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UNIVERSITY RESEARCH

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Sandia National Laboratories

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Abstract

Sandia National Laboratories has traditionally contracted for university research to expand its science and technology base to assure the performance of its nuclear weapons. Sandia and its strategic university partners are seizing the opportunity to establish enduring relationships that produce world-class joint R&D, educate next generation employees, provide Sandians with continuous learning opportunities, and build national visibility and name recognition. Sandia's university research investments are made, for the most part, by individual technical programs. The University Research Office serves as the point of contact for all university research issues and creates and implements those processes and tools that enable university partnerships. The office also manages several university-related programs (Campus Executive Program, Sandia University Research Program, and the Presidential Early Career Award for Scientists and Engineers), through which investments are made in students and faculty via contract research and graduate research fellowships. In addition, the University Research Office, in partnership with Human Resources, oversees a distinguished postdoctoral program entitled the President Harry S. Truman Fellowship in National Security Science and Engineering (Truman Fellowship Program) and exploratory programs that explore niche technical areas of interest and forge new strategic relationships in critical skills areas. The FY2006 University Research Annual Report details the projects supported by Sandia in these university-related partnerships programs.

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An Overview of Sandia National Laboratories' University Research Investments

Marie L. Garcia

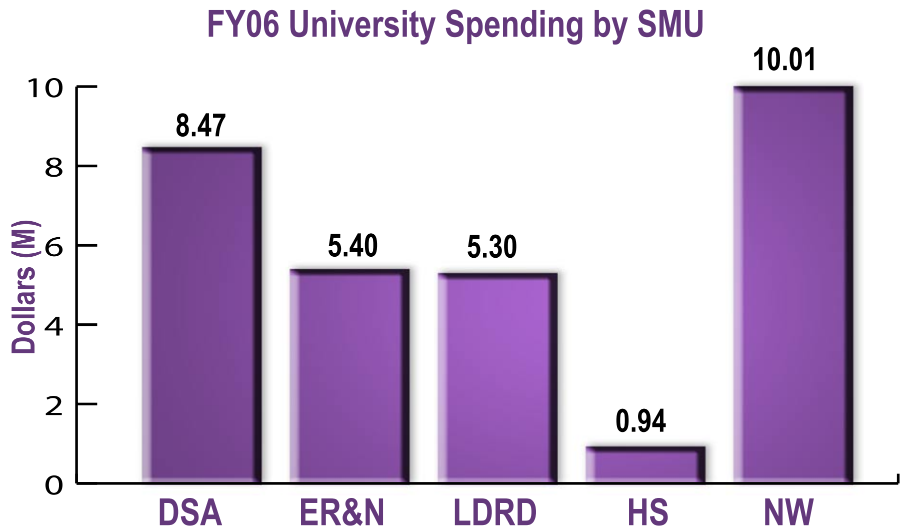

Figure 1. Sandia investments in university research in FY06, by Strategic Business Units[3]

Prior to the 1940s[1] , most of the best basic, or fundamental, scientific research was performed in European universities, and much of the best practical, or applied, technological research was performed in corporate laboratories. During World War II, the U.S. government began to provide significant funds for university research spanning the fundamental-to-applied spectrum, and after the war, Vannevar Bush, science advisor to Presidents Franklin D. Roosevelt and Harry S. Truman, urged that the government should continue investing in university research. In November 1944, President Roosevelt asked Bush, "What can the Government do now and in the future to aid research activities by public and private organizations? Bush replied, "We must strengthen the centers of basic research which are principally the colleges, universities, and research institutes. These institutions provide the environment which is most conducive to the creation of new scientific knowledge and least under pressure for immediate, tangible results." The outcome of the President's request and Bush's response became the seminal study, *Science: The Endless Frontier*, issued by the Executive Office of Scientific Research and Development in 1945, and the establishment of the National Science Foundation in 1950.

Not until the Soviet Union launched the first Earth-orbiting satellite, Sputnik, in 1957 did the level of federal funding for university research begin to approach Bush's intentions. From 1960 to 1966, driven largely by the space program, federal non-defense research spending grew from approximately $6 billion to nearly $35 billion a year, a sizeable portion of which was spent on university research. Since peaking in 1966, federal funding for non-defense research has never dropped below $20 billion annually, while substantially declining as a percentage of overall federal funding.[2]

The nation's investment in science has been in crisis for some time, especially in the physical and engineering sciences. Federal support has declined significantly and R&D investment from industry has not filled the gap, perhaps because industry views such investments as strongly slanted toward development, when application is a closer match to their shareholder-driven requirements. In addition to leading to a weakened technology base for both U.S. industry and the national defense enterprise, these declines in support set the stage for future challenges in attracting the scientific research talent we need in this critical area.

Our nation's business and academic leaders came together in 2005 to issue a series of reports that convincingly document the threats to continued U.S. economic primacy and, more important, offer an action agenda to address the many global challenges facing our country today. In particular, the National Academies released a report, "Rising Above the Gathering Storm" which reinforces an urgent message: If trends in U.S. research and education continue, our nation will squander its economic leadership, and the result will be a lower standard of living for the American people.

Many other countries are pouring money into building their science and technology enterprises. In fact, many of these countries are emulating our innovation model-leveraging investment in science and technology to create market leadership—with remarkable success. America's leaders and its citizens have traditionally pursued policies that encouraged innovation by funding federal investment in basic research, improving education at all levels, allowing the U.S. to attract the best and the brightest from around the world. Today, we must following those footsteps and take the actions necessary to keep the U.S. at the forefront of an increasingly competitive global economy. Partnerships with universities, industry, and other national laboratories are essential to address this issue.

[1]Historical data in the succeeding two paragraphs from "Working Together, Creating Knowledge." 2001. The University-Industry Research Collaboration Initiative. American Council on Education. Washington. p. 19.
[2]Figures are in constant FY98 dollars.
[3]Defense Systems & Assessments (DSA), Energy, Resources & Nonproliferation (ER&N), Laboratory Directed Research and Development (LDRD), Homeland Security (HS), Nuclear Weapons (NW)

For over fifty years, Sandia National Laboratories (Sandia) has focused on being the laboratory that the U.S. turns to first for technology solutions to the most challenging problems that threaten peace and freedom for the nation and the globe. University partnerships have been and will continue to be a critical element in achieving this goal. Sandia has traditionally contracted for university research to expand its science and technology base to assure the performance of its nuclear weapons.

Sandia and its strategic university partners are seizing the opportunity to establish deeper, enduring relationships that produce world-class joint R&D, educate next generation employees, provide Sandians with continuous learning opportunities, and build national visibility and name recognition. In FY2006, Sandia invested approximately $30.3 million in 523 joint research projects with 105 universities (Figure 1) in five mission-related areas. Sandia invests additional monies for graduate student support, tuition assistance for employees, and university and K-12 science outreach. The strategic partnerships of the future will be additionally be directed towards those joint activities that will help ensure national competitiveness in the twenty-first century.

In response to the President's American Competitive Initiative, Sandia National Laboratories hosted a Summit on Accelerating Engineering Innovation in Albuquerque, NM (May 31 - June 2, 2006) to explore the opportunities for jumpstarting a national response to the this Initiative. The Summit brought together leaders from industry, academia, government, and the national laboratories to examine today's innovation dilemma and consider new approaches for the future. As a result of this workshop, Sandia's university and industry partners began working to develop the concept for Discovery Science and Engineering Innovation Institutes (DSEII). The prototype DSEII is the National Institute for Nano Engineering (NINE).

Sandia's university research investments are made, for the most part, by individual technical programs. The University Research Office serves as the point of contact for all university research issues and creates and implements those processes and tools that enable university partnerships. The office also manages several university-related programs (Campus Executive Program, Sandia University Research Program, and the Presidential Early Career Award for Scientists and Engineers) through which investments are made in students and faculty via contract research and graduate research fellowships.

The University Research Office explores new tools, processes, and programs in an attempt to better enable university partnerships. In FY2006, a distinguished postdoctoral program entitled the President Harry S. Truman Fellowship in National Security Science and Engineering (Truman Fellowship Program) entered its third year. This new program provides an opportunity each year for exceptional scholars to join Sandia in the continuation of Sandia's tradition of excellence. Two new Truman Fellows joined Sandia in late 2006. They came from the University of Colorado at Boulder and Oxford University. They joined four other Truman Fellows in conducting cutting-edge research.

To assist Sandia in meeting its mission-related needs, the University Research Office also supports interactions with some universities that do not have official "key" or "regional" status. Such interactions, called "Exploratory Programs," explore niche technical areas of interest and forge new strategic relationships in critical skills areas. Currently, Sandia has exploratory programs at Harvey Mudd College and with the University of Texas System. These programs are evaluated regularly to determine their contribution toward achievement of Sandia's mission objectives.

Investments in university research continue to pay off handsomely for Sandia and for U.S. taxpayers. This University Research Annual Report showcases the excellent results of these investments. Our joint accomplishments can be measured by the number of journal articles published, patents and copyrights issued, and new employees hired. New collaborations include the U.S. Council for Automotive Research, the Office of Naval Research, the U.S. Bureau of Reclamation, and the Paso del Norte Watershed Council. Over the years, the projects have generated follow-on work with Department of Defense programs, including the U.S. Army, the Air Force Office of Scientific Research (AFOSR), Defense Experimental Program to Stimulate Competitive Research (DEPSCoR), Defense University Research Instrumentation Program (DURIP), and Defense Advanced Research Projects Agency (DARPA). Other continuing work has been funded by the National Science Foundation (NSF), the Science and Technology Center for Sustainability of semi-Arid Hydrology and Riparian Areas (SAHRA), and the NSF Center of Research Excellence for Bioinformatics and Computational Biology. The U.S. Department of Agriculture and the National Aeronautics and Space Administration (NASA) have funded research, as have DOE's Office of Science, the National Energy Technology Laboratory, Los Alamos National Laboratory, and Strathclyde University (Scotland). The U.S. Army Corps of Engineers, Lockheed Martin Shared Vision Program, National Institute of Mental Health, Institute of Space Nuclear Power, and the New Mexico Water Resources Research Institute have also funded additional research.

As a national laboratory, Sandia is proud to continue on the path established by Vannevar Bush when he asserted that the federal government should facilitate science and technology by funding researchers in the nation's universities and national laboratories, and by supporting the training of the next generation of scientists.

CAMPUS EXECUTIVE PROGRAM

Sandia's Campus Executive Program helps create strategic relationships with select universities to further our research programs, help recruit the very best technical and administrative talent, support science and engineering education, and continue the development of the nation's science and engineering infrastructure. The program increases Sandia's visibility as a national laboratory with our industrial, academic, and political constituencies.

Since 1977, the Campus Executive program has paired Sandia executives with top university officials at schools that share synergistic research interests and capabilities with Sandia. The Sandia Campus Executives are developing strategic relationships in focused research. They choose Sandia's investments by providing financial support to either research contracts or graduate research fellowships. Those investment decisions are based on making the best choices for the Labs' current and future needs in direct research, employee development, and collaborative partnerships with the universities.

The typical Campus Executive relationship includes conducting a full inventory of existing relationships between Sandia and a university. This includes research collaborations, recruiting efforts, special initiatives, alumni (both Sandians who graduated from the school as well as former Sandians working at the school), intern and co-op students, and graduate fellows. An action plan is developed with input from the school, which includes a shared vision, long-term goals, and short-term objectives. The Sandia vice presidents and other executives who serve as Campus Executives continually build relationships with their assigned universities, visiting the schools' campuses, and inviting deans and faculty members to the Labs.

Each Campus Executive has a small amount of Laboratory Directed Research and Development (LDRD) funding earmarked for investments in either graduate research fellowships or contract research at their university. Based on the plan developed for each university, the Campus Executive determines the appropriate investment of that money. At some schools, the Campus Executive, working with the deans of engineering or arts and sciences, may employ the strategy of establishing graduate research fellowships for doctoral students doing research in areas in which the Labs has an interest. In these instances, the student and a Sandia Principal Investigator are matched to identify a research project and conduct the research. In many cases, the Sandia Principal Investigator or the Campus Executive becomes a member of the student's doctoral committee. With the Sandian on the doctoral committee, the Labs not only builds relationships with other professors but also is able to offer direct input in the research direction. The desired result of these fellowships is to develop a long-term relationship with students that show promise of becoming future Sandia employees, educated and trained in areas of importance to Sandia. At other universities, the Campus Executive elects to invest his/her money in a research project as a means to "seed" an area that looks promising, with the strategy of Sandia and the university eventually collaborating for third-party funding.

For 2006, the following were the Campus Executive/University assignments.

University	Campus Executive
Arizona State University	
California Institute of Technology	Gerry Yonas
Carnegie Mellon University	Steve Roehrig
Cornell University	Gerry Yonas
Georgia Institute of Technology	Jill Hruby
Massachusetts Institute of Technology	Julia Phillips
New Mexico Institute of Mining and Technology	Joan Woodard
New Mexico State University	Jerry Langheim
Purdue University	Joe Polito
Stanford University	Joan Woodard
Texas A&M University	Les Shepherd
University of Arizona	Peter Davies
University of California at Berkeley	Mim John
University of California at Davis	Mim John
University of Colorado at Boulder	Frank Figueroa
University of Florida	Tom Hunter
University of Illinois at Urbana	Dave Carlson
University of Michigan	Rick Stulen
University of New Mexico	Rick Stulen
University of Texas at Austin	Jerry McDowell
University of Texas at El Paso	Gil Herrera
University of Utah	
University of Wisconsin at Madison	John Stichman
Washington State University	

Kinetics and Mechanisms of Nanowire Synthesis

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Arizona State University

Julia Hsu (Org. 1114)
Sandia Principal Investigator

Project Purpose

This project seeks to develop a mechanistic understanding of the heteroepitaxial growth of semiconducting nanowires and nanowire arrays for potential applications in nanoscale electronic, photonic, and sensor devices. Our studies focus on systematically investigating and understanding nanowire growth kinetics of epitaxial silicon and germanium nanowires by ultrahigh vacuum (UHV) chemical vapor deposition (CVD) using the vapor-liquid-solid (VLS) growth technique, such that we can controllably grow specific nanowire heterostructures.

These investigations show that in situ real-time monitoring of nanowire nucleation and growth is essential to understanding nanowire growth kinetics, and as such, we developed an observation method using optical reflectometry to measure nanowire growth in real time. In this technique, treating the growing nanowire layer as an effective dielectric layer and correlating scanning electron microscopy measurements and optical reflection modeling, we show that the technique has surprisingly good sensitivity in observing quantitatively the onset of nanowire growth, the nanowire growth rate, and the average length of the nanowires.

This technique is expected to allow us to accurately control, in situ, the fabrication of nanowire heterostructures. By manipulating the inherent strains within specific Si/Ge heterostructures, we can controllably tune the band structure properties of the nanowires. With Arizona State University, we focus on the key issues, such as the nucleation and growth of the nanowires, the spatially specific location of nanowires into lithographically defined arrays, the factors affecting the synthesis of sharp epitaxial nanowire heterointerfaces, and the resulting strain in these novel structures.

Accomplishments

We continued investigations into the nucleation and growth kinetics of Si and Ge nanowires and Si/Ge heterostructures on Si(111). These studies focus on understanding the fundamental mechanisms of vapor-liquid-solid synthesis of Group IV semiconducting nanowires and exploiting this understanding for the synthesis of novel Si/Ge nanowire heterostructures with new materials properties. We are conducting the research in a specially designed UHV CVD system at Arizona State University. We developed an optical reflectometry technique for in situ monitoring during VLS nanowire growth, and demonstrated Si/Ge nanowire growth for both linear and core-shell heterostructures. The CVD system has the unique capabilities of in situ metal deposition for the formation of Au catalytic seeds on atomically clean surfaces, and has been extended to provide for millitorr regime growth with up to four precursors (silane, germane, disilane, and digermane) simultaneously.

Our project accomplishments include:

- Developing two new tools for understanding and characterizing nanowire growth: a) first in situ optical reflectometry growth monitoring (using a 635 nm laser) of nanowire growth revealing the presence of an incubation time for nanowire growth, and b) first strain mapping approach for nanowires demonstrating good agreement between experiment and theory for our Si/Ge core shell nanowire heterostructures.
- Using the in situ tools to initiate synthesis studies for axial Si/Ge nanowire heterojunctions, specifically investigating silane and germane in addition to our original disilane and digermane gases; energetic differences in such gases enable specific nanowire heterostructures to be grown. This effort is currently underway. Preliminary evidence for a growth method to obtain atomically sharp interfaces by thermal cycling of the Au eutectic between liquid and solid states has been revealed.
- Using finite element modeling of the strain in Si/Ge heterostructures along with deformation potential modeling of the resulting band-structure, we developed scaling predictions for core/shell nanowire strain-engineered bandgap tuning for Si and Ge for the first time.

Our results indicate that for [111] oriented Si/Ge core-shell nanowire heterostructures it will be possible to “tune” the bandgap of Ge cores or shells by up to a factor of two through the ratio of core-to-shell thicknesses. This unprecedented level of bandgap modification results from the unusually large strains possible in nanowire heterostructures and the fact that the conduction band minimum for Ge is determined by the L direction, which is particularly sensitive to strain along the [111] direction. In contrast, the Si bandgap is only modified by a few 10s of meV. This contrast points to the importance of controlling the nanowire orientation in conjunction with nanowire heterostructure design. The tuning of the bandgap opens the door to increased bandstructure control and novel electronic properties, such as one-dimensional hole gas structures. In addition, we initiated a collaboration to grow nanowire arrays using Au seeds patterned by electron beam lithographically. This approach is the first step to exploiting heterostructure designs to fabricate advanced nanodevices.

Significance

A key research and development accomplishment of this project is the determination that the electronic band structure of semiconducting nanowires can be tuned over a significant range of properties. Large modifications in the electronic band structure can be achieved through the growth of nanowire core-shell and axial heterostructures using conventional electronic materials such as silicon and germanium. The changes in bandstructure are predicted to make possible electronic and optoelectronic properties not previously attainable. These modifications in electronic properties are due to the large strains that can be incorporated without the introduction of strain-relieving defects, something that cannot be achieved in normal semiconductor processing such as conventional CVD or MBE layered growth.

While additional work is needed to clearly demonstrate the various aspects of this important result, it is apparent that new electronic properties will be achievable in nanowire electronics. Potential implications and future applications of this result include room temperature resonant tunneling diodes made from Si/Ge, nanowire logic circuits at ultrasmall dimensions, ultrasensitive chemical sensor arrays, and high-performance thermoelectric devices. Such advances would have beneficial impact on national security and energy utilization missions.

Refereed Communications

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A. Egatz-Gomez, S. Melle, A.A. Garcia, S.A. Lindsay, M. Marquez, P. Dominguez-Garcia, M.A. Rubio, S.T. Picraux, J.L. Taraci, T. Clement, D. Yang, M.A. Hayes, and D. Gust, "Discrete Magnetic Microfluidics," *Applied Physics Letters,* vol. 89, pp. 34106-1-3, July 2006.

