrays (the "neuronal network," that will process this information) and transmission of resultant neuronal signals to a digitally-controlled robotic arm capable of complex manipulations (motor output). The neuronal cultures will therefore function as a rudimentary central nervous system. These cultures are capable of long-term *potentiation*, which is the basis for learning. Established training regimens will be utilized to refine the response capabilities of the neuronal network, including differential responses following observation of friendly or potentially hostile targets prior to retaliation. The extent of training and responsiveness will be correlated with that of standard artificial neural networks in order to improve performance of artificial neural networks.

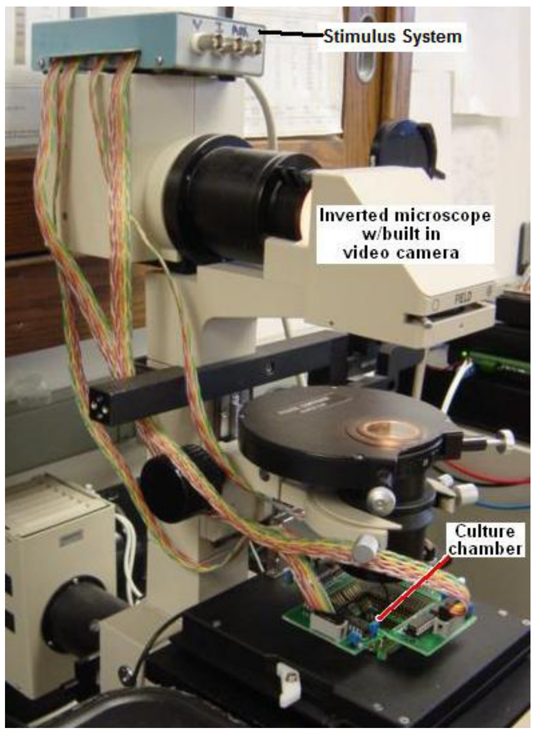

FIGURE 6

Cultured Neural Network - Multi-Electrode Array. It is anticipated that in FY12, under Professor Shea's leadership, a self-contained system will be developed in which cultured neurons receive sensory input from the environment, process this input, and generate motor functions.

D. Modeling Motivational and Action Attitudes

Professor Yoav Shoham, Stanford University, Single Investigator Award

Modern warfare assigns an increasingly important role to robotic soldiers, and thus requires effective methods to harmonize the activities of human and robotic fighters. Professor Shoham is investigating one facet of the interaction between these different types of fighters, namely the mutual modeling of their mental state. In contrast to previous work that focused on informational attitudes such as knowledge and belief, Professor Shoham will focus on motivational (e.g., preferences) and action attitudes (e.g., intentions). Given that any attempt to formalize intentions must account for goals and plans, the researchers generalized calendars as temporal spreadsheets, with events and conditions, in which change in conditions lead to new events being added or old (planned) events being removed. It is anticipated that in FY12 the investigator will extend traditional modal logics for belief and belief revision to include intentions and intention revisions, and use the new logic to explain the semantics of temporal spreadsheets. Finally, the investigator, in collaboration with social scientists, will begin to anchor this modal logic work in theories of behavioral psychology.

VI. DIVISION STAFF

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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 2011* is to provide information on the programs and basic research efforts supported by ARO in FY11, 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 FY11.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Physics Division supports research to discover and understand exotic quantum and extreme optical physics. The Division promotes basic research that explores the frontiers of physics where new regimes of physics promise unique function. Examples such as ultracold molecules, complex oxide heterostructures, attosecond light pulses, and quantum entanglement all represent areas where the scientific community's knowledge of physics must be expanded to enable an understanding of the governing phenomena. The results of these research efforts will stimulate future studies and help to keep the U.S. at the forefront of research in physics.

2. Potential Applications. Beyond advancing the world understanding of exotic quantum physics and extreme optics, the research efforts managed by the Physics Division will provide a scientific foundation upon which revolutionary future warfighter capabilities can be developed. The Division's research is focused on studies at energy levels suitable for the dismounted Soldier: the electron Volt and milli-electron Volt range. In the long term, the discoveries resulting from ARO physics research are anticipated to impact warfighter capabilities in the area of Command, Control, Communications, Computers, Intelligence, Surveillance, and Reconnaissance (C4ISR). Research advances in the Division can be readily visualized to impact sensor capabilities for increased battlespace awareness and Soldier protection, enhanced navigation, ultra-lightweight optical elements and low-power electronics for decreased Soldier load, and advanced computational capabilities for resource optimization and maximal logistical support.

3. Coordination with Other Divisions and Agencies. To meet the Division's scientific objectives and maximize the impact of discoveries, the Physics Division coordinates and leverages efforts within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multidisciplinary research topics, and evaluate the effectiveness of research approaches. For example, research co-funded with the Mathematical Sciences Division seeks coherent-feedback quantum control of collective hyperfine spin dynamics in cold atoms. Collaborative efforts with the Electronics Division are also underway with a goal of developing the science of magnetic materials and the engineering of agile radio frequency device concepts. The Physics Division coordinates efforts with AFOSR and DARPA in pursuit of forefront research advances in atomic and molecular physics, including ultracold molecules and optical lattices. The Division also coordinates certain projects with Intelligence Advanced Research Projects Activity (IARPA), the Joint Technology Office (JTO), and the Joint IED Defeat Organization (JIEDDO). These interactions promote a synergy among ARO Divisions and impact the goals and improve the quality of the Division's research areas.

B. Program Areas

To meet the long-term program goals described in the previous section, the Physics Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY11, the Division managed research efforts within these four Program Areas: (i) Atomic and Molecular Physics, (ii) Condensed Matter Physics, (iii) Optical Physics and Imaging Science, 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 becomes cold enough, they lose their identity and the gas behaves like a wave 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 gravitational sensing and ultra-high resolution lithography for future electronics. The specific research Thrusts within this Program Area are: (i) Quantum Degenerate Matter, (ii) Ultracold Molecular Physics, and (iii) Optical Lattices. 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" based on atoms and molecules, but with statistics, mass, charge, and many additional handles not available in conventional electronics. The Molecular Physics 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 is new for 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 Imaging Science. The goal of this Program Area is to explore the novel manipulation of light and the formation of light in extreme conditions. Research is focused on physical regimes where the operational physics deviates dramatically from what is known. The specific research Thrusts within this Program Area are: (i) Negative Index Materials (NIMs), (ii) Transformation Optics, and (iii) Extreme Light. Negative index materials (NIMs) are artificially fabricated materials whose collective response to light culminates in backward refraction. This program has a particular interest in the development of NIMs that are functional at visible wavelengths and some success has been achieved in this area. Advances have led to research in transformation optics, in which the index of refraction (both positive and negative) of optical materials, is a controllable function of position and possibly time. Possible applications include sub-wavelength imaging, flat or conformal optics, cloaking, and light collection. The Extreme Light Thrust involves investigations of ultra-high intensity light, light filamentation, and femtosecond/attosecond laser physics. High-energy ultrashort pulsed lasers have achieved intensities of 10^{22} W/cm^2. Theoretical and experimental research is needed to describe and understand how matter behaves under these conditions, including radiation reactions and spin effects, from single particle motion to the effects in materials, and how to generate these pulses and use them effectively. One consequence of ultra-high power lasers is light filamentation. Short, intense pulses self focus in the atmosphere until the intensity reaches the breakdown value where nitrogen and oxygen are ionized, creating a plasma. This new form of radiation creates a supercontinuum of coherent light across the visible spectrum. Ultra-short intense pulses can be utilized to develop attosecond pulses by combining them with high harmonic generation. Potential long-term applications of these pulses include imaging through opaque materials, laser pulse modulation, and "observing" electron dynamics.