T. Clement, S. Ingole, S. Ketharanathan, J. Drucker, and S.T. Picraux, "In Situ Study of Semiconductor Nanowire Growth Using Optical Reflectometry," to be published in *Applied Physics Letters*.

Other Communications

J.L. Taraci, M.J. Hÿtch, T. Clement, A. Batwal, D.J. Smith, P. Peralta, M.R. McCartney, J. Drucker, and S.T. Picraux, "Strain Mapping in Si-Ge Nanowire Heterostructures," presented at the American Physical Society Four Corners Meeting, Boulder, CO, October 2005.

T. Clement, J.L. Taraci, J. Drucker, and S.T. Picraux, "Growth of Si/Ge Strained Heterostructures using In Situ Optical Reflectometry," presented at the Spring Materials Research Society Meeting, San Francisco, CA, April 2006.

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S.T. Picraux, A. Batwal, P. Peralta, J.L. Taraci, M.J. Hÿtch, T. Clement, D.J. Smith, M.R. McCartney, and J. Drucker, "Strain Mapping in Semiconductor Nanowires," presented at the 7th MEMS and Nanotechnology Symposium, 2006 SEM Annual Conference, St. Louis, MO, June 2006.

T. Clement, J.L. Taraci, A. Batwal, P. Peralta, J. Drucker, and S.T. Picraux, "Nanowire Bandgap Engineering through Highly Strained Si/Ge Heterostructures," presented at the TMS Electronic Materials Conference, EMC2006, State College, PA, June 2006.

Neural Correlates of Attention and Intention in Decision-Making of Macaques and Humans

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Project Purpose

During decision-making, there are three serial processing steps:

- an initial perceptual representation of the stimuli
- a subsequent association of this perceptual representation with motivation and reward expectancy
- a final central representation of an organism's dispositions and preparations to behave towards the stimuli.

An important aspect of decision-making is the prior allocation of attention and intention before an action is performed. Decision-making is a spatiotemporal process, requiring spatial elements of sensory information and motor planning as well as temporal elements of reward expectancy and learning (error correction).

Prior research in the Andersen lab (Caltech) and elsewhere has shown that posterior parietal cortex is necessary for such sensorimotor integration, representing target locations, intended actions, and even reward-related signals. A recent technique of selective, reversible lesioning in primate cortex using muscimol (GABAa agonist) will help elucidate the influence of various functional areas within the intraparietal sulcus during electrophysiological recording, with particular emphasis on parietal reach region (an area encompassing macaque area 5 and Medial IntraParietal area) and lateral intraparietal area.

The technique of transcranial magnetic stimulation will be employed for equivalent experiments in humans, with brain activity recorded using functional magnetic resonance imaging. An extensively used stimulus of cued target locations with asynchronous onsets, variable delay periods, and reward schedules will be adapted in initial experiments to probe attention and intention during sensorimotor integration. This work is in collaboration with Caltech.

Process Science and Engineering for Thermomechanical Nanomanufacturing

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Sandia Principal Investigator

Project Purpose

Embossing and molding are simple techniques for molecular-scale replication. Recent studies have shown replication of single-walled carbon nanotubes with diameter 2 nm via molding and crack tips of size 0.4 nm via casting. Nanoimprint lithography (NIL) offers scalable embossing or molding of sub-10 nm features over large areas. In the nanoimprint embossing process, a nanopatterned mold is heated and pressed into a thermoplastic polymer film, replicating a negative relief of the mold in the polymer sample. Often, the replicated features are close in size to the polymer radius of gyration (R_g). Atomic force microscope (AFM) nanoindentation is one type of nanoembossing process whereby a sharp conical tip forms indents into a thin polymer layer. As film thickness and feature sizes shrink to 20 nm in AFM nanoindentation, polymer thermomechanical behavior may deviate from that of bulk.

Reliable design of molecular-scale molding processes will require a deep understanding of fundamental polymer mechanics occurring at the nanometer level. This work presents continuum GOMA simulations that model polymer flow during AFM nanoindentation where an atomically sharp tip of specified radius of curvature indents thin films of high molecular weight (MW) polymer. The simulations identify bulk polymer thermomechanical properties that govern nanometer-scale polymer transport in isothermal and nonisothermal AFM nanoindentation. This work is being performed in collaboration with the Georgia Institute of Technology.

Accomplishments

Simulations predict isothermal polymer flow in 35 nm 350k MW polymethylmethacrylate (PMMA) film atop a silicon substrate due to constant velocity indentation of a silicon AFM tip of radius 20 nm. Simulations of AFM nanoindentation into the Carreau Williams-Landel-Ferry polymer produce both local and nonlocal deformation, dependent on shear rate and temperature. For indents at a given temperature, deeper penetration depths result in higher polymer shear rates. Polymer shear rates resulting from constant velocity indentation remain nearly constant as temperature changes, but the localized viscosities move from the Rouse viscosity transition region at low T to the power law rubbery regime at higher T. Force-distance curves from simulation well match reported experimental force-distance curves of polydisperse PMMA over a range of temperatures.

The modified continuum simulations accurately predict subcontinuum polymer mechanical deformation due to an AFM tip of radius ~ R_g indenting a polymer film from initial thickness above the polymer molecular diameter 2 R_g to below the unperturbed R_g. The agreement of simulation force-distance curves and indentation slope to measurements reported in literature suggests that material deformation for high MW polymer films during isothermal AFM nanoindentation closely follows shear-thinning bulk material behavior with a full-slip polymer-tip interface. The continuum simulations allow for optimization of AFM nanoindentation processes based on bulk viscoelastic material properties and extend continuum descriptions of polymer mechanics to length scales below R_g.

The continuum material model developed for isothermal AFM nanoindentation also investigated polymer deformation and heat transfer during nonisothermal AFM thermomechanical data bit formation. The simulations show highly localized deformation in the temperature dependent shear-thinning polymer. The tip locally heats the polymer, creating a temperature gradient spanning from the specified tip temperature to room temperature over radial distance ~ 50 nm from the polymer-tip interface. The resulting temperature dependent complex viscosity ranges orders of magnitude over the same radial distance. The steep spatial gradient of the temperature shift factor results in highly localized polymer deformation resembling lubrication, with only the most mobile polymer layer at highest temperatures deforming. Applied load only slightly affects the rate of indentation as the temperature-dependent viscosity dominates the nanoindentation process. The simulations well match measurements of nonisothermal AFM indentation into 600k MW PMMA at cantilever heater temperature 380 °C. The simulations suggest Tint ~ 240 °C predicts measured material response and 25 °C increments in Tint significantly impact timescale of indentation.

Simulations of nonisothermal AFM nanoindentation with material properties based on bulk polymer physics model experimental measurements and explain high-cantilever heater temperatures required for indentation formation due to localized polymer deformation. The simulations present a modeling tool to further compare with experiment to inform subcontinuum heat transfer models of polymer-tip interface temperature and characterize the bit writing process.

Significance

This work is synergetic with several mission-critical areas within Sandia's science and technology community. First are the advances in nanotechnology research and second, the advances in simulation technology. Nanoembossing using an AFM tip is already revolutionizing the field of lithography. The ability to understand the material response based on continuum-based simulations will enable us to engineer materials that would have required experiments that are expensive to perform.

Refereed Communications

H.D. Rowland, W.P. King, A.C. Sun, and P.R. Schunk, "Simulations for Process Design of Nanoembossing and Atomic Force Microscope Thermomechanical Nanoindentation," in *Proceedings of the 2005 MRS Fall Meeting*, p. 200, November 2005.

File System Performance Optimization for Supercomputing Applications

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Georgia Institute of Technology

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Sandia Principal Investigator

Project Purpose

Scalability demands on the file systems of future supercomputers are giving rise to new system-level technologies. The purpose of this work with the Georgia Institute of Technology is to explore and experiment with ways in which applications interface to and make use of future scalable file systems, in particular addressing quality of service guarantees. Specifically, in many scientific and engineering applications, there is a collection of sinks; each with differing needs for the same data provided by some source (e.g., the file system). Often, different sinks need different portions of the data, or they need slightly transformed data versions. Traditionally the work to adjust data has either been done on the server (e.g., storing multiple versions of the same file) or at the sinks. The result is an increased level of data replication, and/or increased loads on recipients' CPU (central processing unit) resources, and/or increased demands on the aggregate network resources required for data transport.

Our approach is to create richer interfaces between applications and data sources like the file system. The purpose is to: 1) enrich data sources with application-specific functionality that manages the data being streamed out on behalf of individual clients, and 2) take advantage of nodes "in between" the source and the sinks to perform processing and data movement actions that benefit sinks and reduce bottlenecks from resource contention.

Essentially, by automatically decomposing the transformations and generating code according to the CPU resources and network bandwidth available along the network overlay connecting sources and sinks, including the sources, sinks, and even intermediate nodes, we can combine identical operations and reduce composite CPU loads yielding overall improvements in the quality of service experienced by applications. It also affords us the opportunity to investigate other operations, such as siphoning off portions of the written or read data for immediate analysis or additional, off-line processing.

Accomplishments

- Studied extensively various existing file systems and data transformation services to develop a better understanding of existing work in both of these areas.
- Developed a prototype integration of the data transformation engine with the lightweight file systems tools.
- Studied the data storage usage and file formats of typical high-performance computing applications to gain an understanding of current requirements and potential future needs for data transformation services.
- Deployed the lightweight file systems tools from Sandia into a Georgia Tech computing cluster and began educating others within the Georgia Tech community on the philosophy and use of the tools for use in their own storage-related research.
- Learned about additional high-performance computing applications that may be accessed for testing new techniques and applications of this technology.

Significance

More in-depth knowledge of various existing high-performance file systems, the Sandia lightweight file systems tools, and various high-performance computing applications affords the opportunity to focus research efforts to better suit the needs of Sandia applications. The prototype system, once complete, will ultimately lead to applications enabling more efficient use of resources. The techniques, in general, can lead to applications becoming more streamlined and focused on the task at hand and much less concerned with coding of data manipulation tasks. Some offline data processing can be done automatically as part of the storage operation with only a description of the required transformation, accelerating the time from an application run completing and the data being in a usable form.

Reliable and Secure Communication in Wireless Sensor Networks

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Sandia Principal Investigator

Project Purpose

This research addresses the general problem of how to efficiently coordinate multiple inputs to a single-source computational unit. This general problem is more complex in sensor networks where reduced bandwidth and increased efficiency in the network are critical to the successful performance of the system. We consider the optimal compression achievable in sensor networks where these resource constraints hamper the overall design of the sensor network coordination process.

There are two main avenues of compression. First, one can exploit the correlation between the data collected at the various nodes. Second, one can exploit the relative simplicity of the function to be computed at the receiver side. Slepian and Wolf made precise the exploitation of the correlation in the data. However, contemporary distributed data-compression schemes fail to account for the receiver-side goal, often the computation of a simple function of the data received. This research will address this problem to make precise the exploitation of the function and implement such a compression scheme.

This compression scheme will probably introduce a small probability of error. We seek to better understand of this probability of error in order to ensure it will always be "small." This will involve more extensive simulations of the scheme with more varied functions and more than two sources.

Understanding the types of functions that give better compression is a primary component of this research. Certainly, a one-to-one function gives no coding gain and the scheme is not worth implementing under these conditions. But, between such a function and a unary function, there is quite a bit of variability. We will develop a means to classify functions as simple enough or not simple enough to use this scheme approach.

This work will be performed in collaboration with the Massachusetts Institute of Technology.

Accomplishments

We concentrated on narrowing the focus of this research and began to design and develop the methodology for how the data compression will be accomplished.

Algorithm design is based on the following steps:
1. Based on the knowledge of the given function, use graphs to distinguish amongst the function values.
2. Given a function and the statistics of a set of sources, construct a graph for each source that carries all the information relevant to distributed encoding. Each vertex for the graphs would identify with a particular source word. The compression then comes from the idea of coloring the vertices of the graph. The graph is constructed in such a way that the colors are sufficient statistics of the sources.

The two-part scheme, using two binary functions, was simulated using vehicle-tracking data. The results showed coding gains of twenty percent or more over contemporary methods when using a simple greedy coloring algorithm (with probability of error less than 0.1 percent).

Significance

There are two key accomplishments for this initial year of research starting with the scoping of the problem space to deal with distributed data compression. The initial problem statement for this research broadly covered numerous communication issues from the distributed sensor networks field. By narrowing the focus, we began to address a major difficulty associated with the resource limitations of these distributed sensor networks. The initial development of methodology to explore how to share large amounts of data across limited bandwidths is the second key accomplishment of this research. The eventual results of this research will benefit researchers focusing on multiple-input-single-output systems, where data needs to be compressed in a distributed manner.

Within the Sandia mission space, this research is applicable to the many distributed systems used to address security of nuclear weapons, borders, and simulations that deal with vast data repositories.

Catalyst Development and Microreformers for Fuel Processing

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Sandia Principal Investigator

Project Purpose

The purpose of this project with the New Mexico Institute of Mining and Technology is to develop new supported catalysts for high-efficiency liquid-phase conversion of carbohydrates to hydrogen.

Production of hydrogen (H_2) from biomass and organic wastes is considered an effective approach to mitigating the environmental problems caused by pollutant emissions from fossil fuel combustion and allaying our dependence on the limited oil reserves. However, current technological inefficiencies render such biomass utilization economically unviable. A promising alternative to realizing the goal of hydrogen from renewable sources is to convert biomass-derived carbohydrates to H_2. Recently, γ-Al_2O_3 supported platinum (Pt/γ-Al_2O_3) catalysts have been successfully demonstrated for the liquid phase reforming of various carbohydrates into hydrogen at temperatures below 300 °C. However, the throughput of the catalytic conversion is low and the cost of the catalyst is high because of the high load of Pt metal, typically in a range of 3 to 5 wt.%. To make the process economically attractive, catalysts with higher performance and low cost need to be developed.

The main objective of this research is to develop new Pt/NaY zeolite catalysts for high-efficiency liquid (water)-phase conversion of biomass-derived carbohydrates to H_2. The specific tasks of this research include:

- Designing and establishing a packed-bed reactor system for high-pressure liquid-phase reaction
- Synthesizing and characterizing Pt/NaY and Pt/γ-alumina catalysts.
- Selecting catalysts for catalytic performance evaluation.
- Evaluating catalytic performance and stability
- Testing the selected Pt/NaY catalyst for conversion of both ethanol and glucose in liquid phases.

Accomplishments

We synthesized, characterized, and evaluated particulate platinum-loaded Y-type zeolite (Pt/NaY) catalysts for H_2 production from methanol. The catalysts were also tested for liquid-phase reforming of ethanol and glucose to hydrogen. Our accomplishments include:

- We designed and established a packed-bed reactor system for high-pressure liquid-phase reaction. The reactor system was tested by using a similar catalyst (i.e., Pt/γ-alumina) to that reported in the literature.
- We synthesized and characterized Pt/NaY and Pt/γ-alumina catalysts. Synthesis procedures were developed and optimized for both Pt/NaY and Pt/γ-alumina catalysts. X-ray diffraction (XRD) was used to confirm the structure of both catalysts. Microprobe analysis was employed to determine the composition of both catalysts. Scanning transmission electron microscope (STEM) was used to determine the Pt cluster size in the Pt/γ-alumina catalyst. Scanning electron microscope (SEM) was used to determine the size

and morphology of the catalyst particles. Brunauer-Emmett-Teller (BET) N_2 adsorption and desorption was used to measure the catalyst surface areas. Carbon monoxide chemisorption was measured to determine the Pt dispersion.
- We selected catalysts for catalytic performance evaluation. Catalysts were selected based on methanol conversion for Pt/γ-alumina and Pt/NaY catalysts with different Pt load levels. The reaction tests were conducted at elevated temperature.
- We evaluated catalytic performance and stability of the selected catalysts for extended periods of operation time (total continuous reaction time over two hundred hours).
- We tested the selected Pt/NaY catalyst for conversion of both ethanol and glucose in liquid phases.

Significance

We have developed several methods for preparing nanoplatinum-supported catalysts showing good catalytic activity. The catalytic performance of the Pt/NaY catalysts has been compared with that of the Pt/γ-Al_2O_3 catalysts reported in the literature as well as those synthesized in this work. The Pt/NaY catalyst with a Pt load of 0.5 wt.% was found to outperform the Pt/γ-Al_2O_3 catalysts with a Pt load of about 3 wt.% for conversion of methanol to H_2. The Pt/NaY catalyst was demonstrated to be active for ethanol reforming in liquid phase, but incapable of catalyzing glucose because the ringed glucose molecules are too large to effectively transport into the zeolite pores (~ 0.7 nm diameter), where the Pt metal clusters locate. Our research results indicate that the transition metal loaded Y-type zeolite catalysts have great potential for use in catalytic reforming of carbohydrates to H_2.

Catalytic Membrane Development for Microscale Glucose Reforming

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Project Purpose

Glucose and ethanol have emerged as the best candidates for biomass derived hydrocarbon processing for hydrogen. Glucose is a major component of biomass; the fermentation of sugars such as glucose produces ethanol, which can then be easily reformed. A fuel-cost analysis indicates that glucose is a more cost effective fuel from any source.

This research with the New Mexico Institute of Mining and Technology examines both the scientific and economic feasibility of microscale glucose aqueous phase reforming for the production of hydrogen. We are conducting experiments to determine optimal conditions for glucose processing. Ethylene glycol is used as a test feed molecule as it contains the same functional groups as glucose and can be processed more expeditiously. We are using the optimal conditions for ethylene glycol reforming in glucose reforming. We are evaluating reactor temperature, pressure, flow rate and fuel concentration for glucose reforming using Pt supported on –325 mesh Al_2O_3 as the catalyst. We are evaluating the surface activity of the catalyst by irreversible CO absorption.

Accomplishments

We evaluated several approaches for immobilizing catalysts on the support. A primary consideration in this regard is effective adhesion of the Pt microstructured catalyst under the high sheer stress fields associated with the flowing liquid phase in the microreactor environment. We used resistance of the catalyst coating to tape adhesion and removal to gauge binding effectiveness.

We developed both electrophoretic deposition and dip coating methods. Electrophoretic deposition is carried out using a Pt-Ru electrode and a stainless steel plate holder with a fixed distance between the two. A potential of 9 V was applied across the electrodes to drive the catalyst to the stainless steel plate in the holder. The dip coating method necessitated development of a mechanized assembly that allowed sample immersion at a rate of 1 mm/minute. Each sample plate remained in the suspension for 1 minute before being removed. After electrophoretic or dip coat deposition of the catalyst suspension, we heat treated each sample plate at 800 °C for 2 hours. Samples prepared in this way show poor adhesion.