4. Quantum Information Science. The objective of this Program Area is to understand, control, and exploit nonclassical, quantum phenomena for revolutionary advances in computation and in secure communications. Three major Thrusts are established within this program: (i) Foundational Studies, (ii) Quantum Computation and Communication, and (iii) Quantum Sensing and Metrology. Research in the Foundational Studies Thrust involves experimental investigations of the wave nature of matter, including coherence properties, decoherence mechanisms, decoherence mitigation, entanglement, nondestructive measurement, complex quantum state manipulation, and quantum feedback. The objective is to ascertain current limits in creating, controlling, and utilizing information encoded in quantum systems in the presence of noise. Of particular interest is the demonstration of the ability to manipulate quantum coherent states on time scales much faster than the decoherence time, especially in systems where scalability to many quantum bits and quantum operations is promising. Quantum computation entails experimental demonstrations of quantum logic performed on several quantum bits operating simultaneously. Demonstrations of quantum feedback and error correction for multiple quantum bit systems are also of interest. There is particular interest in developing quantum algorithms for solving NP-complete problems for use in resource optimization and in developing quantum algorithms to simulate complex physical systems. Research in the Quantum Computation and Communication Thrust involves studying the transmission of information through quantum entanglement, distributed between spatially separated quantum entities. Long-range quantum entanglement, entanglement transfer among different quantum systems, and long-term quantum memory are of interest. An emerging field of interest is quantum sensing and metrology using small entangled systems. Entanglement provides a means of exceeding classical limits in sensing and metrology and the goal is to demonstrate this experimentally.

C. Research Investment

The total funds managed by the ARO Physics Division for FY11 were $59.8 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY11 ARO Core (BH57) program funding allotment for this Division was $4.6 million. The DoD Multi-disciplinary University Research Initiative (MURI), Defense University Research Instrumentation Program (DURIP), and Presidential Early Career Award for Scientists and Engineers (PECASE) programs provided $10.3 million to projects managed by the Division. The Division managed $13.0 million provided by the Defense Advanced Research projects Agency (DARPA), and $28.1 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $0.6 million for contracts in FY11. Finally, $3.2 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which encompasses OSD-matched funding for active BH57-funded (Core) HBCU/MI projects, DoD-funded Partnership in Research Transition (PIRT) projects, DoD-funded Research and Educational Program (REP) projects, and/or DoD-funded Instrumentation awards to Tribal Colleges and Universities (TCU).

II. RESEARCH PROGRAMS

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

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). 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. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. Topological Insulators (Austin, TX, 19 November 2010). This workshop assessed future scientific opportunities with topological insulators. The workshop brought together leading theorists and experimentalists with discussions emphasizing interactions, different symmetry classes, defects, new numerical techniques and experimental progress and novel probes. An emerging theme was the interplay between correlations and topology in the band structure, which has yet to be explored either theoretically or experimentally.

2. Complex Oxide Interfaces Workshop (San Jose, CA; 29-30 August 2011). The purpose of this workshop was to assess the progress and future research directions of fundamental research in emergent phenomena at complex oxide interfaces with some cross-fertilization fostered by some presentations and discussions on topological insulators. The workshop highlighted key advances in the field and revealed that several aspects of the community's current understanding of complex oxide physics is likely incorrect and in need of revision. The workshop brought together academic leaders in the field to discuss phenomenological and *ab initio* theory, epitaxy, defect modeling and mitigation, and materials characterization to include scanning tunneling electron microscopy, x-ray spectroscopies, optical studies and transport.

C. Multidisciplinary University Research Initiative (MURI)

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

1. Imaging Beyond Classical Limits. This MURI began in FY05 and was awarded to a team led by Professor Robert Boyd at the University of Rochester. The objective of this research is to employ quantum optics and effects to devise unique imaging methodologies that can exceed classical constraints.

Recent advances in quantum optics and in quantum information science have created the possibility of entirely new methods for forming optical images with unprecedented sensitivity and resolution. This research focuses on exploring quantum new methods for image formation enhanced by quantum mechanics (or possibly by exploiting previously-undiscovered analogies with quantum mechanics). Four specific approaches for quantum imaging are being explored: (i) optical coherence tomography, in which quantum effects are used to increase the axial resolution of the imaging system and are used to extract useful information regarding the dispersion of the material, (ii) ghost imaging, in which one can use coincidence techniques to form images using photons that have never interacted with the object to be imaged, (iii) laser radar, for which a noise-free quantum preamplifier might be developed with increased detection sensitivity, and (iv) lithography, where the use of quantum-entangled photons can enable one to write structures at a resolution exceeding that imposed by classical diffraction theory.

2. Advancing Fundamentals in Optics. This MURI began in FY06 and was awarded to a team led by Professor Vlad Shalaev at Purdue University. The objective of this MURI is to advance the field of optics through the construction of negative-index materials (NIMs) operational at visible wavelengths.

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 offer the possibility of developing a perfect lens that in principle could allow an experimenter to see objects at a nanometer scale - much smaller than the diffraction limit. These lenses could be used for sensors, microscopy, and for production of ultra-resolution lithographic structures. NIMs can be designed through the use of metamaterials (artificial materials engineered to provide specific properties not available in naturally-made structures) or by the construction of photonic crystals. The team has already produced NIMs that function at both infrared and visible wavelengths. Although this MURI is in its final year of funding, the overarching goals of this program will be continued and expanded by a new MURI led by Professor David Smith, with Professor Vlad Shalaev contributing as a co-PI (see Subsection 7: Transformation Optics - Exploring New Frontiers in Optics).

3. Quantum Many-body Physics from Biological Assembly. This MURI began in FY07 and was awarded to a team led by Professor Rick Kiehl at the University of California - Davis. The objective of this research is to employ biological assembly to study nanostructures exhibiting quantum phenomena.

Numerous novel quantum phenomena resulting from many-body interactions are present in condensed matter systems with a length scale at or just beyond the reach of current lithographic technology (<10 nm). Biological mechanisms, however, naturally operate on such length scales. The specific goals of this program are: (i) to use studies of biological assembly of individual and multiple nanostructures for systems exhibiting quantum many-body phenomena and to do so in such a way that the phenomena are accessible, and (ii) to demonstrate the systematic study of such phenomena. These goals will be pursued by research involving (a) DNA and protein-based directed assembly of nanostructures, (b) chemical modification of the nanostructure surfaces for protection of the inorganic core and for binding to biological macromolecules, and (c) transport and spectroscopic studies of nanostructure arrays and devices exhibiting quantum phenomena. It is anticipated that the MURI will open a new avenue to study many-body phenomena and will accelerate research toward a fundamental understanding of these phenomena. Results from this MURI are expected to lead to new opportunities for technological development based on novel quantum phases of matter that are as-of-yet inaccessible.

4. 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.

5. 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.

6. 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.

7. 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 NIMs.

Advances in NIMs, many of which were developed by the MURI team led by Professor Vlad Shalaev (refer to Subsection 2: Advancing Fundamentals in Optics), have led to 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 began to explore this new frontier in physics and the research team includes Professor Shalaev as a co-investigator. The MURI team will investigate 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.

8. 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 20th 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.

9. Multi-Qubit Enhanced Sensing and Metrology. This MURI began in FY11 and was awarded to a team led by Professor Paola Cappellaro at the Massachusetts Institute of Technology. The objective of this research is to explore and demonstrate imaging, sensing and metrology beyond the classical and standard quantum limits by exploiting entangled multi-qubit systems.

Precision measurements are among the most important applications of quantum physics. Concepts derived from quantum information science, such as quantum entanglement, have been explored for the past decade to enhance precision measurements in atomic systems with important potential applications such as atomic clocks and inertial navigation sensors. Quantum information science has also enabled the development of new types of controlled quantum systems for the realization of solid-state qubits. These systems could potentially be used as quantum measurement devices such as magnetic sensors with a unique combination of sensitivity and spatial resolution. However, progress towards real-world applications of such techniques is currently limited by the fragile nature of quantum superposition states and difficulties in preparation, control and readout of useful quantum states. The power of entangled and squeezed states for quantum sensing lies in their sensitivity to the external parameter to be measured.