Sputter deposition of Pt onto an oxidized stainless steel substrate is also being developed and is expected to produce a sufficiently bonded catalyst coating. Experiments in this area are ongoing. We integrated a mass spectral residual gas analyzer into the microreactor assembly.

Significance

We completed the microreactor and integrated residual gas analysis system. This will allow characterization of the catalyst structures under conditions of use. Practical advantages of microreactors include safety, "easy modulation," and numbering up as a means for increasing throughput. Heterogeneous reactions can be carried out efficiently due to short diffusion paths and high surface-to-volume ratios. There are also features that may enable more selective control over chemical synthesis. Reactions run in macroscale batch reactors are usually slow (reaction times of minutes to hours), as fast reactions are difficult to control. The superior mixing and heat and mass transfer in microreactors give the control necessary to carry out fast reactions (reaction times from microseconds to seconds), leading to huge increases in production efficiency.

Heat transfer is one of the more important elements of chemical reaction kinetics. Efficient heat transfer is particularly desirable for fast, highly exothermic reactions. The heat generated by a chemical reaction is proportional to the volume of reagents used, and hence the volume of the reactor. Conversely, heat removal capability decreases with increase in reactor size. Heat produced by the reaction is often removed through the reactor wall, and so the ratio of wall surface area to reactor volume is crucial to efficient heat dissipation. The conduction of heat from highly exothermic reactions and extremely fast reactions in macroscale batch reactors often leads to heat removal as the limiting factor. The high surface-to-volume ratio in microreactors eliminates this problem.

Other Communications

J. Monroe, "Development of a Platinum-Loaded Y-Type Zeolite Catalysts for High-Efficiency Conversion of Biomass-Derived Carbohydrates to Hydrogen," New Mexico Institute of Mining and Technology Master's Thesis, June 2006.

Modeling River-Aquifer Interaction with Application to the Rio Grande

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Project Purpose

This work addresses a fundamental shortcoming in traditional modeling projects: groundwater and surface water are modeled in essentially different spatial, dimensional, and temporal domains, requiring modelers to focus on either surface or groundwater, with an oversimplified representation of the other. This work focuses on modeling the interaction between surface water and groundwater and its implications for resource management.

Regional groundwater models tend to be three-dimensional (3D), finite element/finite difference models with cell sizes on the order of a kilometer. The temporal resolution is often limited to seasonal or even annual time frames, making support for within-season management decisions difficult. Surface water models tend to represent the river as nodes, which simulate diversions, inflow points, and so on. These nodes are connected by links that roughly simulate the hydrologic behavior of the river between the nodes. Time steps may be days, hours, or even minutes for flow-routing calculations.

The discrepancies between the conceptual representation of surface and groundwater models can be overcome with integrated surface water–groundwater modeling, but the data needs and computational requirements are far greater than for a single domain model. With the rise of advanced code development and geometrically increasing computing power, such model development on a regional scale is now becoming feasible.

This work includes hydrologic modeling of the Rio Grande Project, extending from Caballo Dam in New Mexico to Fort Quitman, Texas, and including diversion of surface water to Mexico at Juarez. Teaming with researchers from New Mexico State University, the Army Corps of Engineers, Bureau of Reclamation, and the Paso del Norte Watershed Council, we will use this data for the formulation and calibration of a coupled hydrologic routing model and groundwater flow model. The resulting model can then be used initially for examining flood routing and ultimately for improving and managing operations of the Rio Grande Project.

Accomplishments

In order to continue development of the Riverware model for the Rio Grande between Caballo Dam and the Rio Grande at El Paso, relationships between the major drain return flows and diversions in the Mesilla Valley reach are needed. We performed analyses to determine if a regression model with autoregressive moving-average (ARMA) errors would adequately describe these relationships. We found that the major drain return flows in this reach were highly correlated to diversions from the river, and we developed ARMA equations for incorporation into the Riverware model

We performed an extensive literature review on stream-aquifer flow interactions. Many subtopics related to this issue were also researched, some of which were:

- governing equations for flow in open channels
- governing equations for ground-water flow

- aquifer depletion as a result of well pumping near stream
- stream-aquifer interactions in the hyporheic zone
- effects of aquifer recharge on stream-aquifer interactions
- effects of sediment characteristics at the interface (thickness, heterogeneity, and permeability)
- effects of bank storage on modeling coupled systems
- methods of numerical modeling of the governing equations both as separate systems and as a coupled system
- techniques of software development for object-oriented code modules.

We reviewed and classified a variety of existing models of coupled stream-aquifer systems according to the assumptions that they make with respect to key mechanisms driving the interactions. The primary mechanisms we identified as possibly being important in stream-aquifer interactions were:

- the bathymetry of the channel
- the sinuosity of the channel
- the dimensionality of the equations of state
- the distance of the aquifer from the stream
- distributed recharge to the aquifer
- pumping from the aquifer
- aquifer heterogeneity
- stream penetration
- sediment thickness and heterogeneity
- time scales of flow
- total versus net water exchange at the interface
- bank storage.

We are developing a Riverware model for the Mesilla Valley portion of the Rio Grande using monthly flow data, and regression models that define the relationships between the diversions and the major drain return flows in this reach. Additionally, we will document the results of the literature review and classifications in a review article. Based on the classifications, the framework for numerical analysis of high-resolution modeling will be developed. The software coding and baseline analysis to verify and validate the software will also be done. Finally, we will devise a plan that describes the method that will be used to analyze the assumption sets. This plan will start with a system that has few or no assumptions on a hypothetical 3D stream/3D aquifer system with a sinuous stream over a heterogeneous aquifer, and progress to the next simpler assumption set until all assumptions sets have been analyzed.

Significance

Water scarcity has the potential to undermine the nation's economic, energy, and agricultural security. Significant tension exists over water allocations across international and interstate boundaries as well as the distribution of water among irrigators, urban developers and environmentalist. This research will help quantify the magnitude as well as the spatial and temporal variability in exchanges between streams and their adjoining aquifer. For most water courses, these exchanges represent a significant contribution to the overall water budget. Additionally, these exchanges play an important role in defining water quality (including temperature) as well as controlling biologic processes in the hyporheic zone. Unfortunately, it is very difficult to accurately measure these exchanges. Significant difficulties often arise in water planning exercises over uncertainties in surface-groundwater exchanges. To further complicate the water planning process, these uncertainties extend to issues concerning how these exchanges respond to changes in agricultural practices and/or land use within the flood plain.

This research focuses on developing computational tools that better quantify surface water-groundwater exchanges. We have compiled an extensive base of literature on the subject that is being synthesized and documented in a comprehensive review article. This article will help organize this knowledge around computational themes and help define the advantages and shortfalls of different schemes according to their underlying assumptions. Once resource gaps are identified, we will develop the next generation of computational tools for modeling river-aquifer interaction. Such models will provide the technical foundation for water resource decision support modeling tools to support of Sandia's goals for water systems.

Maximally Autonomous Autodirective Antenna Array Technology

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Project Purpose

Electrically steerable passive array radiator (ESPAR) antennas feature dramatically reduced size, complexity, and power consumption relative to other array types while retaining the ability to achieve high-accuracy beam-forming, direction-of-arrival determination, adaptive tracking, and interference suppression. For example, a typical ESPAR as reported in the open literature uses quarter-wave element spacing, which is one-half of a typical phased array, and achieves electrically steerable gain in the 8-10 dB range over all azimuth angles with the use of only a single receive chain. Direction-of-arrival accuracy has been reported in the subdegree accuracy levels, and adaptive null formation of better than 25 dB is readily achieved, again all with just the single active receive chain. Although previously verified through prototype measurements, this relatively new technology requires additional development to realize its full potential.

This project, with New Mexico State University, focuses on enhancing the gain, bandwidth, and size advantages of ESPAR technology through enhanced analysis and characterization of a wider variety of array configurations than treated in previously published work, which has focuses almost exclusively on a single, inherently limited array configuration. The analysis approach seeks to come full circle by carefully scrutinizing closed-form approximations of "exact" electric field integral equation (EFIE) formulations of the array system in order to in turn develop reduced-complexity design techniques.

This work has already resulted in one design technique for beam forming that uses radically simplified computations to directly synthesize array element load values necessary for any azimuthal look angle in arbitrary array configurations. We verified the basic validity of the technique through numerical analysis. Additional work will continue along this paradigm to provide for design techniques that directly treat array bandwidth and gain. The ability to design for both impedance and pattern bandwidth response is especially valuable, and challenging.

Alternate complex analysis configurations, based on using different forms of the EFIE impedance kernel combined with accurate approximations such as the geometric theory of diffraction (GTD), will be used to develop the new reduced-complexity design formulas. Several newer definitions of antenna Q are based on actual element patterns or feed-point impedance trajectories, and will be incorporated into the analysis approach. The results of this work have relevance for all medium-gain, scanned-array applications, and can be used to not only replace larger, more power-hungry existing scanned arrays, but will also allow for scanned arrays to be used in applications where the system cost of such functionality was previously too high.

Accomplishments

We analyzed, simulated, and made measurements with near-earth and subsurface radio frequency (RF) communications. This included analyzing the surface mode traveling waves along the earth-air interface, determining ideal excitation methods for surface waves, and designing hardware for auto-directive antenna arrays and self-matching antenna structures. The results show the potential for overcoming nonideal terrain in diffraction-limited frequency bands, establishing links over non-line-of-sight channels, and decreasing the likelihood of eavesdropping by confining most RF energy, preventing free-space transmission. We built and characterized a prototype auto-tuning proportional-integral-derivative (PID) feedback circuit. The preliminary results verified the applicability of the approach.

We verified the performance and behavior of a basic ESPAR architecture according to the present state of the art. Design techniques have focused more on initial validation of the most simple ESPAR configuration and application of the architecture to various methods of direction-finding and adaptive beamforming. We also completed a thorough review of the ESPAR antenna literature and completed a summary document detailing the measured performance achieved by various researchers. The document serves as a basis for future research to be performed in this area. We developed a custom two-dimensional method of moments solver to analyze the interelement mutual coupling of an arbitrarily configured ESPAR antenna.

Significance

Many Sandia flight test technologies require advanced antenna structures for satellite and wireless network applications. These applications impact advanced concept opportunities for Sandia. Technology developed in this project can benefit intelligence and military applications of network unattended ground sensors and high-gain, electronically steerable antennas for satellite telemetry applications. The results of this work have relevance for all medium-gain, scanned array applications, and can be used to not only replace larger, more power-hungry existing scanned arrays, but will also allow for scanned arrays to be used in applications where the system cost of such functionality was previously too high.

Tunnel Gap Modulation Spectroscopy: An Ultrasensitive Technique for Measuring Small Mass Change

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Project Purpose

We are exploring the feasibility of using carbon nanotubes (CNTs) as ultrasensitive mass sensors using the newly developed technique of tunnel gap modulation spectroscopy (TGMS). TGMS accurately measures the natural frequency of oscillation of a single CNT at room temperature by monitoring the electron tunnel current between the CNT and a conducting substrate. Since the magnitude of the tunnel current is exponentially dependent on the CNT-substrate separation, small changes in the CNT's motion can easily be detected. Our collaborators in the Reifenberger Nanophysics Lab at Purdue University demonstrated the feasibility of using TGMS as a novel nanoscale oscillator that detects a radio frequency (RF) signal derived from the tunnel current of an oscillating CNT.

To develop chemical vapor sensors, we will functionalize individual CNTs with Sandia's unique enabling diazonium/iodonium sensor chemistries that will selectively bind various analytes. When ultralow amounts (< 1 fg) of a target analyte bind to a functionalized CNT, the CNT's natural frequency of oscillation will dramatically shift due to the CNT's small mass (< 1 pg). As an example, we estimate that using a functionalized CNT, a frequency shift of 0.57 MHz will result when a single virus (10-15 g) is attached to the end. Although initial experiments will be conducted using multiwalled carbon nanotubes (MWNTs), the method seems generally applicable to most nanowires. Successful completion of this project will enhance Sandia's ongoing nanosensing programs by enabling fundamental research in carbon nanotube-based sensing and device development.

Accomplishments

We obtained atomic resolution scans of highly orientated pyrolytic graphite (HOPG) with a scanning probe microscope. These atomistic scans provide a stability benchmark to evaluate the resolution of Purdue's custom RF-STM head.

We refined the experimental apparatus needed for tunnel gap modulation spectroscopy. We will conduct initial TGMS measurements by attaching a MWCNT to an STM tip and holding the MWCNT within tunneling range (~ 1 nm) of a conducting substrate. The RF signal (10s of MHz) generated by the thermally excited vibrating MWNT will be amplified and detected with a spectrum analyzer. A custom RF-STM amplifier will be used to measure the tunnel current.

We also modeled the mechanical behavior of the nanotube tip by:

- Calculating the oscillation amplitude, frequency, and mode shapes of a carbon nanotube using the Euler-Bernoulli equation and the equipartion theorem.
- Using ANSYS, a finite element analysis program, to model the CNT as a cantilevered beam. Point masses added to the CNT simulated the presence of a bonded analyte.
- Using Matlab to calculate the frequency spectra of the oscillating MWNT's tunnel current.

We used a circuit-modeling program, ORCAD Capture, to design a custom RF-STM head. ORCAD simulations of the hybrid RF-STM preamplifier showed that the gain of the high-frequency converter is 10^5 (1-100 MHz range) while the gain of the low-frequency (tunnel current-to-voltage) converter is 10^8. STM scans of step edges on graphite show the custom RF-STM head has a fast and stable response and the tunnel current-to-voltage converter has a gain of 10^8. We designed an oscillator circuit that uses a quartz transducer as a 5 MHz reference to test the high-frequency amplifier.

We improved techniques to attach MWNTs to STM tips by refining the procedures to etch nickel STM tips. MWNTs were attached to Ni STM tips using nanomanipulators. Initial tests show the MWNTs are robustly attached to the Ni STM tips. We characterized these tips using a scanning electron microscope (SEM).

Significance

In order to increase the sensitivity of cantilevered microsensors and nanosensors, the mass of the cantilever needs to be decreased. MWNTs are ideal cantilevered nanosensors because of their small mass (~ 1 picogram) and high quality factor (Q ~ 500). Even the smallest amount of analyte bonded to a MWNT will cause a detectable shift in the MWNT's oscillation frequency. With the unique enabling diazonium/iodonium sensor chemistry developed by Sandia, MWNTs will be functionalized to detect the presence of chemical warfare stimulants and toxic industrial compounds. Once we demonstrate the reliability of measurements of the oscillation frequency of MWNTs, the MWNTs will be functionalized for use as nanoscale chemical and biological sensors. In addition to their improved sensitivity, cantilever nanoscale sensors offer a low-power (microwatts) sensing platform. Sandia's nonproliferation mission area, specifically monitoring and detection of chemicals, will benefit from the sensitivity and low-power consumption of these MWNT-based sensors.

Other Communications

L. Biedermann, C. Lan, R. Reifenberger, and J. Therrien, "Tunnel Gap Modulation Spectroscopy: A Scanning Probe High-Frequency Oscillator," in *Proceedings of the 6th IEEE Conference on Nanotechnology*, p. 06TH8861C, June 2006.

Optical Properties of Plasmonic Metal-Dielectric Composites

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Project Purpose

Our project is applying plasmonic resonances of small metal particles to enhance stimulated Raman scattering and thus improve the sensitivity of Raman spectroscopy. The fabrication of thin films containing the particles will be optimized for this application. We are also exploring the application of plasmonic resonance to developing negative refractive index material. Such material might be useful in subwavelength resolution near-field imaging. This project is a collaboration with Mark D. Thoreson, a student at Purdue University.

Accomplishments

We studied semicontinuous metal/dielectric composites for use as infrared obscurants and the effect of different dielectric sublayers on the characteristics of random metal/dielectric films. Subsequent photomodification of these films showed it is possible to create a controlled transparency window in these plasmonic structures. Our goal is to increase the selectivity and spectral shape of these transparency windows.

Previously, we studied various dielectric sublayers, including oxides of silicon, aluminum, and titanium. As expected, the dielectric sublayer material affects the structure of the subsequent evaporated metal film. We varied the metal layer thicknesses to match the plasmon absorption characteristics across differing film materials. Subsequent photomodification then produced windows of transparency. We found that samples with a silicon dioxide sublayer proved to be most useful for photomodification, as the photomodification process altered other sublayer materials.

We studied semicontinuous metal/dielectric films for use as surface enhanced Raman scattering (SERS) substrates. The first commercially produced prototypes were fabricated from a process developed at Purdue. These prototypes were characterized using scanning electron microscopy, spectrophotometry, and other methods. The commercially fabricated substrates show promise as nanoplasmonic structures. Obtaining large quantities of high quality SERS substrates will allow the study of the time dynamics of the adaptation process these substrates undergo during analyte deposition.

Studies of negative refractive index in semicontinuous films continue. Preliminary simulation results indicate the possibility of incorporating semicontinuous metal/dielectric films into more complex structures to create conditions for negative refraction at optical wavelengths. Initial experimental results indicate that composites made from multiple thin metal/dielectric layers show appropriate surface roughness for use in negative index studies, and might be useful for imaging with super-resolution near-field lenses.

Significance

We showed that photomodification of evaporated, semicontinuous metal/dielectric films can produce spectral transparence windows. This might have applications in tunable infrared filters.

We developed prototype metal/dielectric films for use as surface enhanced Raman substrates that are being developed for commercial production through industry/university collaborations.

If negative refractive index films can be developed using the techniques under study, such films might be applied to super-resolution imaging in submicron lithography.

Refereed Communications

V.P. Drachev, V.C. Nashine, M.D. Thoreson, D. Ben-Amotz, V.J. Davisson, and V.M. Shalaev, "Adaptive Silver Films for Detection of Antibody-Antigen Binding," *Langmuir*, vol. 21, pp. 8368-8373, August 2005.

Other Communications

V.M. Shalaev, V.P. Drachev, V. Nashine, M.D. Thoreson, E.N. Khaliullin, D. Ben-Amotz, and V.J Davisson, "Adaptive Silver Films for Bio-Array Applications," presented at PITTCON 2005, Orlando, FL, February 2006.

Cohesive Zone Modeling of Failure in Geomaterials: Formulation and Implementation of a Strong Discontinuity Model Incorporating the Effect of Slip Speed on Frictional Resistance

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Project Purpose

Modeling failure in geomaterials due to various loading and environmental conditions is a challenging problem and requires the latest in experimental constitutive modeling and computational solution method technology. Current geomaterial constitutive models and computational methods are incapable of predicting the transition of continuous to fractured geologic material. As one approach to modeling this transition, in collaboration with graduate student Craig Foster at Stanford University, we developed physically based cohesive zone models for geomaterials and implemented these models within a simulation code that uses the finite element method. This tool advances Sandia's goal of developing a predictive, computational modeling program for failure analysis of geomaterials.

Accomplishments

We developed a new constitutive formulation for modeling the loss of cohesive strength as a material transition from intact continuum to one with a fully coherent macrocrack. This stage, termed slip weakening, has been coupled with the rate- and state-dependent friction law implemented the previous year, and embedded into the strong discontinuity finite element, also implemented last year. We tested the numerical implementation to ensure proper convergence of the numerical scheme and to verify that no spurious mesh dependence exists. The element was then used to simulate experimental data to validate its performance. We implemented the element in a way that makes it fully compatible with the available continuum material models; it was tested with Von Mises, Drucker-Prager, and Sandia GeoModel options. Finally, we developed an efficient algorithm and tested it to track multiple localized surfaces throughout a given body.

The results of these simulations were very positive. However, we found that a "kinematic locking" phenomenon, that is partly nonphysical, occurs for curving failure surfaces. Allowing the element to open under tensile loading can relieve this phenomenon.

Significance

Two problems that would be better understood with this modeling capability are the defeat of hard and deeply buried targets (HDBT) and the long-term performance of deep geologic nuclear waste repositories. It would be useful to be able to predict the behavior of these buried structures when subjected to extreme dynamic loading conditions, such as high-velocity penetration events, explosive blasts, or seismic events. At present, the mechanics of rock penetration are poorly understood, and there are no empirical data that can be used to forecast long-term performance (over thousands of years) of deep geologic nuclear waste repositories. The advanced model and methods developed in this project overcome limitations of existing methodologies, allowing for more accurate reliability and performance analyses needed for such repositories

In addition to modeling the defeat of HDBT and the long-term performance of nuclear waste repositories, the resulting computational analysis tool will be useful for understanding fracture and fragmentation in geomaterials such as concrete, rock, frozen soil, and heavily over-consolidated clay encountered in fault propagation, tunneling construction, oil and natural gas production, and depleted reservoirs used for subsurface sequestration of greenhouse gases.

Refereed Communications

C.D. Foster, R.A. Regueiro, A.F. Fossum, and R.I. Borja, "Implicit Numerical Integration of a Three-Invariant, Isotropic/Kinematic Hardening Cap Plasticity Model for Geomaterials," *Computer Methods in Applied Mechanics and Engineering*, vol. 194, pp. 5109-5138, December 2005.

Other Communications

R.A. Regueiro, A.F. Fossum, R.P. Jensen, C.D. Foster, M.T. Manzari, and R.I. Borja, "Computational Modeling of Fracture and Fragmentation in Geomaterials," Sandia Report, SAND2005-5940, Livermore, CA, 2005.

C.D. Foster, R.I. Borja, and J. Oliver, "Strong Discontinuity Modeling of Slip Weakening and Variable Friction in Geomaterials," presented at the International Union of Theoretical and Applied Mechanics Seminar on Discretisation Methods for Evolving Discontinuities, Lyon, France, September 2006.

C.D. Foster and R.I. Borja, "Brittle Fracture, Slip Weakening, and Variable Friction Modeling in Geomaterials Using an Embedded Strong Discontinuity Finite Element," presented at the ALERT Geomaterials Workshop, October 2006.

C.D. Foster and R.I. Borja, "Capturing Slip Weakening and Variable Frictional Response in Localizing Geomaterials Using an Enhanced Strain Finite Element," in *Proceedings of the Third European Conference on Computational Mechanics*, June 2006.

C.D. Foster, R.I. Borja, and D.D. Pollard, "Continuum Mathematical Modeling of Slip Weakening in Geological Systems," presented (poster) at the American Geophysical Union Fall Meeting, December 2005.

Atmospheric Aerosols

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Bernie Zak (Org. 6338)
Sandia Principal Investigator

Project Purpose

The purpose of this project is to develop a new "smog chamber" technique for investigating the formation and evolution of ambient aerosols from primary gaseous air pollutants, and/or the evolution of a known primary aerosol when exposed to gaseous air pollutants from the ambient environment.This project is in collaboration with Crystal Reed, graduate student at Texas A&M University.

Atmospheric aerosols have major impacts on climate, both directly through scattering and absorption and indirectly through cloud processes. Understanding these impacts can be challenging given the complex nature and composition of the atmospheric aerosol. In order to better understand the effects of aerosols on the environment, we must study the processes of aerosol transformation in the ambient environment. Such processes include the transformation of soot, which can result in changes occurring to the radiative properties of black carbon and alter our understanding of its effects on the environment.

Another process of concern includes the formation of secondary organic aerosols in which an otherwise hygroscopic particle may undergo changes via the condensation of nonhygroscopic organic vapors. During this transformation, the hygroscopicity of the particle may decrease, leading to an alteration in cloud microphysical processes.

Aerosol chambers have been used in previous laboratory experiments to investigate the coating of gas phase species on existing aerosols. However, laboratory results may not be completely representative of the ambient environment. Captured air experiments, which are more representative of the ambient environment, involve trapping ambient air in several identical chambers and injecting a single compound with varying concentrations into successive chambers in order to investigate the impacts of the compound addition. However, due to the closed nature of the system, processes that take an exceptional amount of time will not be accurately represented since the captured air concentration will decay with time.

Therefore, the purpose of this project is to develop a new chamber type, the ambient aerosol chamber for evolution studies (AACES), in order to better understand the ambient effects on aerosol transformation. AACES construction will allow for measurement periods beyond 24 hours without depleting the gas concentration within the chamber.

Accomplishments

We completed a prototype of the AACES in early April 2006. AACES is a roughly cubical chamber constructed of a rigid Acrylite OP-4 acrylic outer shell, which transmits ultraviolet (UV) radiation both in the UV-B (280-215 nm) and UV-A (315-400 nm) ranges. FEP Teflon lines the inside of the chamber on all sides and the top, while expanded PTFE (ePTFE) Teflon is used on the bottom of the chamber. The fibrous structure of the ePTFE acts as a barrier to particulates, while allowing gas molecules to move virtually unimpeded from one side of the chamber wall to the other, creating an initial environment inside the chamber that is free of particles and continuously mimics the ambient air.

In order to create an environment within the chamber that is well mixed, we discovered a new environmental chamber mixing technology. Internal Teflon coated fans have been the preferred method of mixing in environmental chambers. However, due to their invasive nature, such fans lead to an increase in surface area within the chamber, which may lead to an increase in depositional loss. Through the use of subsonic sound at 20 Hz using an external, noninvasive 12-inch subwoofer, we were able to completely mix the chamber efficiently with little effect on the particle loss rate.

We conducted a series of tests to verify AACES ability to perform in the field:

- Particle Filtration: PTFE membrane has an estimated 96 percent filtration efficiency for particles larger than 10 nm under typical filtration conditions. The particle filtration efficiency as tested under chamber conditions resulted in over a 99 percent removal of ambient particles. This was tested using a TSI 3760A Condensation Nucleus Counter.
- Ambient Gas Penetration Efficiency: We tested ozone penetration efficiency using a Thermo Electron Corp. O_3 Gas Analyzer. Since ozone is highly reactive, its penetration efficiency across the ePTFE membrane reveals the general penetration efficiency of many other species. Resulting ozone concentration within the chamber was above 90 percent of ambient.
- Particle Deposition/Wall Loss: Many processes that lead to particle evolution have time scales on the order of hours to days. Therefore, we tested the depositional loss of particles within the chamber. First, the chamber was completely flushed with zero air to ensure an initial clean environment. Second,

we injected 70 nm uncharged ammonium sulfate particles, and monitored the concentration on an hourly basis using a differential mobility analyzer (DMA). In order to inject only uncharged particles, a tandem differential mobility analyzer (TDMA) was used. Ammonium sulfate particles generated using a TSI atomizer were first dried, passed through a charger, and size-selected using the first DMA. The size-selected particles were then passed through a charger prior to entering the second DMA set at a high voltage sufficient to remove all charged particles. Particle loss rate was less than 10 percent per hour.

Upon the successful completion of all chamber tests, a second chamber was created and AACES deployed in the field in August 2006.

Significance

Numerous studies have utilized laboratory and smog chamber results in model analysis to predict the behavior of the atmospheric aerosol. However, the simplistic treatment of aerosols in models, coupled with the difficulty in interpretation of ambient aerosol measurements due to source variability, makes a comparison between model results and measurements difficult at best. By introducing a monodisperse aerosol of known composition into the AACES, we can monitor the growth rate due to such processes using a DMA system. With this new knowledge, chemistry models will be better equipped to predict the behavior of the atmospheric aerosol. Furthermore, results from these studies will aid the development of future aerosol modeling techniques designed for comparing the ambient aerosol with model predictions.

With the growing concern regarding organic aerosol concentrations, the effects of low volatile organic species on aerosol properties can be better understood by monitoring changes occurring to the hygroscopic aerosols over time. Through the use of AACES, we will be able to separate the hygroscopic growth of an aerosol from variability in source region and history prior to sampling, providing a better understanding of the ambient effects on aerosols, including soot, and increase the certainty of aerosol classification and composition inferred from hygroscopic growth measurements. Also, field studies often result in data that is difficult to interpret due to the variability in both the temporal and spatial scales. Through collaborative efforts, AACES may be utilized in the interpretation of such field data.

Internal mixing devices implemented in environmental smog chambers create both design challenges and the opportunity for leaks. Furthermore, the placement of these devices may create concerns with turbulent mixing and particle loss rates. By implementing the newly developed subsonic mixing technology, future Teflon chambers will be more efficiently constructed and better equipped to more accurately represent heterogeneous reactions in the ambient environment. Moreover, the use of subsonic sound to move air will open new doors to innovation and technology.

The techniques developed here are applicable to hazardous aerosols that are of concern to Sandia: routine aerosol emissions from new or modified energy systems; routine aerosol emissions from new or modified elements of the nuclear fuel cycle; and accident-related aerosols from either the nuclear fuel cycle or nuclear weapons.

Application of Advanced Laser Diagnostics to Hypersonic Wind Tunnels and Combustion Systems

Andrea Hsu
Texas A&M University

Jonathan Frank (Org. 8351)
Sandia Principal Investigator

Project Purpose

We propose to conduct experimental research on nonequilibrium phenomena in hypersonic flows. This research is part of a multidisciplinary university research initiative (MURI) that involves collaboration between the Chemistry and Aerospace Engineering Departments at Texas A&M University. The MURI project is a fundamental study of supersonic combustion ramjet (SCRAMJET) propulsion and includes both experimental characterization and theoretical modeling of thermal and chemical non-equilibrium systems in hypersonic shear layers.

In hypersonic flight conditions, gas molecules are in a state of non-thermochemical equilibrium (NTE). This research will study the interactions of non-equilibrium gas molecules with hypersonic shear flows. The experimental results from this project will be coupled with computational fluid dynamics simulations in an effort to develop a novel hypersonic flow model that can bridge the gap between Lattice-Boltzmann and conventional Navier-Stokes methods while accommodating NTE.

We will use laser-based imaging diagnostics to study non-reacting hypersonic flows. We will use planar laser-induced fluorescence (PLIF) imaging of NO seeded into the flows to measure rotational and vibrational temperatures as well as pressure. We will measure velocity fields with particle imaging velocimetry. We will introduce non-equilibrium conditions into the flows and measure the subsequent equilibration of the gases.

We will investigate two different approaches for producing non-equilibrium conditions: one uses a capacitively coupled radio frequency system to produce a plasma; the other uses photodissociation of NO_2 to produce vibrationally excited NO molecules, where the timescale for vibrational energy transfer is expected to be of the same order as the hypersonic flow timescales.

Sandia's Combustion Research Facility will provide expertise in state-of-the-art imaging diagnostics for turbulent flows. A portion of this research will be conducted in the Advanced Imaging Laboratory at Sandia.

Precise Distributed Control and State/Parameter Estimation for Multi-body Satellites and Satellite Formations

James Fisher
Texas A&M University

Jeff Spooner (Org. 5338),
Sandia Principal Investigator

Project Purpose

Reconnaissance and surveillance satellites use sensor payloads that require accurate pointing and extremely low line-of-sight residual jitter. These sensor payloads are usually not the primary payloads of the spacecraft, requiring them to point accurately despite unknown maneuvers of the primary spacecraft bus. Maintaining pointing accuracy in the face of unknown main body maneuvers, despite incomplete knowledge of the spacecraft dynamics, and under the influence of unknown disturbances, is a very challenging and important problem.

The more precise the knowledge of the parameters of a system is, the better performance the control law has. Higher performance can also be achieved, for example, by modeling disturbances due to sudden changes in disturbance forces and thermal expansion effects that occur when the satellite passes in and out of the Earth's shadow. The control problem is further complicated due to the requirement that solar panels of such satellites must continuously track the sun with the help of gimbals. This requirement is often in conflict with the primary goal of payload pointing and assuring the stability of the satellite.

The proposed research, to be conducted at Texas A&M University, will develop novel control and estimation methods for multibody satellites as well as formations involving multiple, dissimilar satellites. The key elements to be researched are accurate modeling of the vehicle dynamics, space environment, and the associated uncertainty in attitude and orbit. Multibody satellites require stability/partial stability analysis using multiple measures (Vector and Matrix Lyapunov functions). The limits of performance, propagation of uncertainty, and parameter/state estimation must be addressed. Methods for formation orbit control, collision avoidance, as well as altitude control of the individual satellites will be developed.

Interactive Water Quality Modeling to Assist Regional Water Planning

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Vince Tidwell (Org. 6313)
Sandia Principal Investigator

Project Purpose

While freshwater supplies are finite, demand has tripled since 1950. This growing disparity between supply and demand necessitates difficult decisions that often directly impact groundwater levels and stream flows. Perturbations to water supply in turn may result in unexpected impacts on water quality and the riparian ecosystem. Unfortunately, making these decisions is complicated by the differing values placed on water by the different sectors of our society (industrial, agricultural, environmental, municipal). While many models serve water resources managers in day-to-day operations, there is a lack of integrated modeling tools to assist in regional water planning and to facilitate public involvement in the decision process. We take a novel approach to community-mediated water planning, employing a cooperative modeling process formulated within a system dynamics decision framework.

Water quality often limits the potential uses of scarce water resources in semiarid and arid regions. Consequently, changing water quality, particularly nutrient levels, is often an important concern with many water resource decisions. Chronically elevated nutrient loads may result in eutrophication of reservoirs and changes in riparian vegetation. To best manage water quality, one must understand the sources and sinks of both solutes and water to the river system. Therefore, modeling efforts will need to include biogeochemical processes both within the river and within the shallow alluvial aquifers of the riparian corridor. Incorporating these processes and feedback is paramount to modeling and evaluating the water quality dynamics that may result from changing land use practices, waste water treatment policies, watershed/range management, and reservoir operations.

We are pursuing this work cooperatively with the University of Arizona and the NSF Science and Technology Center for the Sustainability of semiArid Hydrology and Riparian Areas (SAHRA). SAHRA is a multi-institutional, multidisciplinary research center working to improve understanding of the hydrologic cycle, provide improved tools for decision makers, and raise the level of hydrology literacy.

Accomplishments

We developed relationships between discharge, land use, and nitrogen sources and sinks using five years of synoptic sampling along a 300 km reach of the Rio Grande in central New Mexico. Average discharge in the river was significantly higher ($p = 0.01$) during 2001 and 2005 "wet years" (15.0 m^3/s, standard deviation [S.D.] = 0.88) than during the drought years of 2002 – 2004 "dry years" (8.85 m^3/s, S.D. = 1.77). Wastewater treatment plants (WWTPs) were the largest and most consistent source of nitrogen to the river (1331 kg/day, S.D. = 19.8). Agricultural drain returns contributed less nitrogen than WWTPs in both wet (262 kg/day, S.D. = 54) and dry years (82 kg/day, S.D. = 38). Average total dissolved nitrogen (TDN) concentration downstream of the WWTP was 1.18 mg/L (S.D. = 0.22) in wet years and 0.52 mg/L (S.D. = 0.40) in dry years.

Possible explanations for the constant elevated TDN concentrations include continuous low flows, minimal channel vegetation, and large suspended sediment loads. Somewhat surprisingly, agricultural return flows had lower average nitrogen concentrations than river water originally diverted to agriculture in both wet (0.81 mg/L, S.D. = 0.17) and dry years (0.19 mg/L, S.D. = 0.18), indicating that the agricultural system is a sink for nitrogen. Lower average nitrogen concentrations in the river during the dry years are mostly due to the input of agricultural returns, which comprise the majority of river flow in dry years.

These findings imply that the hydrology of the river system is crucial in determining nitrogen removal rates in the river and agricultural system and must be included in the model. Furthermore, these changes in water source in the river during wet and dry years must be included in the model to accurately model nitrogen concentrations and cycling in the river.

Significance

Water scarcity has the potential to undermine the nation's economic, energy, and agricultural security. Significant tension exists over water allocations across international and interstate boundaries as well as the distribution of water among irrigators, urban developers, and environmentalist. This project focuses on developing tools to better manage our limited resources and engage the public in the water planning process.

In particular, this research will help quantify nutrient cycling processes and their impact on water quality. Nutrients represent the leading anthropogenic source of pollution in surface and groundwater supplies. Nutrients are contributed to the environment through agricultural chemicals, urban storm and wastewater streams, atmospheric deposition, and natural pathways. The chemistry and ultimate fate of these nutrients undergoes a complicated process of transformation, dispersion, and uptake in the environment. Because of this complexity in the nutrient cycle, tools are needed to understand how changes in the natural and anthropogenic environment impact nutrient loads. Tools are also needed to assess how changes in nutrient loads impact the environment, and how they may limit water use and increase treatment costs.

Our work provides a comprehensive data set with which to explore the complexities of nutrient cycling in a large semiarid watershed, and we are analyzing and modeling these data. The resulting relations are being implemented within a decision support framework, allowing decision makers, stakeholders, and the public to explore a wide range of water use scenarios while understanding the downstream consequences in terms of water quality change. Such models will provide the technical foundation for water resource decision support modeling objectives for Sandia's water security programs.

System Dynamics Modeling to Assist Regional Water Planning: Modeling the Nonmarket Value of Water

Matt Weber
University of Arizona

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Sandia Principal Investigator

Project Purpose

Fresh water is central to the vitality of our society; however, current demands are increasingly being met through unsustainable practices.

Establishing new sustainable practices is complicated by the differing values placed on water by the disparate sectors of our society (industrial, agricultural, environmental). Integrated modeling tools are needed to assist in regional water planning and to facilitate public involvement in the decision process. We take a novel approach to community-mediated water planning, employing a cooperative modeling process formulated within a system dynamics decision framework.

This work is being performed cooperatively with the University of Arizona and the National Science Foundation (NSF) Science and Technology Center for the Sustainability of semiArid Hydrology and Riparian Areas (SAHRA). SAHRA is a multi-institutional, multidisciplinary research center working to improve understanding of the hydrologic cycle, provide improved tools for decision makers, and raise the level of hydrology literacy. Through this collaboration, we gain access to extensive expertise and data from unique studies on valuation of water conducted in the Rio Grande and San Pedro river basins.