This MURI effort aims to overcome three major obstacles to practical quantum sensor operation: the difficulty to experimentally create desired entangled many-qubit input states to the sensing device, the fragility of the states during signal acquisition, and low fidelity of the readout process. The results of this research may ultimately lead to dramatic improvements in imaging, sensing, and metrology.

10. 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.

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

No new starts were initiated in FY11.

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

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. High-speed Room-temperature Single-photon Counters. Two Phase II STTR contracts were awarded to NuCrypt, LLC and Princeton Lightwave, Inc. to develop and validate innovative compact near room temperature systems for high speed (GHz) single-photon counting at telecommunications wavelengths. Single-photon detectors are used in various applications including quantum communications, hyperspectral imaging, and florescence spectroscopy. Currently, silicon based avalanche photodiode devices (APDs) are effective and convenient options below 1 micron wavelength. These STTR efforts are attempting to achieve improvements to detector device design, materials, and near-room-temperature operation. This research may ultimately lead to a prototype counter that may impact future applications in quantum communication, and compact sensors for imaging and spectroscopy.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) – 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). The FY11 new starts within these programs are described here, while the missions of each of these programs were described *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. DoD REP Awards. As described in more detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, REP awards aim to enhance or increase the programs, capabilities, and graduates in scientific and engineering disciplines in universities serving underrepresented minorities. In FY11, the Physics Division managed six new REP projects, totaling $3.2 million. The equipment purchased with this award is promoting research in areas of interest to ARO, such as determining the optical properties of aerosols composed of mixtures of different absorbing and non-absorbing species, and to advance state of the art algorithms for large-scale electronic structure and atomistic simulations through the study of quantum phenomena in nanowire sensors.

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

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Exploring Strong Coupling Regime of Superconducting Qubit and Microwave Cavity. The objective of this new PECASE award, led by Professor Andrew Houck at Princeton University, is to explore the strong coupling regime of a superconducting qubit and a microwave cavity.

Quantum mechanics has played an increasing role in electronics over the past several decades, beginning with materials and devices that were designed from quantum mechanical principles, and extending to devices that store and manipulate quantum bits (qubits) of information. However until recently, these qubits have been controlled with classical signals. A fully quantum mechanical circuit, in which both the components and the control signals are fundamentally non-classical, opens the possibility of scalable quantum computing architectures and enables a full range of quantum optics capabilities, all on a single chip. This research will explore the strong coupling regime of a superconducting qubit and a microwave cavity through three specific aims: (i) core building blocks for scalable quantum computation, (ii) new techniques for quantum control, and (iii) implementation of quantized non-linear optics. This research may ultimately enable more secure financial transactions, optimal airline routing, and efficient telecommunications networks.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY11, the Physics Division managed eight 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 research to obtain electron spectroscopies of complex oxide heterostructures, study the growth, surfaces and interfaces of topological insulators, analyze and image entangled photons, and to explore the optical properties of materials.

I. DARPA Information in a Photon (InPho) Program

The goal of the DARPA InPho Program 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.

J. DARPA Optical Lattice Emulator (OLE) Program

The DARPA OLE Program seeks 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 program.

III. SCIENTIFIC ACCOMPLISHMENTS

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

A. First Functional Atomic Circuit Will Enable Atomtronic Devices

Professor Ian Spielman, University of Maryland - College Park, MURI Award

The goal of this research project is to investigate and demonstrate "atomtronic" concepts, envisioning atom-based rather than electron-based physics, analogous to and extending beyond electronics. The MURI team, along with scientists from ARL-SEDD and researchers from the Joint Quantum Institute, have created the first functional atomic circuit using ultra-cold gases cooled to near absolute zero using focused lasers. The researchers created this circuit using a ring-shaped Bose-Einstein condensate. The condensate is a unique superfluid-like state of an atomic gas that exhibits a quantum behavior that can be observed and studied only at temperatures near absolute zero.

To create this ring or donut-shaped loop of atoms, the team crossed laser beams such that the highest light intensity was at the edge and smoothly tapered down toward the center of the intersecting beams. This laser arrangement formed an optical bowl-shaped trap for the atoms. The researchers further chilled the atoms to less than 10 nK (*i.e.*, 10 billionths of a degree above absolute zero). Another laser beam was then directed into the center of the bowl, forcing the cloud of atoms into a ring along the edge, with a radius of about 20 micrometers. The researchers further included an adjustable barrier (circuit element) that can control the flow of atom current to specified values, similar to a control switch in an electrical circuit. The investigators created an atom circuit with a stationary barrier to study the stability of the atom current (see FIGURE 1) and a tunable barrier that can be dynamically controlled (see FIGURE 2). This research marks the first example of a functional atomic circuit.

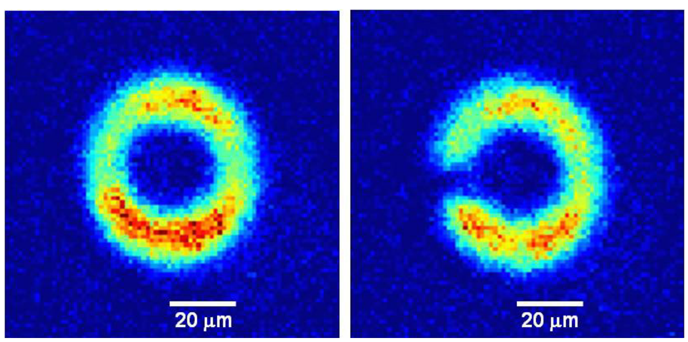

FIGURE 1

Functional atomic circuit with stationary barrier. The researchers created this "atom circuit" composed of ultra-cold sodium gas, as shown in these false-color images. A focused laser beam creates the circuit element, which is a barrier across one side of the ring and constitutes a tunable "weak link" that can turn off the current around the loop. A laser-based barrier can stop the flow of atoms around the circuit (left), while the atoms can circulate around the ring in the absence of the barrier (right).

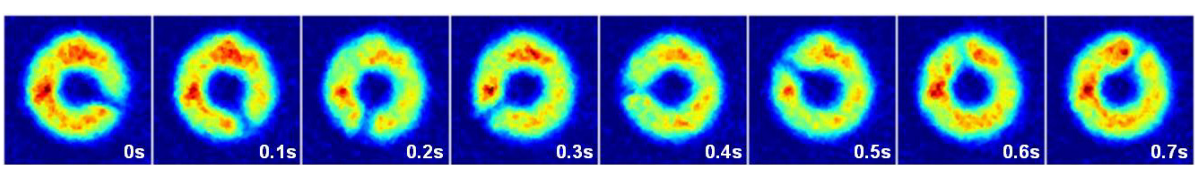

FIGURE 2

Atomic circuit with rotating barrier. The researchers have also implemented a control switch that is tunable and can be rotated at a desired speed, as shown in these time-lapse images.

Just as the ability to control electrons led to the electronics revolution, this method for controlling atoms—no longer limited to a single mass, spin, and interaction—is a key initial step in a future "atomtronics" revolution. This atom-circuit is analogous to a superconducting quantum interference device (SQUID). SQUIDs use superconducting electrons in a loop to make highly sensitive measurements of magnetic fields.

This simplest of atomtronic circuits could one day be used as a sensor for atomic rotation. It may ultimately provide a 100,000-fold improvement in precision of inertial navigation, which has tremendous implications for operations in GPS-denied environments. Atomtronics should also enable compact fieldable sensors, such as mobile gravity gradiometers and miniaturized optical-grade clocks that will be able to break classical sensing limits. Such a revolutionary new technology would enable capabilities such as detecting underground structures like tunnels and bunkers from an overflying aircraft and quantum-based encryption for ultra-secure communications.

B. Role of the Laser Magnetic Field in Ultra-intense Fields: Semi-Classical Calculations of Ionization

Professor Barry Walker, University of Delaware, Single Investigator Award

The goal of this project is to understand ultra-high field dynamics, including the dynamics of ionization, photoelectrons and radiation in the new ultra-strong field regime (10^{17} W/cm^2 to 10^{20} W/cm^2). This research is led by Professor Walker at the University of Delaware and is providing some of the first detailed, high dynamic-range measurements of the ultra-strong field-atom interaction. Understanding the physics of the interaction of ultra high intensity laser beams with matter is essential for control of and protection from X-rays and THz radiation.

In FY11, Professor Walker developed a classical Monte Carlo simulation where he numerically integrated the classical equations of motion for single-electron atoms interacting with an external laser pulse. Atoms with atomic numbers $1 < Z < 15$ were studied to determine the influence of the laser magnetic field on the ionization process. The research team found the dipole approximation (B=0) is valid up to intensities of 10^{22} W/cm^2 for calculating the ionization rate. A small Lorentz deflection is seen in the angular distribution of ionized electrons as the intensity is increased well into the relativistic regime as the magnetic field begins to deflect the electron as it tunnel ionizes (see FIGURE 3).

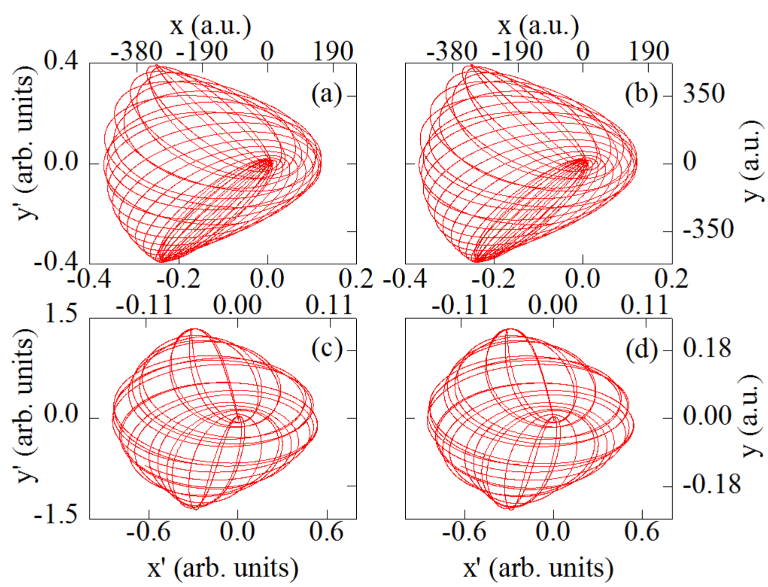

FIGURE 3

Procession of electron orbits. The x' and y' effective coordinates have been rescaled by the square root of the electric field strength. Classical, nonrelativistic Rydberg trajectories are shown in (a) & (b) are for Z = 1, Rydberg state (n,l = 18,s) with and without magnetic field respectively. The trajectories for (c) & (d) are for tightly bound (n,l = 1,s) state for Z = 8, with and without magnetic field, respectively (a.u. = atomic units).

Despite the increase in the field magnitude by more than 10^9, the trajectories are similarly unaffected by the inclusion of the laser magnetic field. While this is expected for the 18s Rydberg state ionized by microwave radiation, this result was not anticipated at such high intensities (> 10^3 a.u.) and tightly bound states (Z = 8) considered well into the relativistic regime for the laser-matter interaction. They quantified the differences with and without the laser magnetic field by looking at the phase space, configuration space explored by the electron with and without the laser magnetic field, comparing the ionization rates, and finally looking at the momentum in the angular distributions of the outgoing electrons.

The difference in the configuration space visited by the electron during the interaction with the laser field is shown in FIGURE 4. These distributions mark a spatial grid ranging from $-4n^2/Z < x, y, z < 4n^2/Z$. The coordinates of the electron are averaged over time for 10^4 electrons. The investigator subtracted the distributions calculated with the laser electric and magnetic field (denoted E&B) from the calculated distribution calculated including only the laser electric field (denoted E). To set the numerical accuracy estimate the researchers calculated the configuration space for two different random number launches of the 10^4 electrons and subtract the two calculations, such as $(E\&B)_1 - (E\&B)_2$.

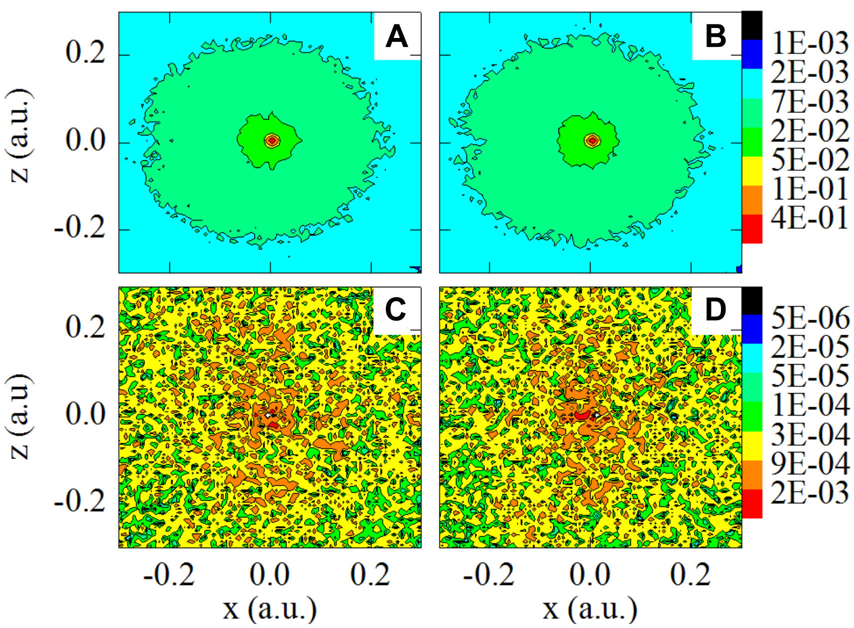

FIGURE 4

Configuration space distributions for Z = 4. (A) Distribution in the dipole approximation. (B) Distribution with magnetic field included. (C) Difference in normalized distributions Sqrt[$(E\text{-}E\&B)^2$]. (D) Difference in two sets of distributions Sqrt[$(E\&B)_1\text{-}(E\&B)_2)^2$].

The investigators found no differences in the configuration space when including (E&B) and neglecting (E) the laser magnetic field. Any differences were at the level of 10^{-4}, which is similar to the noise from the numerical calculations and different random number launches. Therefore, there is no appreciable difference in the configuration space distributions. Surprisingly, this result shows the ultrastrong external field of order 10^3 a.u. is actually very weak compared to the relevant bound state interactions and result in no significant perturbation of the electron. This is consistent with the ionization critical field, were no significant difference was found in the critical field required to achieve ionization at the intensity changes from 0.001 a.u. to 10^6 a.u. of intensity.

The investigators also calculated the angular distributions using the coordinates of the electron as it ionizes (see FIGURE 5). With the inclusion of the magnetic field, the magnetic field can cause the electron trajectory to deflect via the Lorentz force. The change in the range of angles can give an indication of the amount of deflection the electron experiences. For Z < 3 the relative difference in the range of angles is almost negligible for all intensities considered. When Z > 3 the range of angles increases.