Accomplishments

A riparian valuation project for Aravaipa Canyon Wilderness in southern Arizona continues in its second phase. Visitation data over a 14-year span have been prepared and linked to census socioeconomic data, environmental time series data, and a constructed travel cost variable. This project will increase the resolution of instream-flow recreational usage data, which likewise will be incorporated in the system dynamics framework for riparian value.

A bosque restoration survey instrument canvassed public values for the Middle Rio Grande corridor and recorded bosque recreational usage patterns. The survey was designed to supply new inputs for the riparian valuation module within the larger watershed decision support tool. Final survey responses have been coded, and analysis is in process. Valuation of restoration allows improved analysis of water allocation in the Middle Rio Grande, results of which may be applicable to other southwestern areas with competing human and environmental usage.

Significance

Water scarcity has the potential to undermine the nation's economic, energy, and agricultural security. Significant tension exists over water allocations across international and interstate boundaries as well as the distribution of water among irrigators, urban developers, and environmentalists.

Our project provides data that allows direct comparison of water valuation between its use for irrigated agriculture, residential consumption, or in industrial applications. Specifically, the data and models developed from this project will be implemented within a decision support framework allowing decision makers, stakeholders, and the public to explore a wide range of water allocation strategies. Such models will provide the technical foundation for water resource decision support modeling objectives for Sandia's water security programs.

Other Communications

M. Weber and G. Woodard, "Shades of Grey: Modeling Tucson Area Residential Water Use," presented at the Arizona Hydrological Society, Flagstaff, AZ, September 2005.

M. Weber and S. Stewart, "Restoration Preferences for the Middle Rio Grande Bosque," presented at the 5th Annual Meeting of SAHRA, Tucson, AZ, October 2005.

M. Weber and S. Stewart, "Restoration Preferences and Management for the Middle Rio Grande," presented at the Universities Council on Water Resources, Santa Fe, NM, July 2006.

M. Weber, R. Berrens, and S. Stewart, "Quantifying the Value of Instream Flow in the Desert Southwest," presented at the Natural Areas Conference, Flagstaff, AZ, September 2006.

Tribological Studies of Microelectromechanical Systems

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Bonnie Antoun (Org. 8776)
Sandia Principal Investigator

Project Purpose

Polysilicon micromachines were designed to study the tribological properties of microelectromechanical systems (MEMS). A device for characterizing interfacial adhesion and a device for characterizing friction were developed at the University of California at Berkeley (UCB). We used these devices to develop an understanding of the physics controlling the interfacial behavior that is critical to the reliability and efficiency of micrometer-scale devices. We conducted this research with Shannon Timpe at UCB.

Accomplishments

Two MEMS tribology-testing devices were successfully designed and implemented, one for testing adhesion alone and a second capable of testing both adhesion and friction. We completed the first experimental phase, which examined the adhesion force under a variety of loading and environmental conditions. In the second experimental phase, we used the second device and attempted to determine the effect of high-adhesive forces on the frictional behavior of the MEMS structures.

Once we established these working devices and experimental protocols, we performed initial experiments on dynamic friction in a variety of environments.

We are conducting experiments to study the effects of current flow across an interface on the adhesive properties of that interface. This is a particularly important topic for microswitching applications. Initial data shows a combination of charge trapping in native oxide films and eventual catastrophic failure due to microwelding.

Significance

This project benefits the general scientific and technical community by developing an understanding of the tribological behavior of MEMS devices under various environments and conditions. This project further serves to develop collaboration with UCB and enable the development of future engineers and scientists that will enter the S&T community and possibly consider employment at Sandia.

Refereed Communications

S.J. Timpe and K. Komvopolous, “An Experimental Study of Sidewall Adhesion in Microelectromechanical Systems,” *Journal of Microelectro-mechanical Systems*, vol. 14, No. 6, pp. 1356-1363, December 2005.

S. Timpe and K. Komvopolous, “Dynamic Friction in Microelectro-mechanical Systems,” presented at the Materials Science and Technology 2006 Conference, San Antonio, TX, October 2006.

Reconciling System and Application Logs

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Steve Hurd (Org. 8965)
Sandia Principal Investigator

Project Purpose

The purpose of this project is to devise a method that can be used to automate the process of mapping events across systems layers in order to assemble them into useful models of events. Such models will aid in both forensic analysis of compromised machines and intrusion detection systems, as they will provide the templates necessary to create useful, easily analyzable logs. This work is in collaboration with the University of California at Davis (UC Davis).

Computer system event logging is best done as a fine balance between overflow of information and lack of data. Limited logging can hinder intrusion detection systems and forensic analysis, both of which rely on the event logs to provide the data necessary to differentiate between normal machine operation and attack. Overly thorough logging, however, can generate so many superfluous entries that the time needed to manually examine the logs for pertinent data is infeasible. Thus, it is critical to devise and maintain a system that can record sufficient data to differentiate between those events that occur in normal operation and those that allude to malicious intent.

A deeper complexity involves the various sources of logs, including both applications and the system (and in many cases, other sources). How to reconcile the log entries generated by the many sources remains an open question in the field. The ability to do so would allow auditors to conserve effort by consulting a collated log, rather than reviewing each source log individually and manually determining which high-layer event corresponds to which low-level entry. Such aggregation is surprisingly complex in today’s modern computing environment.

Accomplishments

We found that dealing with clock synchronization issues (both within and between systems) is the critical technical obstacle to project success. The two primary issues are “clock skew” and “clock drift.” Without accurate clock synchronization (both within and among systems), it is virtually impossible to effectively perform correlation analysis/ reconstruction on logs. Accordingly, we dedicated all resources to solving this problem.

A promising approach to solving this problem was previously developed at UC Davis. This approach, best described as the MIN-DELAY-SYNCHRONIZE algorithm, searches for an entry in the logfile (one for each host), where the difference between the timestamp generated by the host and the timestamp generated by the log-server is minimal. This is assumed to be where the transmission delay was the least and clock skew is estimated using that as a basis.

The MIN-DELAY-SYNCHRONIZE algorithm had only been verified using simulation, rather than using actual systems and associated logs. Thus, the major task we completed this year was to develop and execute an experiment to verify or refute the results of the approach to solving this problem, then analyze the results.

At first, the results we obtained through testing tended to verify the validity of the MIN-DELAY-SYNCHRONIZE algorithm. However, under further examination, it became clear that while this approach works for dealing with clock skew, it does not address issues related to clock drift.

Following this realization, we considered a number of different potential solutions to the clock drift problem. It appears that the most promising approach is to use linear regression techniques in conjunction with the MIN-DELAY-SYNCHRONIZE algorithm. At this time, we have not completed the detailed analysis as to whether this combined approach will work.

Significance

A significant accomplishment from this year is the demonstration that the MIN-DELAY-SYNCHRONIZE algorithm approach is insufficient to deal with both clock skew and clock drift and could lead to flawed research results.

This project supports the national security mission in cyber security by developing improved tools and techniques to use system logs for both intrusion detection and forensics analysis.

Mobile Agent Abstractions, Methods, and Infrastructure for Efficient Sensor Network Tasking Over Heterogeneous Networks

Leo Szumel
University of California at Davis

Nina Berry (Org. 8961)
Sandia Principal Investigator

Project Purpose

This research, in collaboration with Ph.D. candidate Leo Szumel at the University of California at Davis (UC Davis), addresses the programming of efficient, scalable, fault-tolerant networks of wireless sensor nodes. These networks are made up of several nodes: elements characterized by a sensor suite, a power source, processing capability, and a radio. There are several challenges in programming these networks.

First, because no single node has complete knowledge of the world environment, nodes of the network must collaborate with each other in order to solve problems with sufficient fidelity and scalability. Second, a network's full potential is only attainable by multiplexing several users or applications, and doing so decreases the effective deployment cost of the network. A third challenge is that limited power means that nodes must spend most of their time sleeping and must perform rapid and efficient collaboration to accommodate that need.

This work integrates the former two challenges into that of "programming," and the latter challenge into that of "communication." This work develops a mobile agent-programming model to solve the first challenge and a pheromone-inspired smart flooding communication primitive to solve the second problem.

This approach is to be demonstrated in a real, physical sensor network deployment. The network will be deployed at the UC Davis McLaughlin Reserve to enhance traditional plant ecology studies with new data that would not be attainable via human sampling. The network will measure air, surface, and soil temperatures and soil moisture content.

This deployment has interesting network properties that distinguish it from many experimental networks. First, the network is not in range of wired or wireless data communications. Second, the nodes are placed according to existing experiment sites and cannot be moved to improve radio frequency (RF) connectivity. Third, the terrain and the RF landscape are expected to change considerably as plants grow from foot-high to waist-high. Lastly, a mobile node will visit the site every 1–2 weeks.

This deployment is a specific example of a class of networks that mimics unattended operation in a harsh environment and hybrid static/mobile modalities.

Accomplishments

We examined the efficiency, scalability, and fault-tolerance of sensor network tasks built with the virtual pheromone (VP) primitive, comparing them against state-of-the-art algorithms built using traditional communication methods. VP is found to provide comparable performance while resulting in fewer lines of code.

A high-level network simulator was specifically tailored to the design of agent algorithms and novel communication primitives in sensor networks. The agent high-level pythonic simulator (AHLPS) is based on Python and the SimPy discrete event simulation module. AHLPS allows rapid prototyping and high-level analysis of these algorithms. Implementation in TinyOS and deployment on physical nodes is still used for verification of functionality, but AHLPS provides the unique ability to test algorithms at scale (thousands of nodes) in a reasonable timescale.

At Sandia, we developed and demonstrated a hardware prototype of an adaptive image tracking sensor network (DISCERN). We will continue to work on DISCERN and explore a case study in applying an agent programming model and virtual pheromone communication primitive to the DISCERN sensor nodes. This study will provide valuable data and enrich DISCERN capabilities.

Significance

This research focuses on the challenges posed by the programming of large sensor networks. The interest in such networks is quite easy to understand – the more measurements we can collect from our environment, the better we can understand and control it. This argument applies across many fields, including environmental monitoring, physical security, and basic science research. What has become clear over the last few years, however, is that we are approaching a time when these large networks are affordable from an equipment standpoint but remain a huge logistical challenge, largely because of software development difficulty. These difficulties arise from the need to handle heterogeneous nodes, the spatial and temporal decoupling of nodes, and scaling challenges, among others.

How do we design algorithms that can be tested in simulation and small-scale deployments, then be expected to work well under adverse (perhaps unpredictable) conditions and at a scale that increases over time? How do we amortize infrastructure cost by sharing the network between multiple users? How do we enable adaptation of the network code once it is deployed, in a way that is efficient and does not interfere with existing components that do not need to be updated?

This research is answering these questions by providing a framework for the tasking of, and communication between, sensor nodes in large-scale deployments. This framework is scalable, efficient, and can support multiple applications on a single network. The application(s) can be updated independently and/or concurrently.

A specific example of how this research can be applied to Sandia's mission objectives is being demonstrated in the case study. The DISCERN nodes have the ability to detect objects and share their information with neighboring nodes–this is a scalable and efficient design. However, the network is of limited use if all decision synthesis occurs outside the network because doing so limits scalability and increases latency. We will use the agent framework to program the DISCERN nodes, allowing synthesis to occur inside the network. For example, the user (existing outside the network) can inject an agent that knows how to identify a particular threat and has an action profile dictating how to handle threat detections. The agent then "lives" inside the sensor network, using multi-hop communications only when necessary. A key advantage to this approach is that the learning process can continue long after network deployment; as new threats emerge, new agents can be tailored and injected into the network, at minimal cost, without disturbing the other agents already existing in the network.

Refereed Communications

L. Szumel and J. Owens, "The Virtual Pheromone Communication Primitive" in *Proceedings of the IEEE/ACM International Conference on Distributed Computation in Sensor Systems*, pp. 135-149, June 2006.

MEMS Reconfigurable Intelligent RF Circuits

Patrick Bell
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Chris Dyck (Org. 1742)
Sandia Principal Investigator

Project Purpose

Switched impedance networks are essential in developing reconfigurable systems, however "tuner" networks are more complex and produce many points over a targeted impedance range. Such networks could be used as chip-level load-pull networks in order to increase the efficiency of high-power systems, reduce design cycle times, and enable dynamic system optimization. Conventional power amplifier design uses mechanical source and load tuners to determine the optimal operating impedances for highest power and efficiency. However, high-power applications often require several amplification stages, and there exists no method to determine the optimal interstage impedance in these multistage amplifiers. A MEMS (microelectromechanical system) tuner network could be placed between each amplifier stage and used to vary the impedance for optimal power and efficiency. These networks could either remain in the amplifier to allow it to be dynamically optimized with changing signal and environmental conditions, or removed and used solely as a measurement tool.

Accomplishments

We designed and fabricated a novel design of an impedance transform network at the University of Colorado at Boulder. The design was an electrically reconfigurable double-slug network consisting of 22 RF MEMS ohmic switches. We designed this network to cover large portions of the Smith chart while dramatically improving on the loss of previous impedance transform network topologies. The system was designed using Agilent's Advanced Design System. Masks were ordered and the circuits were fabricated at Sandia using the baseline RF MEMS ohmic switch process. Testing was not completed.

Significance

This development of reconfigurable active networks benefits the DOE by developing a knowledge base and infrastructure at Sandia to address national security and nuclear weapon needs in the area of high-performance miniaturized microwave systems. Potential applications in communications, radar, and surveillance include switched-mode operation, frequency hopping for antijamming, and dynamic adaptive reconfiguration in response to environmental changes.

Patrick Bell completed his PhD thesis on MEMS reconfigurable networks while supported by this project, and graduated from the University of Colorado at Boulder during FY 2006.

Other Communications

P.J. Bell, "Reconfigurable Microwave Power Amplifiers," PhD dissertation, University of Colorado at Boulder, 2006.

Fourier Analysis and Synthesis Tomography

Dan Feldkhun
University of Colorado at Boulder

Michael Sinclair (Org. 1824)
Sandia Principal Investigator

Project Purpose

We propose to develop a new microscopic imaging technique that will be of great benefit to Sandia's efforts in microelectromechanical systems (MEMS) development and biological research. The new approach, called FAST, is a full-field "synthetic aperture" microscopy technique.

FAST does not require a lens to form an image. Instead, it samples the spatial frequencies and phases of an object by sequentially illuminating it with interfering pairs of pulsed laser beams at different angles, detecting the response with a fast non-resolving detector, and using a novel optical processor to perform Fourier synthesis to reconstruct the object. FAST can be used in fluorescence mode for studying biological samples, or in coherent scattering mode for measuring synthetic objects such as MEMS.

FAST can be used to form a three-dimensional reconstruction of the object by rotating the illumination axis. By performing Fourier analysis sequentially, FAST makes possible full-field imaging with millimeters of depth of field, inches of working distance, and submicron resolution. By replacing mechanics with optoelectronics, it is possible to acquire a frequency sample every 100ns, achieving KHz imaging rates.

FAST can also be used to detect object motion with very high spatial (nm) and temporal (ns) resolution by tracking the phase of its Fourier components. These capabilities are important for biological applications, such as real-time imaging of signals propagating through neurons and rapid screening of cellular and DNA microarrays, as well as for full-field imaging and motion characterization of microstructures such as MEMS.

Personnel at the University of Colorado's Optoelectronics Computing Systems Center initially proposed this new approach to microscopy. The initial development of a FAST instrument, including theory development, simulations, algorithm design, optical and mechanical system implementation, and electronic hardware and control software development will be performed at the University of Colorado, Boulder.

Modeling and Design of Microstructures with Tailored Adhesive Properties

Kevin Sylves
University of Colorado at Boulder

Dave Reedy (Org. 1526)
Sandia Principal Investigator

Project Purpose

This project is concerned with the analysis and design of micro- and nanostructures with responses dominated by adhesive forces. A multiscale adhesion model will be developed that takes into account van der Waals, friction, capillary and electrostatic force mechanisms at the micro- and nanoscale. This model will be implemented into a finite element analysis framework through nonlinear constitutive laws that accurately capture adhesive effects between surfaces. The constitutive model will incorporate internal parameters that capture hysterisis effects and rate dependencies. Additionally, a contact model based on the Lagrange multiplier approach will be developed to prevent surface penetration. Microbeam/plate example problems that incorporate tailored force-displacement characteristics that can be verified experimentally will be constructed.

In order to develop a formal design approach applicable to a broad range of problems, the above analysis method will be integrated into a design optimization framework. This tool will allow designers to create devices that integrate tailored surface properties in novel ways such as robust microdevices that are insensitive to detrimental adhesive behavior, multiphysics problems such as behavior of multiple particles immersed in flow, and self-assembling micro- and nanosystems.

Gradient-based optimization algorithms already integrated into the finite element code will be employed for shape and topology optimization of adhesive characteristics of surfaces. The nonlinear program will include an objective such as a specific force-displacement characteristic in adhesion/decohesion and constraints such as maximum surface adhesion energy.

Both adjoint and direct sensitivity analyses are implemented for computational efficiency for problems with large numbers of optimization variables or criteria. Finite element problems tend to have a large number of variables, making the adjoint method more attractive. This work will be performed at the University of Colorado, Boulder.

MEMS Dual-Backplate Capacitive Microphone

David Martin
University of Florida

Kent Schubert (Org. 1723)
Sandia Principal Investigator

Project Purpose

The purpose of this project is to develop a dual-backplate microphone using Sandia's ultraplanar, multilevel MEMS Technology (SUMMiT V™) fabrication process. A dual-backplate microphone consists of a diaphragm and two porous backplates, one on either side of the diaphragm. These three plates are conducting, thus creating two capacitors. The holes in the backplates allow the incident pressure to pass through the backplates and impinge on the diaphragm. As the incident pressure deflects the diaphragm, the capacitances of the top and bottom capacitors change. An electrical bias is applied to the microphone; therefore, the change in capacitance causes an electrical output. This can be either a voltage or a charge depending on how the microphone is biased. The microphone is packaged with interface circuitry to amplify the output and produce the buffered output voltage.

The fabrication of this device presents several challenges. First, three independent conducting layers must be fabricated to construct the diaphragm and the two backplates. The diaphragm should be compliant to increase the sensitivity of the device. The thickness of the gap between the plates, as well as the thickness of the plates themselves, must be uniform and well-controlled. The SUMMiT V fabrication process is unique in that it can meet the fabrication needs of this project. The SUMMiT V process has been optimized to provide compliant mechanical layers that are ideal for the construction of the microphone's diaphragm. Furthermore, the use of chemical mechanical polishing results in extremely flat structural layers and uniform spacing between the layers, both of which are critical to the successful fabrication of the MEMS microphone.

This microphone is designed for aero acoustic applications, which have vastly different specifications than typical audio microphones. An aero acoustic microphone should be capable of operating up to sound pressure levels (SPL) of 160 dB due to the high SPLs radiated by jet engines. Furthermore, the frequency range of interest for aero acoustic measurements extends up to 90 kHz because experiments are often conducted on scale models. In order to have diffraction-free measurements at high frequencies, the microphone size must be small; at 90 kHz, the microphone radius should be less than 0.6 mm. MEMS microphones are well suited for this application because of the desired small size and high frequency range.

The majority of previous research in MEMS microphones has focused on audio microphones. However, this project will improve on previous MEMS-based aero acoustic microphones and is the first dual-backplate capacitive MEMS microphone developed for aero acoustic applications.

Accomplishments

We focused on documentation of research results and the release of more microphones. We developed a complete electromechanical lumped-element model for the dual-backplate microphone. In addition, we developed a noise model for the microphone and completed the analysis for the microphone packaged with a charge amplifier. To enable the reliable packaging of the released microphones, we modified the release process to include bond pad metallization. Initial attempts to wire bond to the polysilicon bond pads proved unreliable and resulted in many damaged devices. The bond pad metallization is not trivial, as the metal is exposed to the release etchant. This etchant is some form of HF mixture to etch the sacrificial oxide; initially, 49% HF was used for the release etch.

The first metallization we attempted was gold with a chromium adhesion layer. These metals were chosen because of their resistance to HF. However, devices released with the Au/Cr metallization did not function properly. After a thorough investigation of the device failure, including a literature search and analysis using scanning electron microscopy (SEM), we determined that the presence of gold increases the HF etch rate of polysilicon. Based on the literature, we believe that Au nanoparticles released by the Au metallization act potentially as a catalyst for HF. This results in damage to a critical feature of the microphone, an electrical connection from the bottom backplate to the bond pad in POLY0.

The latest work focused on developing a release process that utilizes aluminum bond pads. However, typical HF solutions readily attack aluminum. We found that an oxide etchant, Silox Vapox III produced by Transcene Company, Inc., provides a sufficient etch rate for oxide while providing a selectivity of about 50:1 to aluminum. Initial testing shows that this etchant should be able to successfully release the microphone with aluminum metallization.

Significance

There are several contributions of this research to the general scientific and technical community. As part of this work, we completed detailed modeling of a dual-backplate microphone. A lumped element model for a dual-backplate microphone was developed. This model considers the effects of the microphone structure and includes the transduction elements to give an electrical output. We also developed a noise model of the microphone. This can be analyzed with either a voltage amplifier or charge amplifier to study the noise sources of a dual-backplate microphone. These models will be useful to researchers developing future dual-backplate microphones for any of a variety of applications, including those specific to national security issues.

This device shows the feasibility of a dual-backplate capacitive microphone for aero acoustic measurements. The designed microphone has achieved a high bandwidth and a wide dynamic range. Furthermore, this device demonstrated a novel use of the SUMMiT V process and the viability of this process for MEMS microphones.

Refereed Communications

D.T. Martin, J. Liu, K. Kadirvel, R.M. Fox, M. Sheplak, and T. Nishida, "Development of a MEMS Dual-Backplate Capacitive Microphone for Aero acoustic Measurements," presented at the 44th AIAA Aerospace Sciences Meeting and Exhibit, Reno, NV, January 2006.

J. Liu, D.T. Martin, K. Kadirvel, T. Nishida, L. Cattafesta, M. Sheplak, and B.P. Mann, "Nonlinear Model and System Identification of a Capacitive Dual-Backplate MEMS Microphone," to be published in the *Journal of Sound Vibration*.

Other Communications

J. Liu, D.T. Martin, K. Kadirvel, T. Nishida, M. Sheplak, and B.P. Mann, "Nonlinear Identification of a Capacitive Dual-Backplate MEMS Microphone," presented at the 2005 ASME International Design Engineering Technical Conferences, Long Beach, CA, September 2005.

J. Liu, D.T. Martin, K. Kadirvel, T. Nishida, L.N. Cattafesta, M. Sheplak, and B. Mann, "Nonlinear System Identification of a MEMS Dual-Backplate Capacitive Microphone by Harmonic Balance Method," presented at the 2005 ASME International Mechanical Engineering Congress and Exposition, Orlando, FL, November 2005.

Design, Analysis and Control of MEMS Devices for Micromanipulation Tasks

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Project Purpose

The objective of this research is to develop advanced microelectromechanical systems (MEMS) micromirror arrays for use in adaptive optics applications such as optical communications and imaging systems. In order to realize the full capabilities of MEMS optical systems for the demands of next-generation technologies, MEMS micromirror components need to be robust and agile to the changing needs of performance and environment with precise and accurate positioning. Micromirror arrays are one of the most successful and versatile MEMS applications, including optical switches for telecommunications, scanning and imaging for projection displays, diffraction gratings for spectroscopy, and adaptive optics for wave front correction.

Many of these devices require large arrays of micromirrors and it is desirable to ensure accurate positioning capabilities for each mirror in the array despite the presence of outside disturbances or variations from the fabrication process such as small deviations in dimensional or material properties across the array. Many of today's emerging technologies require true analog positioning capabilities and in order to guarantee precision and accuracy of the mirror position for analog operation, closed-loop feedback control techniques are needed.

Feedback control has long been used in many macroscale systems to correct for such factors, yet limited work has been done to apply these techniques to MEMS systems. Current state-of-the-art micromirror arrays either rely on discrete open-loop actuation that may limit the device to on/off binary operation or require extensive calibration to simulate analog performance. For applications that require continuous analog positioning of very large arrays of mirrors (on the order of millions), these are not optimal or efficient solutions. The device performance must be robust with respect to parametric uncertainties from the fabrication process as well as environmental noise and uncertainties in the feedback-loop from the sensor.

This research is focused on the development of micromirrors with closed-loop control to ensure accurate position tracking across an array of devices in the presence of parametric uncertainties and external disturbances. This goal will be achieved by considering both optimized design of the actuators as well as developing closed-loop control schemes to meet the unique needs of MEMS systems. The success of this project will lead to new capabilities for MEMS optical systems and provide means for increased reliability and precision.

Accomplishments

We filed for a patent on a mechanism design that seeks to eliminate the problem of electrostatic pull-in on the micromirrors. Pull-in is a common feature of electrostatic actuators and limits the range of analog motion of the mirror and also creates hysteresis in the motion of the device. Eliminating this problem will ensure greater range of motion and stability for the micromirror arrays.

We completed designs of new micromirror arrays that incorporate on-chip piezoresistive position sensing. The new designs have been fabricated in SUMMiT V™ and await further testing. The designs will establish the capabilities of creating piezoresistive sensing within the standard SUMMiT process by utilizing the process layers in a novel fashion. In addition, the new arrays will be used to study the effectiveness of using either distributed (i.e., every micromirror's position is sensed) or localized (i.e., only a few mirrors' positions are known) sensing to achieve active control of the entire micromirror array.

We continued development of the device model for use in design and simulation of the closed-loop control system and identified expected sources and values of uncertainties to incorporate into the model for robust control design. We developed an optical testing method to obtain real-time data and create a test bed for experimentation.

Significance

The full impact of microsystem technology has thus far been limited by a lack of reliable, accurate, and high-precision MEMS devices. This project will lead to new capabilities for MEMS optical systems and provide a means for strengthening Sandia's national security capabilities by integrating more reliable and precise microsystems into next-generation communication and imaging technologies.

Our accomplishments have provided the fundamental modeling as well as the design and fabrication of an experimental module that will enable viable demonstration of passive and active control methodologies. The objective is to achieve micromirror arrays with precise and accurate positioning enabled by use of robust, optimized design and control techniques. The successful completion of this work will allow micromirrors for adaptive optics applications that are robust to parametric uncertainties that commonly arise through microfabrication processes as well as to disturbance rejection and plant instabilities.

The application of optimal design methods and closed-loop control techniques will enable cost reduction as the devices will no longer require extensive calibration for open-loop performance, as well as improved performance and reliability. Further, the incorporation of on-chip sensing mechanisms into the device will allow for compact realization of complete microsystems. This method for using piezoresistive methods within SUMMiT V fabrication is novel and its success will open up new areas of device applications.

Other Communications

J.R. Bronson, G.J. Wiens, and J.J. Allen, "Modeling and Alleviating Instability in a MEMS Vertical Comb Drive Using a Progressive Linkage," in *Proceedings of the ASME International Design Engineering Technical Conference*, September 2005.

J.R. Bronson and G.J. Wiens, "Control of Micromirrors for High-Precision Performance," in *Proceedings of 2006 Florida Conference on Recent Advances in Robotics*, May 2006, Miami, FL.

Capture and Utilization of Prosody in Disambiguating Spoken Speech

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Project Purpose

A large amount of work has gone into statistical and semantic analysis of text to support many different national security applications. However, the words themselves are only one aspect of text that people use to convey meaning in spoken dialog. This project with the University of Illinois at Urbana-Champaign investigates some of the other aspects.

The goal of the project is to gain a better understanding of how people use other types of information to deal with ambiguous speech. A critical avenue of research in this area is how people use prosody, including cues like fundamental frequency, harmonics, and amplitude. By conducting experiments investigating human use of prosodic cues, technologies may be developed that help resolve ambiguities the same way people do. Our research focuses on modeling how people use prosody to resolve ambiguity, using electroencephalography to track brain responses to sentences containing ambiguities.

Accomplishments

We are pursuing two related lines of research in our laboratory. The first explores the consequences of ambiguous information in language processing and cues that readers or listeners can use to navigate ambiguity. Although ambiguity is highly common in language, our studies show that readers are often unaware of it. This leads to processing difficulty and misunderstandings in which the readers never realize that they have failed to reach the correct interpretation of a statement. The potential consequences of these errors are important, so we are laying the groundwork for studies of cues, such as prosody, that could help listeners avoid ambiguity altogether.

Our second line of research also relates to errors of which people are unaware. We conducted a series of memory studies that investigates the impact of context and study strategies on memory for verbal materials. We found that readers make high numbers of memory errors when tested on lures that are similar in either meaning or visual form to words on a study list. In both cases, the readers are highly confident in saying that they had studied words that never actually appeared. However, we found that changing the context in which the words were studied had a dramatic impact on the types of lures that readers were susceptible to, probably because of differences in their study strategies when faced with different kinds of materials.

The information we are gathering from both of these lines of research is potentially useful for helping people to become aware of these unconscious errors. Once they are aware of these pitfalls, they could change their information processing strategies in order to avoid them.

Significance

These accomplishments are helping advance the basic science of understanding how people use language, specifically how they disambiguate language. As this work matures, we anticipate that it will yield an understanding of language that will help advance Sandia-developed capabilities for building models of individuals based on their speech. Increasing our ability to automatically process this type of information will help advance analysis and decision support tools and benefit national security related programs at Sandia.

Refereed Communications

L.E. Matzen and A.S. Benjamin, "Remembering Words Not Presented in Sentences: How Study Context Changes Patterns of False Memories," submitted to the *Journal of Experimental Psychology: Learning, Memory, and Cognition*.

Pareto Optimization Techniques

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Project Purpose

Multiobjective optimization presents a number of significant technical challenges. The first challenge occurs when conflicting multiple objectives lead to multiple optimal solutions. Second, given that multiple optimal solutions are inherent in multiobjective optimization, evaluating solutions will be significantly more difficult than single objective optimization problems, requiring the need for additional post-optimality analysis of the solution space.

The research focus of this project can be summarized into two parts. The first part of the research consisted of investigating multiobjective optimization algorithms in the field of reliability analysis. The second part of the research focused on post-optimality analysis, which is the analysis of solutions obtained after the optimization process. These two areas of research are two integral parts of the general multiobjective optimization analysis framework. The project team includes a doctoral student at the University of Illinois.

Accomplishments

We studied several different multiobjective optimization algorithms. These algorithms were applied to different reliability test problems, including those similar to the analysis of the Apache helicopters and the Naval Landing Craft Air Cushions.

In particular, the Nondominated Sorting Genetic Algorithm II (NSGA-II) was compared to other single and multiobjective genetic algorithms. NSGA-II was shown to be superior in the reliability analysis domain. It was able to efficiently generate large diverse sets of Pareto optimal solutions. Finding large sets of diverse Pareto optimal solutions provides the decision makers with a full spectrum of trade-off analyses. In addition, unlike other multiobjective genetic algorithms (MOGA), NSGA-II requires minimal problem dependent adjustments, using only a few user-defined parameters. We are incorporating such multiobjective optimization capabilities into Pro-Opta, a reliability and optimization analysis tool developed at Sandia.

One important objective is helping the decision makers visualize large sets of Pareto optimal solutions. In large and high-dimensional problems, this is not a trivial task. We began investigating interactive approaches to presenting the solutions to the decision maker. This work is also being incorporated into Pro-Opta.

Another important focus is the analysis of the Pareto optimal solutions to enable the decision maker to identify the best solutions across a very large number of Pareto optimal solutions. We focused on finding preferred subsets of Pareto optimal solutions. To do so, we introduced and formulated a new discrete optimization problem to obtain such subsets. We compared and studied two exact algorithms and five heuristics. We are also trying to identify characteristics of Pareto optimal solutions. Such characteristics can help identify solutions that are robust and desirable. Several evaluation metrics were proposed and are under investigation. Other techniques such as clustering are also under evaluation. By gaining more information about Pareto optimal solutions, we expect to achieve overall improvements in the multiobjective optimization process.

Significance

The area of multiobjective optimization presents a number of significant technical challenges: specifically, when conflicting multiple objectives lead to multiple optimal solutions. That is, it is very difficult to find a set of well-distributed optimal solutions that can be evaluated by the analyst within the context of their domain-specific problem. This in turn leads to the need for visualizing complex multiobjective Pareto fronts.

As Sandia extends its GO genetic optimization software into the multiobjective realm, capabilities developed in this project will contribute to the development of a leading multiobjective optimization tool that will provide significant technical benefit to Sandia's nuclear weapons, homeland security, and defense missions.

Refereed Communications

"Finding Preferred Subsets of Pareto Optimal Solutions," accepted for publication in the *Journal of Computational Optimization and Applications (COAP)*.

Rapid Chemical Analysis Using Micropower Gas Chromatographic Columns and Latching Microvalves

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Project Purpose

Chemical sensing is critical for a wide variety of applications, including those in industrial process control, environmental monitoring, health diagnosis, and homeland security. Individual sensors often lack speed, sensitivity, stability, and (especially) selectivity. Gas chromatography (GC) provides a solution to these problems, but commercial instruments are bulky, power-hungry, and inefficient at best. Thus, this project seeks to develop GC components for a high-performance separation and detection, ultraminiature (1 cubic centimeter), micropower gas chromatography system capable of analyzing a wide variety of gaseous mixtures in seconds with high selectivity and part-per-billion sensitivity. We are also investigating electrostatically latching thermopneumatic microvalves for the purpose of pressure and flow tuning and programming the separation. This project is in collaboration with the University of Michigan.

Accomplishments

The microfabricated GC column designed in this project has substantially smaller size and thermal mass, and higher chromatographic performance than any reported in the past. The goal is to perform separations at temperatures above 100 °C, using less than 20 milliwatts of power. A thermal ramp rate on the order of seconds is sought, with the ability to separate 30+ compounds in less than five minutes.

Initially, we used a simple column fabrication process for rapid device design and testing. This process used a deep reactive-ion etch followed by anodic bonding of a glass plate to close the channel. Columns were coated with polar and nonpolar stationary phases to achieve separations of chemical compounds. The nonpolar, three-meter column has separated over 30 components in less than six minutes, achieving over 4000 theoretical plates per meter. These characteristics facilitated miniaturization, but posed significant design challenges. We incorporated integrated pressure sensors with thin boron-doped silicon membranes. The pressure sensors are necessary for repeatability in measurements, as well as for failure detection in the column.

A second approach to column formation used a buried microchannel that we sealed through chemical vapor deposition and then etched back to remove the unnecessary substrate. The column was fully suspended to reduce heating power consumption and to improve its thermal ramping rate. The device requires only 11 milliwatts to maintain the 25-centimeter long column at 130 °C. This low mass, isolated column requires five times less power and is four times faster (thermally) than any other column to date. Furthermore, it achieves over a five-fold improvement in separation performance over previously reported low-power columns.

In order to achieve the aggressive valve goals, we are developing and improving thermopneumatic valves for low power and fast operation. The approach uses a thermally isolated thermopneumatic chamber and an electrostatic latch, harnessing the advantages of both actuation mechanisms. Initial testing for the fabricated microvalves revealed an open flow rate of 8 standard cubic centimeters per minute at a differential pressure of 5 torr, and a leak rate of 0.001 standard cubic centimeters per minute at 860 torr. The thermopneumatic actuator closes the valve in under 430 milliseconds with 250 milliwatts. In conjunction with the electrostatic latch, 60 milliwatts is required to keep the valve closed. The integrated valve plate position sensor has a sensitivity of 1.3 femtofarads per torr and is used to monitor when the valve has closed and, thus, when to activate the electrostatic latch.

Significance

Gas chromatography is one of several highly versatile, highly sensitive chemical analysis methods. It is the most amenable to extreme miniaturization. The research and advances made in this project serve to retain the adequate analytical fidelity of the method as further miniaturization occurs. At present, GC has been miniaturized to a battery-powered hand-held instrument. This is suitable for military and first responders to perform air monitoring for toxic chemicals and chemical warfare agents. To use this instrument, a technician must pause from activities, use a keypad, and wait at least one minute (two minute run-to-run cycle time). Batteries, creating the heaviest mass of the entire system, last approximately four hours. Extreme miniaturization and commensurate savings in power consumption will lead to microGC systems weighing ounces that can run autonomously for days unobtrusively in a package similar to a button. This also opens the door for surveillance using unmanned aerial vehicles, distributed ground sensors, and other leave-behind methods.

Because GC is such a versatile technique microGCs will find use in gas refineries, pharmaceutical manufactures, chemical factories, semiconductor manufacture facilities, etc. GC breath analysis for medical diagnosis is presently under study. These and other applications give this research project impact in energy, as well as military, nonproliferation, and homeland security missions.

Refereed Communications

M. Agah, J.A. Potkay, G.R. Lambertus, R.D. Sacks, and K.D. Wise, “High-Performance Temperature-Programmed Microfabricated Gas Chromatography Columns,” *IEEE Journal of MicroElectroMechanical Systems*, vol. 14, pp. 1039-1050, October 2005.

C.J. Lu, W.H. Steinecker, W.C. Tian, M.C. Oborny, J.M. Nichols, M. Agah, J.A. Potkay, H.K.L. Chan, J. Driscoll, R.D. Sacks, K.D. Wise, S.W. Pang, and E.T. Zellers, “First-Generation Hybrid MEMS Gas Chromatograph,” *Lab on a Chip*, vol. 5, pp. 1123-1131, October 2005.

Other Communications

J.A. Potkay, G.R. Lambertus, R.D. Sacks, and K.D. Wise, “A Low-Power Temperature- and Pressure-Programmable µGC Column,” in *Proceedings of the Solid-State Sensor, Actuator, and Microsystems Workshop,* pp. 144-147, June 2006.