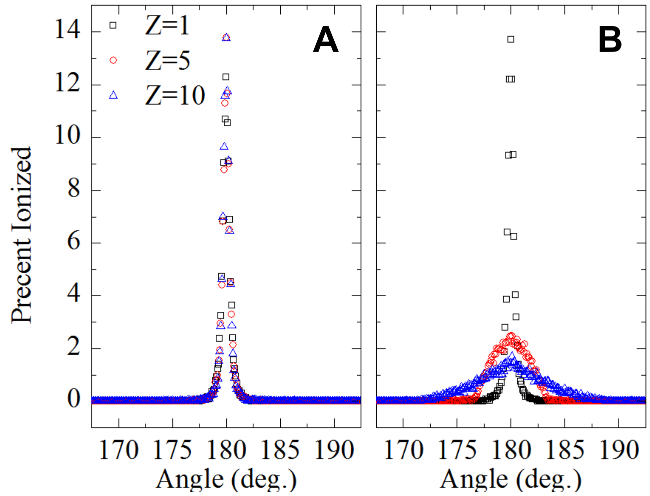

FIGURE 5

Angular distributions for three different Z values for both the dipole approximation and non-dipole approximation. Angle of emission for the ionized electron from Z=1 to Z=10 species (a) without the laser magnetic field and (b) with the laser magnetic field. The intensity for these species is: Z=1 the intensity to ionize is 0.01 a.u., Z=5 the intensity to ionize is 300 a.u., and Z=10 the intensity to ionize is 2 10^4 a.u.

In summary, Professor Walker and colleagues have investigated the influence of including the laser magnetic field on the ionization process. The researchers have shown that the dipole approximation is still valid for intensities up to 10^{22} W/cm^2 and the laser magnetic field has little to no influence on bound state dynamics for the electron. The investigators also found that angular distributions of ionized electrons are slightly affected by inclusion of the laser magnetic field at ultrahigh intensities when the ionized electron is tightly bound.

C. Quantum Computing and Control, and Quantized Nonlinear Optics with Superconducting Circuits

Professor Andrew Houck, Princeton University, PECASE Award

The goal of this project is to explore the strong coupling regime of a superconducting qubit and a microwave cavity, to include execution of high-fidelity quantum coherent operations, chip-scale integration, and exploration of quantized non-linear optics and correlated photon effects. In FY11, the research team focused on properties and control of a new charge qubit for circuit quantum electrodynamics that allows fast and coherent tunable coupling between atomic levels and photons in the cavity. This newly-developed qubit consists of two transmon-like halves (Josephson junctions coupled to a microwave cavity) that are directly coupled with a large capacitor. The resulting hybridized levels suppress or enhance coupling due to quantum interference. By independently tuning flux through two superconducting quantum interference device (SQUID) loops, the investigators were able to independently tune the frequencies and coupling (see FIGURE 6).

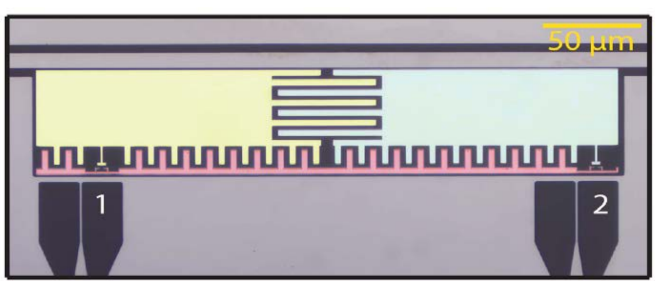

FIGURE 6

Transmon-like charge qubit with tunable coupling to a microwave cavity.

In FY11, the investigator and his research team demonstrated that this qubit can be turned on and off with a fast flux bias line while keeping the qubit frequency constant. Coupling could be turned off by more than three orders of magnitude so that the qubit could not be driven with an applied Rabi drive; however, coupling could be turned back on in tens of nanoseconds, enabling control only when desired (see FIGURE 7). This achievement substantially reduces problems of spectral crowding as "off" qubits are not as affected by crosstalk between control pulses and "on" qubits.

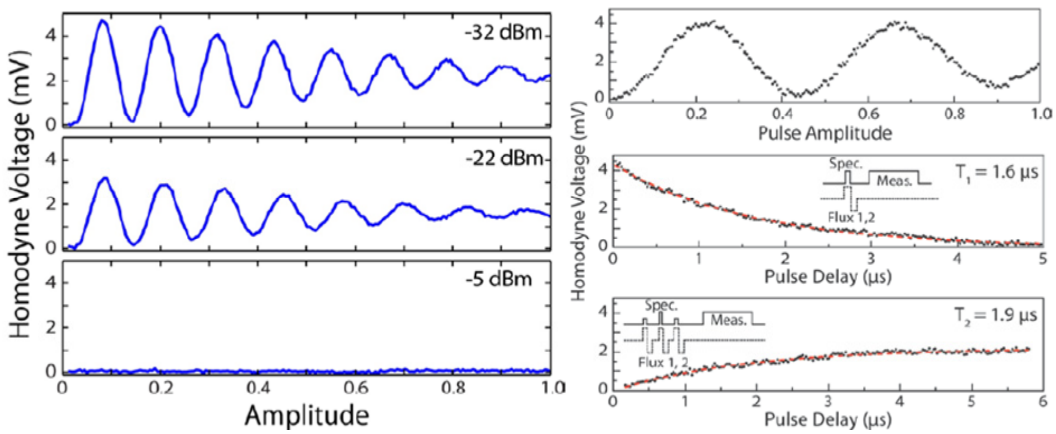

FIGURE 7

Demonstration of qubit turned on and off with a fast flux bias line while keeping qubit frequency constant. The rate of Rabi oscillations can be suppressed (left), even at high drive powers, with a tunable coupling qubit. Coupling can be restored and coherent manipulation made possible through fast flux biasing (right).

Using this qubit, coherent operations were demonstrated with dynamically tuned coupling. The coherence times of the two transmon qubits were 1.6 µs and 1.9 µs as measured with Hahn echo. This Hahn echo experiment demonstrates an ability to apply repeated gates with synchronized RF and flux pulses. These coherence times are comparable to those observed in a single transmon-qubit device. The added complexity of the tunable coupling qubit does not substantially degrade coherence, though operation is more complex due to the dual flux bias.

D. Highest Electron Mobility in a Transition Metal Complex Oxides

Professor Susanne Stemmer, University of California - Santa Barbara, MURI Award

High electron mobility in GaAs two-dimensional electron systems (2DESs) in the 1980s led to a revolution in condensed matter physics by revealing new phases of matter that depended not on a broken symmetry but on the topology of the system. This first discovered topological phases were the integer quantum Hall (QH) states. The more exotic cousins, the fractional quantum Hall states (FQHS), were discovered soon after, in samples with an electron mobility of 90,000 $cm^2/V\,s$. As the FQHS results from electron correlations, this state is often sought in other material systems with stronger correlations. To this end, it is most notable that in 2010, FQHS was observed in MgZnO/ZnO heterostructures, an oxide 2DES with electron mobility exceeding 180,000 $cm^2/V\,s$. Transition metal oxides have the potential to exhibit even more interesting correlated electron physics. The active electrons in these materials originate from transition metal d-orbitals. Many-body phenomena such as ferromagnetic ordering, Mott metal-insulator transition physics and superconductivity may interact with the topological phases of high mobility electrons (in two dimensions) with interesting and unexpected results. Accordingly, Professor Stemmer's demonstration of electron mobilities in $SrTiO_2$ exceeding 128,000 $cm^2/V\,s$ is a tantalizing indication that these expectations may soon be realized. Two components of Professor Stemmer's research have been combined to reach this record. First, Professor Stemmer explored a hybrid molecular beam epitaxy (MBE) approach that greatly improved the material quality. III-V semiconductors, such as GaAs, prefer stoichiometry such that there is a "growth window" of processing conditions over which stoichiometry is easily achieved. Complex oxides, however, are stable over a wide non-stoichiometric range and do not have such a growth window, that is, until Dr. Stemmer explored the hybrid MBE approach. She replaced the standard elemental Ti source with a metal organic precursor. This precursor includes additional oxygen, which is conjectured to assist in achieving stoichiometry. With this metal organic precursor, Professor Stemmer's team has demonstrated stoichiometry and was able to achieve an electron mobility of ~30,000 $cm^2/V\,s$ in $SrTiO_3$.

The second component was to apply strain to doped $SrTiO_3$ samples. This approach has been used in conventional semiconductors to increase carrier mobility resulting in enhanced device speeds. Similarities between the band structures of Si and Ge, and $SrTiO_3$ indicate that a similar enhancement should be possible in the complex oxide. In the semiconductors, compressive strain along the transport direction decreases the effective mass of the carriers, thus increasing the mobility. Professor Stemmer's team grew two samples of La-doped $SrTiO_3$ approximately one micron thick on insulating $SrTiO_3$. The three dimensional electron densities of the two samples were found to be 3.5×10^{17} cm^{-3} and 7.5×10^{17} cm^{-3}. Electron mobility was measured using the standard Hall bar geometry. Uniaxial compressive strain was applied along the transport direction. A strain of approximately -0.3% increased the low temperature mobility by more than a factor of three to reach 128,641 $cm^2/V\,s$ (see FIGURE 8). The mobility did not show signs of saturation with strain and much larger strains are readily feasible in oxide heterostructures. Thus it should be possible to increase this mobility even further. These results indicate the potential for highly functional complex oxides for unique electronic technologies, which may include advanced computational architectures and sensors.

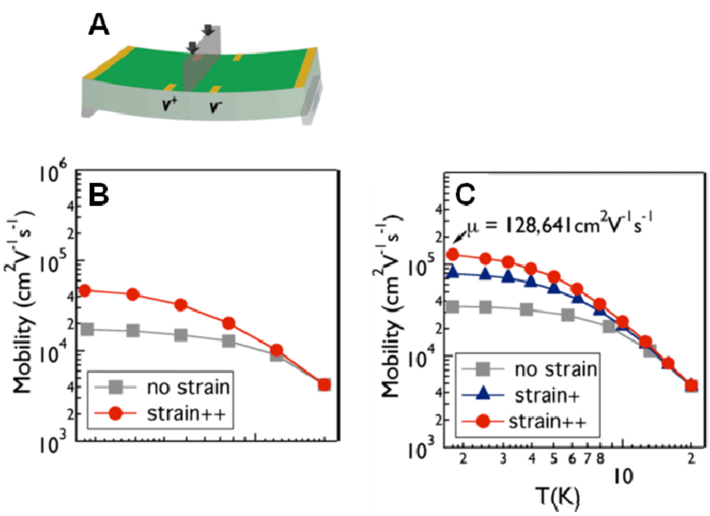

FIGURE 8

Effect of strain on the electron mobility of $SrTiO_3$. (A) Schematic of the three-point bending apparatus used to apply the strain. (B-C) Mobility of La:$SrTiO_3$ as a function of temperature for doping levels of 3.5×10^{17} cm^{-3} and 7.5×10^{17} cm^{-3}, respectively. The maximum strain (red) was approximately -0.3%.

E. Quantum Dot-photonic Crystal Cavity QED-Based Quantum Information Processing

Professor Jelena Vuckovic, Stanford University, Single Investigator and DURIP Awards

The objectives of this research are to increase the efficiency of coherent probing of quantum dot-photonic crystal cavity system, as necessary for implementation of quantum gates, demonstrate optical manipulation of quantum dot states in photonic crystal cavities and demonstrate quantum information transfer between a photon and a quantum dot state.

In FY11, Dr. Vuckovic explored the utility of photon induced tunneling and blockade for non-classical photon state generation. Experimental and numerical demonstrations of the transition from blockade to the tunneling regime in a strongly coupled quantum dot (QD)-cavity system were performed and the signature of higher order dressed states in the measured photon statistics observed. The experimental part of this work was performed with InAs QDs coupled to a linear three hole defect GaAs photonic crystal cavity. At resonance, the QD and cavity mix to generate two polaritons, seen as two Lorentzian peaks in FIGURE 9A. To drive the cavity-QD system, a mode-locked Ti-Sapphire laser was used. The pulsed laser was tuned at the dip in the second-order correlation of the spectrum of light transmitted through the cavity. FIGURE 9B shows the histogram, where the coincidence counts at zero time delay are increased compared to the nonzero time delays. This is a signature of photon bunching and indicates photon-induced tunneling. A similar experiment with the laser tuned to the polariton frequency results in anti-bunching, where the coincidence counts at zero time delay is less than the coincidence counts at non-zero time delay. This is the signature of photon blockade (see FIGURE 9C). The onset of a peak corresponding to the second order dressed states is as predicted by the theory and simulations.

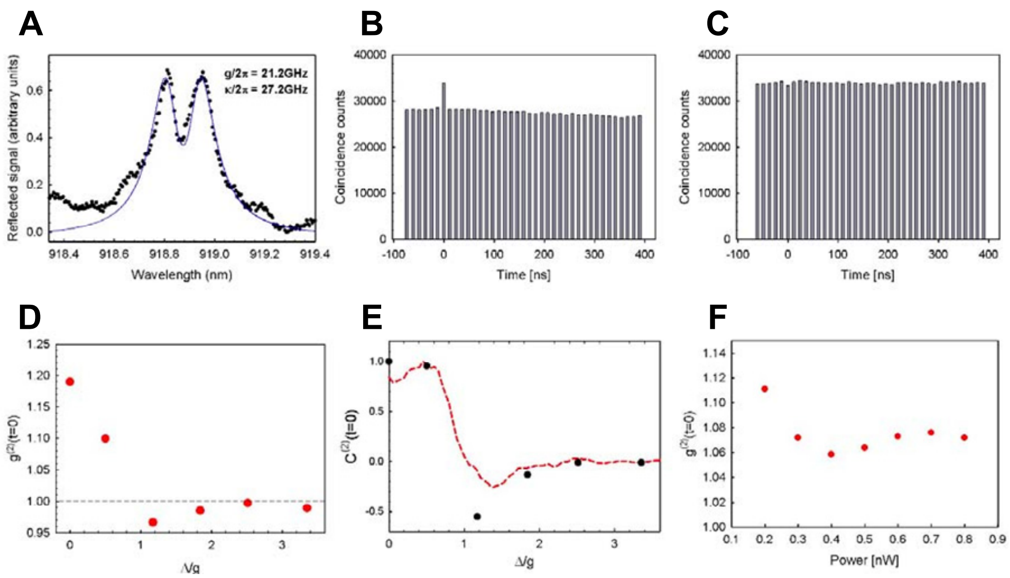

FIGURE 9

Experimental result for photon induced tunneling and blockade under pulsed excitation (τp ~ 24 ps pulses with 80 MHz repetition frequency). (A) The reflectivity spectrum of a strongly coupled QD-cavity system. (B) Coincidence measurement obtained when the laser is tuned to the dip induced by the QD. Increased coincidence counts at t = 0 indicate the photon induced tunneling regime. (C) Coincidence measurement obtained when the laser is tuned to the polariton. The reduced coincidence counts at t = 0 indicate the photon blockade regime. (D) Second order coherence function at t = 0, $g^{(2)}(0)$, as a function of the laser detuning from the empty cavity frequency. We observe transition from the blockade to the tunneling regime. (E) Normalized differential correlation function, $C^{(2)}(0)$, as a function of the laser detuning. The dashed red line shows the result of a numerical simulation based on the system's experimental parameters. The peak at Δ/g ~ 0.5 results from the excitation of the second order dressed states via two-photon process. (F) $g^{(2)}(0)$ in the tunneling regime (Δ = 0) as a function of laser power, Pavg, measured in front of the objective lens. For (b)-(e) Pavg = 0.2 nW.

The research team also demonstrated the controllable charging of a single quantum dot inside an optical nanocavity in FY11. QD charge control is required for the implementation of individual QD spins as qubits for quantum information processing technologies. In bulk QD structures, charge control is typically achieved by embedding the entire sample in a Schottky diode type structure and then controlling the charge via an external bias voltage source. However, in this study photonic crystal structures are fabricated in a 164 nm thick GaAs membrane and the implementation of charge control in such structures remains a challenge. To address this challenge, the investigator implemented a new fabrication procedure by which the charge state of a QD may be controlled by applying a voltage across a PIN junction. The procedure involves wet-etching through the p-doped and intrinsic GaAs layers and then depositing contacts atop the p-doped and n-doped layers to enable QD charge control via an external bias voltage (see FIGURE 10).