Microfabricated Preconcentrator for Microscale Gas Chromatography

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Project Purpose

Cryogenic cooling for sample injection is ubiquitous in large-scale commercial gas chromatography (GC) systems. However for microscale systems, preconcentration via thermal desorption is a superior sample injection solution. The goal of this project is to implement a microscale preconcentrator for use as the analytical front-end of a microGC where the primary application is rapid, complex mixture analysis.

At the University of Michigan's Center for Wireless Integrated MicroSystems (WIMS), a microfabricated preconcentrator was developed to enable high-resolution chromatography with low-parts-per-billion (ppb) sensitivity. The packaging and integration goals for this project include modularity and environmental robustness for reliable integration into a common microfluidic/electrical substrate.

Miniaturization of preconcentrators using packed beds of granular adsorbents for microscale and portable GC systems has not been developed widely due to the difficulty in manipulating micron-diameter granular adsorbents to construct microscale packed beds. The packed bed approach is different from microhotplate-based preconcentrator designs and allows for the accommodation of adequate adsorbent mass to achieve quantitative trapping of trace level volatile organic compound (VOC) mixtures at ppb concentrations for indoor air analysis.

A cavity microheater-based preconcentrator design is used in conjunction with an adsorbent-solvent filling technique and subsequent solvent-compatible wafer-level sealing technology to fabricate preconcentrators capable of quantitative capture of ppb-level VOCs. The preconcentrator design goals are to minimize total analysis time by reducing the preconcentrator sampling times and to reduce the desorbed injection plug width to the microGC column at low column inlet velocities.

Further preconcentrator miniaturization, wafer-level packaging, gas interconnections, and electrical integration with the WIMS microGC are also addressed. Advances in thermal isolation, vacuum packaging, and leak-proof fluid interconnection technologies for the preconcentrator developed in this project benefit other microscale microGC components (columns, substrate, sensor arrays) and portable chemical and biological analysis systems.

Accomplishments

- We built a new preconcentrator measurement system to characterize device performance, including sample extraction and sample injection.
- We demonstrated large adsorptive capacity with our microdevice, including 300 mL exhaustive extraction of octane at 25 mL/minute, room temperature, and parts-per-million concentrations.
- The new effluent curve data are being used in conjunction with a new preconcentrator model to describe the performance limits of packed bed designs.
- Sample injection studies of the micropreconcentrator show injection plug widths on the order of seconds, appropriate for injection onto standard-bore 3 m microcolumns.
- We customized two commercially available packages for use with the preconcentrator to integrate it with macro- and microscale gas chromatography systems. The technology is designed to allow reuse so that a preconcentrator can be tested in a laboratory-scale system for functional verification, followed by microscale integration.

Significance

A combined sample extraction and injection device is key to any real-time gas analysis system, including those for chemical and biological (C/B) warfare agent detection. The microscale preconcentrator results of this project are applicable to the development of these miniaturized C/B detection systems. Key technologies include robust microdevices and electrical interconnects, silicon micromachining techniques, thermal isolation structures and methods, and methods of integration into analytical systems. These leverage Sandia's microsystem efforts.

Results from this research could find use in gas refineries, pharmaceutical plants, chemical factories, semiconductor manufacture facilities, and so on. Gas chromatographic breath analysis for medical diagnosis is another key area presently receiving attention. These and other applications would give this research project impact in defense, energy, nonproliferation, and homeland security.

Analysis of Bead Attached Ion Channels on Optically Addressable Microfluidic Electrode Arrays

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Project Purpose

In order to better understand the fundamental structural dynamics of membrane-bound ion channels and membrane-bound proteins in general, we are collaborating with the University of New Mexico to develop new solid-supported lipid bilayer platforms in which single membrane-bound proteins can be electrochemically and optically interrogated. It has recently been shown that membrane-associated proteins can be incorporated into lipid bilayers supported on silica beads. Expansion of these capabilities through high-throughput parallel and multiplex strategies offers great possibilities for biosensor technology; however, functional reconstitution of complex transmembrane proteins into this platform has yet to be demonstrated.

The introduction of functional transmembrane proteins into supported bilayer-based biomimetic systems presents a significant challenge for biophysics. Among the various methods for producing supported bilayers, liposomal fusion offers a versatile method for the introduction of membrane proteins into supported bilayers on a variety of substrates. We investigate the properties of protein contained in unilamellar phosphocholine lipid bilayers on nanoporous silica microspheres to determine the effects of the silica substrate pore structure and the curvature on the stability of the membrane and the functionality of the membrane protein. Supported bilayers on porous silica microspheres show a significant increase in surface area on surfaces with structures in excess of 10 nm, as well as an overall decrease in stability resulting from increasing pore size and curvature.

Comparison of liposomal and detergent-mediated introduction of purified bacteriorhodopsin (bR) and the human type 3 serotonin receptor (5HT3R) are investigated, focusing on the resulting protein function, diffusion, orientation, and incorporation efficiency. In both cases, functional proteins with near-native diffusion constants are observed, however, the reconstitution efficiency and orientation selectivity are significantly enhanced through detergent-mediated protein reconstitution. The results of these experiments provide a basis for bulk ionic and fluorescent dye-based compartmentalization assays, as well as single-molecule optical and single-channel electrochemical interrogation of transmembrane proteins in a biomimetic platform.

Accomplishments

Our milestones were aimed at characterizing the biophysical properties of the membrane-bound proteins, bacteriorhodopsin and the serotonin type 3 receptor, on the nanoporous silica bead platform. We completed studies on the long-term stability, detergent solubilization, and protein incorporation in nanoporous microsphere supported bilayers (NMsbs) resulting from varying particle diameter and surface porosity. In addition to traditional proteoliposome deposition, we tested a new method for introducing detergent-solubilized membrane proteins into preformed supported bilayers. We completed a comparison of the two methods based upon the incorporation efficiency, orientation specificity, and functionality. Finally, micromanipulation and patch-clamp electrochemical measurements were attempted on the NMsbs.

We made several noteworthy observations while probing the effects of substrate pore size and diameter in phosphocholine-supported bilayers. With respect to curvature, the larger diameter beads displayed the greatest capacity to maintain compartmentalized fluorescent dye and calcium ions and were the most resistant to detergent solubilization. The conclusion that high curvature in phosphocholine-supported bilayer systems can significantly reduce the resulting bilayer stability suggests the potential significance of the intrinsic curvature of the incorporated bilayer components. Thus, adjusting the lipid component mixture to more efficiently match the curvature of a specified supported bilayer system may offer a large increase in bilayer stability.

When considering pore size, we observed that in bilayers with pores less than or equal to 2x the bilayer thickness, fluid bilayers span surface structures much like a bilayer in its gel phase. When the pore sizes are much larger than the bilayer thickness, the membrane is significantly invaginated into the pore, thus increasing the membrane surface area. For various applications, different degrees of invagination may be appropriate; however, the fraction of membrane-bound protein exposed to the surface may be significantly increased and the overall bilayer stability is diminished. In probing detergent solubilization, exposure of porous bead-supported bilayers to increasing detergent concentrations showed reversible detergent saturation of the bilayer; however, even at detergent to phospholipid ratios exceeding 50:1 (above the critical micelle concentration), we did not observe complete bilayer solubilization.

To rule out the possibility of perturbations resulting from surface accessible fluorescent tags, the experiment was repeated with an in-membrane fluorescent label with the same result. The evidence suggests, however, that the platform described is not a case of a detergent-resistant bilayer as seen in many biological systems, but possibly the result of the high surface area for mixed micelle adsorption. Finally, protein reconstitution into preformed supported bilayers was carried out at detergent saturating conditions and resulted in a large increase in reconstitution efficiency and orientation selectivity.

Significance

Porous silica bead-supported bilayers show promise for the future study of a wide range of membrane-bound proteins, providing a stable and size-selective medium that is easily interfaced with current optical and electrochemical technologies, and show promise for new chip-based sensor technology. Single-molecule spectroscopic measurements, in combination with electrical detection, offer a unique opportunity for obtaining a dynamic view of structural/functional relationships on transmembrane proteins. However, the potential impact of combined optical and electrochemical measurements goes well beyond the study of basic biophysical mechanisms and can provide the ultimate in biodetection schemes: using the specificity of biochemical interactions, the sensitivity of single-molecule fluorescence detection, and the enormous electrochemical amplification afforded by the opening of a membrane channel.

Nanostructured Electrocatalyst for Fuel Cells: Silica Templated Synthesis of Pt/C Composites

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Sandia Principal Investigator

Project Purpose

Platinum and ruthenium (Pt-Ru) blacks are the common methanol oxidation electrocatalysts employed in direct methanol fuel cells (DMFCs). Noble metal utilization in these catalysts has been traditionally low in comparison to anode catalysts used in hydrogen/air fuel cells. One of the reasons for that is the relatively low surface area of these catalysts resulting in inefficient mass transport within the fuel cell catalytic layer. By structuring the electrocatalyst on the nanoscale, advantageous local mass transfer properties can be attained. The essential balance of kinetic and transport properties of the electrocatalysts are due in part to the hierarchical structure that combines distinct structural considerations across length-scales. This work with the University of New Mexico will assist in understanding these properties and develop enhanced materials through the synthesis and investigation of novel bimetallic Pt-Ru nanowire networks.

Accomplishments

The primary accomplishment of the work during was the exploration of the synthesis processes and electrochemical activity of nanostructured Pt-Ru nanowire networks. Because the ability exists to alter and fine-tune the Pt-Ru microstructure, fundamental studies of the local structures can be undertaken next year. By controlling the morphology of the Pt-Ru catalyst on the nanoscale, we can study the effects of the local structure on electrochemical activity and a new class of catalysts will be developed.

We formulated and investigated an innovative aerosol-based synthesis approach that involves using silica precursors and/or preformed particles to template the Pt and Ru precursors, which is followed by silica removal. In this method of materials self-assembly, a solution of metal precursors and the silica template are atomized and undergo spray pyrolysis. This process results in colloidal silica particles in the precursor solution that form a mesostructured Pt-Ru network via the silicate precursors, resulting in a final microporous PtRu network. A combination of variables allows a hierarchically structured Pt-Ru nanowire network. Confirmatory studies of the structure and morphology are ongoing.

We performed studies of the electrochemical behavior of these catalysts on a rotating disk electrode. Initial studies show that 70 wt.% samples have an order of magnitude increase in activity compared to the initial formulations. We are benchmarking aerosol-derived catalysts with respect to the most advanced industrial catalysts for methanol oxidation, Pt-Ru Vulcan XC72. While the activity per gram of catalyst is not at the level of a commercial catalyst, improvements in aerosol-derived materials suggest its capacity.

The researchers at the University of New Mexico will continue their effort in developing synthesis methods for high surface-area methanol electro-oxidation catalysts. Optimal formulation of the precursor solution for the aerosol synthesis process will be determined. We will commence model fuel cell investigations in a 5 cm^2 membrane electrode assembly to study the behavior of this new catalyst and to improve the catalytic activity of methanol electo-oxidation catalysts. We will explore promoters such as V and W oxides. These oxides will be included in the sol-gel synthesis route and an integrated synthesis protocol will be developed. We will explore mesoporous materials templating also as a method for nanophase stabilization, and will develop a phenomenological model of catalysis in open frame structured materials.

Significance

An innovative aerosol-based synthesis approach is employed that involves using silica to template Pt and Ru precursors, which is followed by silica removal to form nanostructured catalysts. In this method of assembly, a precursor solution is atomized and undergoes spray pyrolysis. The catalyst precursor solution consists of colloidal silica particles with an average diameter of 20 nm, and metallic-amine Pt-Ru complexes. In this method of synthesis, all phases are in intimate contact during synthesis, which promotes the production of a homogeneous material with a higher degree of alloying. The dried powder is then reduced under hydrogen flow at 300 °C for two hours. This is followed by removal of the silica template with a 7M KOH solution. This research has the potential to access more of the catalytic area than traditional catalysts, thus affording the potential to achieve very low loadings in both methanol and hydrogen fuel cells.

Refereed Communications

E. Switzer, M. Bore, A. Datye, and P. Atanassov, "Hierarchically Structured Platinum-Ruthenium Electrocatalysts for Direct Methanol Fuel Cells," in *Proceedings of the 209th Electrochemical Society*, p. 1145, May 2006.

Dynamics of Propagating Shock Waves and Phase Fronts

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University of Texas at Austin

James Redmond (Org 1525)
Sandia Principal Investigator

Project Purpose

Phase transformations and shocks are developed in many high-energy impact and explosion problems. Understanding the physics of these phenomena in a wide range of materials permits their use in structures designed to mitigate the effects of blast or impact events. This research with the University of Texas at Austin involves a combination of experimental observations, analytical modeling, and numerical simulations of models to examine impacts that generate a fan of elastic waves followed by phase transformation and/or shock wave.

Accomplishments

I. Experimental

- We successfully modified a tensile impact experimental setup to allow visual inspection of a specimen during impact, and to allow the capability to increase impact velocity.
- We ran a series of impact experiments on rubber specimens in the modified tensile impact setup, as well as a series of retraction experiments with the use of a high-speed camera to monitor specimen displacement as a function of time.
- We developed a working code that calculates the strain and particle velocity of the rubber as a function of time using images taken during the experiment of lines drawn on the specimen. This code also estimates the constitutive behavior of and the wave speeds in the material during experiment.
- We obtained NiTi specimens and found the heat treatment that allowed the specimens to undergo the phase transformation from austenite to martensite at room temperature. This eliminates the need for heating devices that obstruct the field of view of a high-speed camera.
- We developed a working code that uses the digital image correlation technique to record the strain history of a specimen during loading and we verified its capability and resolution in quasistatic tensile tests on NiTi.

II. Comparison of Theory and Experiments

- We modified theory developed by Knowles to account for the material properties of the rubber used in the impact and retraction experiments.
- We showed that the theory qualitatively describes the response of rubber to impact and retraction during the elastic fan of waves prior to the arrival of a shock wave, but not quantitatively.
- We showed that during these experiments a partial phase transformation from amorphous to crystalline (impact) or crystalline to amorphous state (retraction) occurs prior to arrival of a shock wave.

Significance

The partial phase transformation of rubber prior to arrival of a shock wave during impact and retraction is a new observation and gives an insight into how to better model the response of rubber. The tensile impact experimental setup and the two codes that can be used to determine strain and particle velocity history provide a new set of tools that can be used to investigate other materials that experience a phase transformation and/or shock wave during impact.

With this new tool set, better models of the kinetic relation can now be developed to fully describe a material's response to a given impact. Knowing the magnitude of the driving force and the speed of the phase transformation front/shock wave, engineers will know when to use these materials and how to design a structure using their material properties for use against certain types of impact.

The accomplishments of this project are beneficial to the scientific and technical community and Sandia mission areas in science, homeland security and nuclear weapons. This work will advance the ability to develop accurate constitutive models that predict the mechanical response of materials to extreme conditions and new advanced computational mechanics codes to simulate the response of nuclear weapon components.

Refereed Communications

J. Niemczura and K. Ravi-Chandar, "Dynamics of Propagating Phase Boundaries in NiTi," *Journal of the Mechanics and Physics of Solids*, vol. 54, pp. 2136-2161, October 2006.

J. Niemczura and K. Ravi-Chandar, "On the Propagation of Finite Deformation Waves in Rubber," submitted to *Journal of the Mechanics and Physics of Solids*.

Adaptive Algorithms for Use in the Rejection of Periodic Disturbances of Unknown Frequency

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University of Utah

Eugene Hertel, Jr. (Org. 1516)
Sandia Principal Investigator

Project Purpose

The objective of this research with the University of Utah is to investigate algorithms for the rejection of unknown disturbances, with a particular interest in active noise and vibration control applications (ANC, AVC, or ANVC). Disturbances are assumed to be the sum of periodic signals with time-varying magnitudes, frequencies, and phases. The control algorithms are of the pure feedback type, where no reference sensor is assumed to be available to give a preview of the disturbance. These problems are more difficult to solve and less well understood. The algorithms are also able to handle systems with unknown dynamics that may change significantly over time.

Specifically, this work involves the development of new algorithms for adaptive disturbance rejection, with particular emphasis on the cancellation of periodic noise disturbances. In the development and implementation of these algorithms, we are using multichannel active noise control experiments to explore issues related to more globalized disturbance rejection, and we are examining the effects of adding additional sensors/actuators to multichannel configurations.

A key emphasis of this project is to treat unknown disturbances as well as unknown systems. Periodic disturbances with unknown frequencies may vary over a wide range. In adaptive feedback control, the rejection of such disturbances can be accomplished by using frequency estimation techniques or by deriving controller structures that obtain this estimate implicitly. Additionally, methods involving modified least-squares identifiers can be derived for identifying plant parameters online. We are investigating these methods for the development and analysis of simple and efficient algorithms for systems where both disturbance frequency and system dynamics are unknown and possibly time-varying. The stability and parameter convergence of all algorithms considered will be examined through averaging theory.

Accomplishments

New algorithms for the rejection of periodic disturbances continue to be developed at the University of Utah. The focus on disturbances that are known to be periodic in nature makes this research relevant to many applications involving rotating equipment. Specifically, we are paying attention to narrowband adaptive feedback control, in which knowledge of the disturbance frequency and plant dynamics allows for perfect cancellation of periodic disturbances. We are considering algorithms that identify and adapt to variations in either disturbance or plant parameters. By assuming that the system dynamics have reached steady-state with respect to parameter update, simple and meaningful algorithms with established convergence properties have been derived.

Since many applications such as those concerning rotorcraft involve unknown and time-varying dynamics due to variations in environmental factors, we developed methods for identifying plant parameters online. Several such methods were implemented and investigated on an active noise control testbed at the University of Utah. A commonly used method involves the use of conventional least-squares techniques to continuously update an estimate of plant dynamics. By deriving a linear expression at the output of the plant, we found an estimate of the disturbance as well as the plant frequency response. This estimate is then used in determining the control input that exactly cancels the disturbance. Estimation of the parameters occurs continuously, whereas previous methods have required the collection of batches of data. We studied algorithms of both a continuous and discrete nature, and we implemented several different controller structures.

Based on this set of linear equations describing the plant output over time, we used recursive least-squares algorithms to achieve 97 percent attenuation of sinusoidal disturbance acting on an unknown system through single-channel ANC experiments. We compared convergence rates among the various controller structures. Also, we investigated the ability to track both slowly and rapidly time-varying system parameters while maintaining considerable disturbance rejection. We used an exploration of various identification algorithms to reduce the effect of transients when rapid parameter variation occurs. The goal in this work is to obtain solutions that are viable in engineering practice.