Having implemented the above procedure, charging of individual QDs was observed as manifestations of discrete shifts in QD emission lines. Such charging is shown for a particular photonic crystal cavity containing two nearly-degenerate cross-polarized modes. Based on the energy shift of the lines, the shift in the photoluminescence energy indicates a transition from a neutral charge state to a state where the QD contains a single electron. In addition to the observation of QD charging, QD emission lines revealed that it is possible to shift QD emission lines by the quantum confined Stark effect via the external bias voltage (see FIGURE 11). The ability to observe the negative charge state of a QD and to shift its emission energy in a photonic structure marks significant progress towards the development of optical initialization, control and readout methods demonstrated on singly-charged QDs in bulk structures.

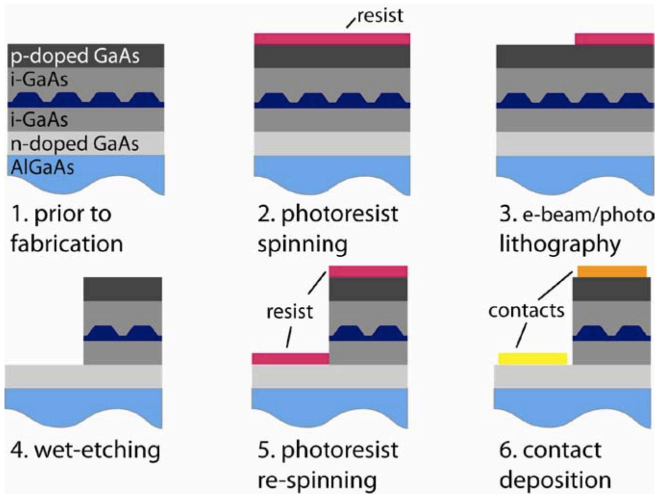

FIGURE 10

Fabrication procedure for PIN junctions enabling charge control of the QD via an external bias voltage. The first portion of the process involves either e-beam or photolithography followed by chemical wet-etching of the p-doped intrinsic GaAs layers. After etching, the photoresist is re-spun on the chip to enable the deposition of metallic contacts atop the p-doped and n-doped layers.

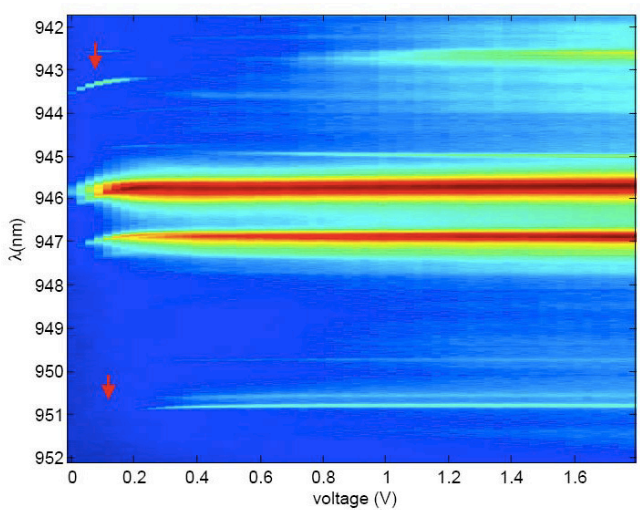

FIGURE 11

Photoluminescence as a function of the bias voltage applied to the vertical pin junction (embedded inside the photonic crystal membrane). Broad stripes correspond to two cavity modes, while narrow stripes correspond to QD lines. A smooth DC Stark shift of QDs is visible. For the QD lines (red arrows), an abrupt wavelength change (from 943 – 951 nm) occurs at the bias voltage of 0.2 V, corresponding to the QD charging event (*i.e.*, an extra electron added to an otherwise neutral QD; therefore, the 943 nm line corresponds to the neutral exciton, while 951 nm line corresponds to the trion [electron + exciton] transition of the QD).

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. Unexpected Astronomical Application of Vortex Lens

Investigator: Professor Grover Swartzlander, University of Arizona, Joint Services Optics Program Award
Recipient: National Aeronautics and Space Administration (NASA)

The research project that led to this noteworthy transition was jointly funded through ARO and the Air Force as an FY03-FY06 Joint Services Optics Program (JSOP) award. The objective of this multi-investigator project was to investigate optical limiting of laser radiation, including theoretical models and experimental validation. Professor Swartzlander, a co-investigator from the previously-completed JSOP award, was investigating optical vortices with the goal of designing a new kind of lens based on vortex beams (*i.e.*, light beams with no light along the axis of propagation). The investigator and his collaborators designed and constructed a new lens to study vortex beams, as proposed. This lens is constructed in a fashion akin to a spiral staircase and forces light to form an optical vortex as it passes through the lens (see FIGURE 12A).

When observing stars, astronomers typically used conventional lenses with an opaque disk to minimize the interference from light directly emanating from the sun or other stars. It was discovered that the dark region created by this lens (see FIGURE 12B) was much darker than the dark region created using an opaque disk. As a result, this lens is more effective in detecting and observing distant planets relative to the traditional opaque disk approach. This lens and the newly-discovered astronomical application of vortex beams recently transitioned to NASA and is being incorporated into telescopes to search for distant planets.

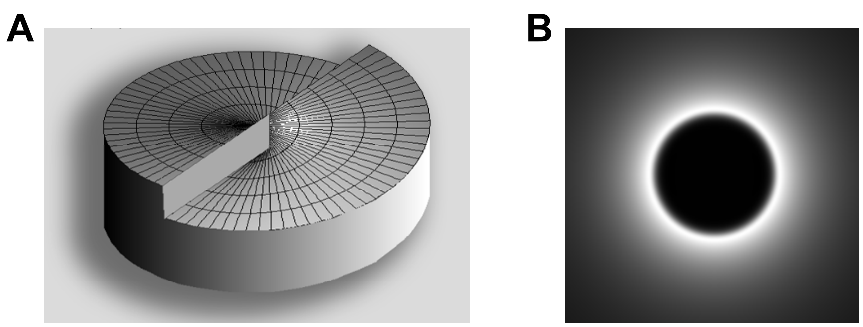

FIGURE 12

Vortex lens and unexpected astronomical application. (A) Coherent light forms optical vortex when passed through the "spiral staircase" structure of the vortex lens. (B) The vortex lens can be used by astronomers for more effective observation due to the reduced light interference relative to a traditional opaque disk.

B. Metamaterials for wireless power transfer

Investigator: Professor David Smith, Duke University, MURI Award
Recipient: Mitsubishi Corp. and Toyota Corp.

Wireless power transfer (WPT) has become a topic of great interest in the commercial world, with the proliferation of handheld and portable devices, and the general expectation that electric vehicles will dominate the transportation landscape in coming years. Electromagnetic frequencies suitable for WPT can readily take advantage of metamaterial ideas originally proposed for optical wavelengths.

The MURI team lead by Professor David Smith is exploring new frontiers in optics made possible by metamaterials (refer to Section II-C.7 *Transformation Optics - Exploring New Frontiers in Optics.*) One particular example is that of a "perfect lens" which can be devised for non-optical frequencies to enhance the efficiency of WPT systems. The idea was proposed to Professor David Smith by researchers from Mitsubishi Electric Research Laboratory (MERL) based on interest in a metamaterials-based approach to WPT. After some initial discussion and investigation, MERL built and demonstrated a perfect lens – formed from split-ring resonators – that increased the efficiency of a WPT system operating in the low-MHz region.

Subsequent to this demonstration, Toyota requested a joint program with Professor Smith's group to repeat the demonstration and begin a more focused effort to tailor the metamaterial perfect lens to electric vehicle charging. In developing various form factors, nearly all the tricks of metamaterials have come in to play, including transformation optics. In an internal Toyota competition in which hundreds of research projects were reported, this project took first place, indicating the importance that Toyota is currently placing on metamaterial-based WPT topics.

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. Towards a Solid-state Optical Clock Based on a Thorium-doped Crystal

Professor Eric Hudson, University of California Los Angeles, Single Investigator Award

The goal of this project is to design, develop and test a solid-state optical clock based on thorium doped crystals, building on existing solid-state analogs (see FIGURE 13). Despite the successes of traditional optical clocks, they are often cumbersome. The high quality (high-Q) oscillator utilized in these clocks is an atomic transition, which may be extremely sensitive to its environment. To mitigate environmental influences, modern clock experimenters routinely employ complicated interrogation schemes such as atomic fountains or 3D optical lattice confinement. An interesting paradigm shift is to consider an optical clock based on a nuclear transition. Just as in atomic clocks, the high-Q oscillator (*i.e.*, the nuclear transition), can in principle be addressed simply by laser spectroscopic techniques, as long as the transition energy is accessible with current laser technology. Furthermore, it is known from Mössbauer spectroscopy that nuclear energy levels are extremely insensitive to their environment. Based on these observations, it may be feasible to build a solid-state optical frequency standard based on an optical nuclear transition. By doping a transparent crystal with the desired nucleus, a high-density sample can be prepared allowing simultaneously good signal-to-noise ratio and narrow linewidth. In this scheme, the complex vacuum and laser cooling apparatus of current clocks could be replaced by a single, room-temperature crystal. It is anticipated that in FY12, the investigator will grow the thorium-doped crystal and perform spectroscopy to determine the clock transition.

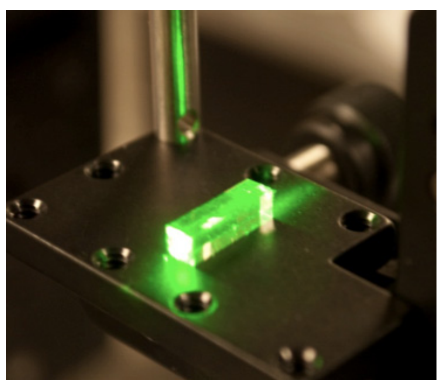

FIGURE 13

Prototype solid-state clock. The investigator is aiming to crystallize a thorium-doped crystal similar to the solid-state analog shown in the image.

B. Quantum Illumination-Based Target Detection and Discrimination

Professor Jeffrey Shapiro, MIT, Single Investigator Award

The objective of this project is to explore, experimentally and theoretically, the role of quantum entanglement as a resource to improve the performance of sensing and measurement systems beyond their classical counterparts in noisy environments. In particular, the project is focusing the theoretical and experimental investigation of applying the concept of quantum illumination (QI) to realizing enhanced performance in target detection and discrimination. The main thrust of this research in FY11 has been to perform theoretical work on QI for improved target detection and spatial resolution to enable target discrimination (see FIGURE 14). The supporting theoretical work to set up the experiment has been performed.

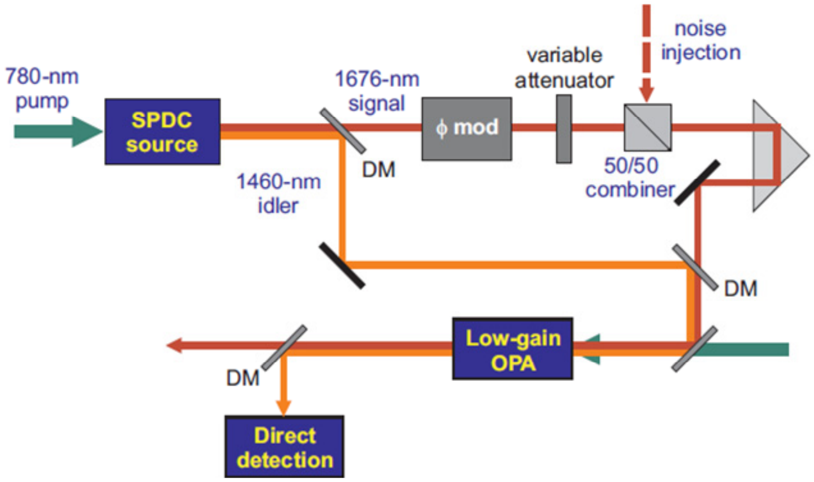

FIGURE 14

Experimental setup for QI-based target detection under high-loss and high-noise conditions. SPDC, spontaneous parametric downconversion; DM, dichroic mirror; OPA, optical parametric amplifier.

The initial theoretical demonstration that quantum illumination could provide improved performance in target detection relied on a probability-of-error performance metric in which target absence and target presence were equally likely hypotheses. Radar target detection seldom, if ever, confronts target detection with equal likelihood of target absence or presence. Instead, the Neyman-Pearson criterion is employed, wherein the probability of detection is maximized subject to a constraint on the false-alarm probability. The advantage of using the minimum error-probability criterion—insofar as quantum illumination performance analysis is concerned—is the availability of the quantum Chernoff bound to circumvent the formidable difficulty of evaluating the eigen values of a high-dimensional mixed-state quantum system. In classical detection theory, there are Chernoff-bound formulas that can be applied for target detection. No such bounds are available in the literature for quantum detection and recent work on this project makes it clear that such bounds may not be obtainable. To demonstrate the QI performance advantage, the optical parametric amplifier (OPA) receiver for quantum illumination is compared with that of the homodyne receiver for coherent-state illumination. The investigator found that the QI advantage is retained over the entire receiver operating characteristic (ROC) range examined in this study (see FIGURE 15).

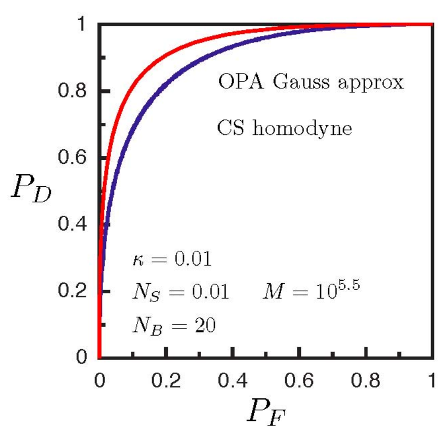

FIGURE 15

QI advantage is retained over the entire receiver operating characteristic (ROC) range. The plot compares the receiver operating characteristic comparison between OPA reception of a quantum-illumination source and homodyne reception of coherent-state illumination. P_D is the probability of detection and P_F is the false alarm probability

In FY12, it is anticipated that the research team will investigate potential measurement fidelity gains in the tunable coupling qubit. The tunable coupling qubit is key to many of the proposed research goals and has the potential for a new method of quantum non-demolition readout. 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 and will be explored in the coming year. In addition, the tunable coupling qubit can serve not only as a qubit but also as a control element in more complex quantum circuits. In particular it 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 tunable coupling qubit can also work to control photon-photon interactions, allowing a new control knob in quantum simulation work.

In optical quantum dots, the main focus in FY12 will be to optically initialize the spin of a charged quantum dot inside a photonic crystal cavity. This would be the first demonstration of a stationary qubit (memory) node coupled to a photon (flying qubit) via an optical interface. To achieve this goal, methods for selective quantum dot charging and mapping of the photon state to the quantum dot state already being developed will be pursued further. Investigation of the phonon-mediated off-resonant dot-cavity coupling will be pursued. This effect could be potentially used to overcome issues resulting from inhomogeneous broadening of quantum dots when attempting to entangle two quantum dots.

In the area of quantum illumination, another line of theoretical inquiry aimed at addressing the need for interferometric phase stability in quantum illumination reception will be started. Here a two-OPA receiver operated in quadrature will be studied and its performance compared with a conventional incoherent second-detection heterodyne receiver for coherent-state light. If quantum illumination can provide a performance advantage in such random phase scenarios, it will broaden the range of its applicability. The first experimental results that test some of the theoretical predictions are expected to be completed in FY12.

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