Significance

There are many examples of applications where disturbance rejection is a primary control objective. Among these applications are a variety of engineering problems including the active control of noise in turboprop aircraft, the reduction of road noise in cars, headphones for noise cancellation, vibration reduction in helicopters, the reduction of optical jitter in laser communication systems, isolation in space structures of vibrations produced by control moment gyroscopes and cryogenic coolers, suppression of gearbox housing vibrations, and track-following despite eccentricity in disk drives and CD players.

In several of these applications, the tracking of time-varying parameters is essential. For example, in helicopters the plant may vary significantly due to changes in environmental conditions during flight. In applications for space exploration, repair is very costly, and it is preferable to have systems that can adapt to changes caused by aging or the harsh environment of space. The objective of this research is to derive simple and efficient algorithms for the rejection of periodic disturbances, with an emphasis on time-varying systems. While existing techniques enable one to tackle known systems, few methods are able to deal with time-varying systems and, typically, they assume the existence of a reference sensor.

Of interest in this project are feedback structures that require no reference sensor to feedforward an uncorrupted measure of the disturbance. Already, this problem has been seriously investigated at the University of Utah. We studied several theoretical techniques and found a method that continuously estimates the system dynamics. By assuming the disturbance is sinusoidal and of known frequency, the number of parameters is much smaller than required to describe the transfer function in ANC systems. From this linear expression, an estimate of both plant and disturbance parameters can be obtained. This estimate can then be used to exactly cancel the disturbance. The ability to track both rapidly and slowly time-varying systems demonstrates the practicality and robustness of this approach. Similar algorithms can be used for active vibration control and active noise control, and this research is, in particular, validated experimentally on an active noise control test bed at the University of Utah.

Data Collecting, Analysis, and Modeling to Better Understand Supercritical Water (SCW) Reactor Safety Technologies

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University of Wisconsin-Madison

Jason Zuffranieri (Org. 6761)
Sandia Principal Investigator

Project Purpose

In order to advance the development of supercritical water (SCW) reactors, mechanisms of heat transfer to supercritical fluids need to be further clarified to improve heat transfer calculations. Currently, there are no detailed velocity, density, or turbulence profiles obtained in water at critical pressures. The purpose of this experimental investigation with the University of Wisconsin is to develop a set of heat transfer measurements along with detailed information on the fluctuating velocities and density, in addition to the thickness of the momentum and thermal boundary layers. The experimental results will serve as a database to compare existing models and aid in the development of new models, which will be used to improve performance and decrease cost by increasing the efficiency of the systems under investigation.

Accomplishments

We built a SCW heat transfer test facility to allow for a detailed study of heat transfer to SCW in a circular annular geometry. The loop dimensions are approximately 2 m wide by 3 m tall and made of 4.29 cm inner diameter Inconel 625 piping. A 3.3 m long heater rod with a diameter of 1.07 cm spans the entire right leg of the loop and protrudes out both ends. This design permits the use of 16 thermocouples evenly spaced along the inner cladding of the 1 m heated length. The center portion of the right leg of the loop serves as the test section, allowing a 76 cm entrance length for both upward and downward flow studies.

The heater can generate up to 50 kW, giving a maximum heat flux of 1.5 MW/m^2. A pump capable of operating at supercritical conditions generates mass velocities in the range of 200 to 2000 kg/m^2s. The current configuration is up-flow, although the facility can be used for flows in either direction with only minor modification. The setup is capable of operating at any steady-state heat flux condition by using a variable heat removal system made up of copper cooling coils. Eight copper coils of various contact area are tightly wrapped to the Inconel piping. Heat removal by the cooling coils can be set to match that supplied by the heater by simply controlling which coils receive cooling water and controlling the respective flow rates.

About 33 percent of the heat transfer measurements for the planned test matrix have been completed. These experiments have been performed at a pressure of 25 MPa, with bulk inlet temperatures of 300 °C to 395 °C, heat flux of 250 kW/m^2 to 1MW/m^2, and mass velocities of 400 kg/m^2s to 1400 kg/m^2s.

Significance

In an effort to improve the efficiency of current light water reactors (LWRs), the Generation IV initiative has included the SCW reactor as one of the next steps in future nuclear reactors. An SCW reactor will achieve efficiencies of about 45-50 percent, compared with current LWR efficiencies of about 33 percent, by operating its coolant at higher temperature (500 °C) and pressure (25 MPa) than current LWRs. These operating conditions are above the pseudocritical temperature of water (defined as the temperature, for a given pressure, at which the specific heat exhibits a maximum) and thus the coolant of SCW reactors will undergo large thermophysical property changes.

Current models and correlations used for water near or at the supercritical region have not been able to accurately predict experimentally measured heat transfer coefficients, which have negative effects on system performance. With the Generation IV reactors set to come on-line in the near future, it is important to have a better understanding of the properties related to SCWR performance. This work serves a vital need in improving this understanding.

An Examination into the Chemical Properties of Supercritical Water

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Jason Zuffranieri (Org. 6761)
Sandia Principal Investigator

Project Purpose

This project with the University of Wisconsin is designed to establish concentrations or G-values of radicals formed per energy (“G-value” usually suggests molecules per 100 eV) for both neutron and gamma radiation as a function of temperature and pressure up to and beyond the critical point. Two separate pieces of data are needed to properly understand and simulate water chemistry at a given temperature and pressure. First, it must be known what concentration of radicals will form based on the dose from high and low linear energy transfer radiation. Second, the recombination rates of these radicals must be known.

In addition to direct water chemistry data, critical hydrogen concentration experiments are also run. These determine the amount of hydrogen necessary to sufficiently prevent the formation of all oxidizing species. Such water chemistry information will prove useful and will aid in the design and performance of Generation IV reactors.

Accomplishments

One of the challenges we have met has been the difficulty in measuring neutron and gamma dose to the water in the irradiation volume. Gamma dose was particularly difficult to measure since instruments and foils typically used to measure such high doses see interference from the high neutron dose. To overcome this challenge, we designed a series of experiments:

1. a neutron activation experiment using a sodium carbonate solution to determine thermal neutron flux
2. a Monte Carlo N-Particle model of the reactor to determine neutron energy deposition as a function of thermal flux
3. a radiolysis experiment measuring the concentrations of aqueous electrons and hydrogen radicals as well as the long-term formation of hydrogen gas at 25 °C or 100 °C
4. a simulation using known values at these temperatures to calculate the G-values for these radicals by both neutron and gamma radiation.

Experiments 1) and 2) can be used to determine total dose, experiment 3) finds total concentrations produced, 4) finds expected concentration from neutron dose, which can be subtracted from 3), thereby leaving gamma produced concentration, which can be translated into dose again by 4).

Significance

The supercritical water reactor, one of the Generation IV reactor designs chosen for research and development in the United States, faces many challenges in the design of materials that will be in contact with the water, especially at the core outlet. Chief issues already addressed in pressurized water reactors are worsened by higher pressure and temperatures as well as additional factors caused by the extreme changes in water properties at the critical point. Water chemistry will play a major role in the feasibility of using different types of steels, nickel-based alloys, and other metals as fuel cladding, pressure vessel lining, and piping of the system. Water radiolysis, which can create oxidizing species and change the corrosion potential of the cooling water, will be a significant aspect in consideration of water chemistry.

The results garnered from these experiments will be helpful in bringing about the implementation of the Generation IV reactors in the US, which will play an important part in defining the role nuclear energy will have in America's future.

Reliability of Materials in MEMS: Residual Stress and Adhesion in a Micro Power Generation System

Molly Kennedy
Washington State University

Neville Moody (Org. 8759)
Sandia Principal Investigator

Project Purpose

This project coordinates the work of a Ph.D. student at Washington State University with mentors at Sandia to determine a self-consistent method to quantify interfacial fracture toughness of thin film systems that contain tensile and compressive stresses. Experimental measurements of adhesion will be coupled with analytical solutions to determine interfacial fracture toughness. These results will provide computational model validation and design parameters and lifetime analysis for microelectromechanical systems (MEMS) structures and thin films in microelectronics the nation's stockpile. We used two of the three desired methods of interfacial adhesion, compressed overlayer buckling and four-point bend testing, to measure the interfacial fracture energy of metal-dielectric interfaces. Tested film systems include both Pt films used in MEMS and Au films used in Sandia microelectronics systems. This past year we focused on experimentally characterizing the effect of film chemistry using compressive overlayers and the influence of the applied stress on the calculated toughness.

Accomplishments

We focused on experimentally characterizing the effect of film chemistry on adhesion. We found the adhesion energy of a mixed chemistry interface to be proportional to the coverage of the film with the highest energy interface. This was shown to be important in determining the adhesion energy for nonuniform coverage of interlayers. In metallic film systems, an interlayer is often used to improve the adhesion. Processing conditions, however, often result in nonuniform coverage. In this set of experiments, the interfacial energy for $Pt/Ti/SiO_2$ initially scaled with nominal thickness of the interlayer and then effectively reached a steady-state value, which suggests a transition from island to uniform film coverage.

We built a four-point bend testing apparatus to measure films at a constant phase angle of 45 degrees. During this test, the film stack of interest is restricted by two elastic substrates on each side and then loaded in a four-point flexure at a constant displacement. With this type of loading, the moment is constant and the energy release rate can be obtained for interfacial cracks in the region between the inner loading spans.

Initial testing of Au and Pt film systems showed that interfacial cracks could be monitored and load plateau could be obtained. These plateaus are proportional to the interfacial fracture energy. In addition, we found that the interfacial fracture energy of film tested with this method needs to have minimum toughness. When the energy is too low, such as in Pt/SiO_2, the interface catastrophically fails and no steady-state crack rate can be measured.

Additionally, we heat treated and analyzed the series of Au films with Cr interlayers using Auger electron spectroscopy to characterize diffusion effects that will impact the toughness measurements. In particular, we identified that Cr acts to improve adhesion both as a complete layer as well as while in solution after heat treated with accelerated aging tests. This suggests that the impact of metallic interlayers on adhesion is a complex phenomenon that will require accurate measurements of both strength and characterization to provide comprehensive data for computational modeling efforts.

Significance

This project is designed to develop self-consistent testing methods and structures for evaluating the reliability of thin films in MEMS and microelectronics with a wide range of properties and stress states. We are producing both experimental methods and analytical models that can provide validation for computational models of interfacial materials properties and design guidelines for MEMS.

The development of testing techniques and analytical models which are rapid, robust, and verifiable will greatly add to the ability of Sandia to evaluate a wide range of critical materials and technologies that currently exist in the stockpile, as well as devices and materials that may exist or be used to monitor these systems in the future. Long-term relationships between Washington State University and Sandia researchers will be enhanced through the campus fellowship. The results from this project are expected to bring a unique capability to Sandia that will enhance our efforts in nanotechnology device design and application.

Refereed Communications

M.S. Kennedy, N.R. Moody, and D.F. Bahr, "Effect of Non-Uniform Chemistry on Interfacial Fracture Toughness," to be published in *Metallurgical and Materials Transactions A*.

M.S. Kennedy, A.L. Olson, J.C. Raupp, N.R. Moody, and D.F. Bahr, "Coupling Bulge Testing and Nanoindentation to Characterize Materials Properties of Bulk Micromachined Structures," *Microsystems Technologies Journal*, vol. 11, pp. 298-302, November 2005.

Other Communications

M.S. Kennedy, R.P. Vance, D.F. Bahr, D.P. Adams, and N.R. Moody "Development of Adhesion Layer Chemistry for Metal Interfaces," presented at the 2006 TMS Annual Meeting, San Antonio, TX, February 2006.

M.S. Kennedy, N.R. Moody, and D.F. Bahr, "Development of Adhesion Layer Chemistry for Metal Ceramic Interfaces," presented at the 2006 Gordon Conference on Thin Film and Small Volume Mechanical Behavior, Waterville, ME, July 2006.

Automated Assembly of Microscale Devices

Carnegie Mellon University

Jack (Red) Jones (Org. 6471)
Sandia Principal Investigator

Project Purpose

Microelectromechanical systems (MEMS), with their ability to integrate moving mechanical parts, electronics, and other functions inexpensively, have had a deep impact on many fields of endeavor. We are just beginning to see their amazing potential to provide tangible benefits for our daily lives. On the other hand, MEMS and their related technologies are drastically limited in several important ways. The key problem is the inability to form true three-dimensional (3D) structures of the needed complexity comprised of heterogeneous materials.

Without solutions to this problem, the range of future applications will be severely restricted. If effective solutions can be found, they will revolutionize the way in which numerous products based on microscale parts will be produced. We are collaborating with Carnegie Mellon University (CMU) to address the main robotic issues regarding the assembly of complex 3D microscale mechanisms and the integration of different microfabrication technologies into hybrid microsystems.

The approach is aimed at the system level, building on previously developed MEMS batch and robotic assembly methods. Unlike previous work, we are applying a robotic-agent-based distributed information architecture for rapidly deployable and rapidly reconfigurable microassembly systems. In contrast to previous robotic systems for microassembly based on individual work cells, this approach uses a modular branching pipeline concept to address scalability in four main dimensions with the same computational and physical system. These dimensions are: product size scalability, fastening process scalability, parallel processing scalability, and assembly process step scalability. Ultimately, this research will provide the basis for modular and scalable microfactories that will enable the economically viable assembly of complex 3D microscale mechanisms and integration of hybrid microsystems relevant to NNSA nuclear weapons applications.

Accomplishments

We developed a new gripper concept for integration into the CMU minifactory environment. We fabricated and functionally tested the new gripper concept. Small grippers such as MEMS-based microgrippers tend to be fragile and easily damaged. Sandia has shown that commercially available nonmagnetic tweezers can be used successfully to pick and place objects such as metal spheres as small as 30 µm in diameter. A significant advantage is the fact that a tweezer with bent or misaligned tips can be easily replaced.

The Sandia system uses a small model airplane servo and linkage to actuate the tweezers. CMU adopted this approach for the new microscope end effectors. In contrast to the prior approach, the CMU system operates the tweezers by a small voice coil actuator. The actuator's magnet assembly is attached to one arm of the tweezers and the voice coil is attached to the other. This enables the tweezer arms to move symmetrically at the center of the microscope's field without any friction. Additionally, the tweezer gripping force is simply proportional to coil current, making control straightforward

Significance

The evolution of 3D heterogeneous microsystems holds promise to enable a range of revolutionary capabilities of interest to national security. These capabilities range from ultraminiature weapon components to highly covert sensor systems. However, the assembly of 3D microscale mechanisms and integration of hybrid microsystems present significant technical challenges. This research contributes to moving toward a practical manufacturing basis for realizing assembled microsystems.

Membrane-Based Water Purification for Removal of Arsenic and Biologically Active Small Molecules

University of Texas at Austin

Mike Hickner (Org. 6338)
Sandia Principal Investigator

Project Purpose

This goal of this project with the University of Texas at Austin was to define some of the unique transport relationships of Sandia membranes and determine their potential for water purification.

Accomplishments

A three-cell cross-flow apparatus was designed and built at Sandia to enhance our membrane characterization capabilities.

Significance

Current commercial membranes for water treatment, mainly composed of cross-linked aromatic polyamides, are improving at the rate of 1-2 percent per year. This improvement is not great enough to spark a revolutionary change in the water treatment industry. Sandia has excellent polymer synthesis and characterization capabilities and has brought these resources to bear on problems such as fuel cells and gas separation membranes. We are beginning to apply our materials knowledge to water treatment and this project is in support of that goal. Our key research and development accomplishments provide a new set of water treatment membrane materials, and application-specific testing capabilities for the general science and technology community. Our results will benefit Sandia's mission areas in energy and water security.

Process and Infrastructure Development for Integrated Three-Dimensional Mesomanufacturing

University of Texas at El Paso

J. A. Palmer, B. D. Chavez
(Org. 2611)
Sandia Principal Investigators

Project Purpose

The purpose of this project with the University of Texas at El Paso (UTEP) was to explore ultrasonic consolidation (UC) layered manufacturing as a possible manufacturing technology for building smaller and lighter steerable antennas of interest to Sandia. The purpose of UTEP's effort was to provide expertise in direct write (DW) of conductive inks so that DW could be combined with UC where applicable to successfully accomplish the antenna assembly. The UTEP research was divided into two focus areas of research: tensile strength of direct write inks, and ink gap depth penetration.

Accomplishments

- Designed tensile test specimens to determine strength of DW inks for securing electrical conductors.
- Inspected tensile test specimens (pre- and post-cure and fracture).
- Performed tensile tests for two DW inks and a standard solder connection.
- Determined the effect of slot width (gap) on ink penetration.
- Determined the mechanism (or mechanisms) that affect penetration depth.

Significance

We conducted this research in coordination with the Sandia team on the passive electronically steerable array (PESA) for miniature synthetic aperture radar (miniSAR) LDRD project 67028. PESA represents a potential novel application of a prior joint Sandia/UTEP LDRD effort in rapid prototyping of high density circuitry in which a SAR assembly may be practically consolidated, miniaturized, and functionally improved by introducing low-mass stereolithography (SL) support members, and ultimately a monolithic body with encapsulated interconnect. UTEP investigated design and manufacture of hybrid SL-DW radio frequency (RF) interconnect in this application. The interconnect was created using an integrated SL-DW apparatus we developed. This led to a separate FY 2006 LDRD project on integrated manufacturing of a MEMS antenna (project 102606), and the first known research in the area of integrated DW and novel ultrasonic consolidation, an aluminum-based solid freeform fabrication (SFF) technology.

This research is significant in that it represents (to the authors' knowledge) an unprecedented application of integrated, ambient-temperature, metallic SFF technologies (three-dimensional printing) in manufacturing of electro-optomechanical and RF systems. Dimensional uncertainties that compound as the square root of the sum of the squares of individual part tolerances are reduced or eliminated by the monolithic approach, thus leading to reduced dimensional compensation and therefore reduced labor cost. The significance of this effort to the war fighter and the taxpayer is faster weapon system delivery at lower manufacturing cost through measurable reductions in parts, material, labor, and scrap. For the Department of Defense, this would also mean a decreased burden for material review board and disposition activities.

Refereed Communications

C.J. Robinson, B.E. Stucker, A.J. Lopes, R.B. Wicker, and J.A. Palmer, "Integration of Direct-Write (DW) and Ultrasonic Consolidation (UC) Technologies to Create Advanced Structures with Embedded Electrical Circuitry," in *Proceedings of the 2006 Solid Freeform Fabrication Symposium*, August 2006.

A. Lopes, M. Navarrete, F. Medina, J.A. Palmer, E. MacDonald, and R.B. Wicker, "Expanding Rapid Prototyping for Electronic Systems Integration of Arbitrary Form," in *Proceedings of the 2006 Solid Freeform Fabrication Symposium*, August 2006.

PRESIDENTIAL EARLY CAREER AWARDS FOR SCIENTISTS AND ENGINEERS

DOE/NNSA Defense Programs (DP) identifies nominees for the Presidential Early Career Awards for Scientists and Engineers (PECASE) from the most meritorious recipients of the DOE/NNSA-DP Early Career Scientist and Engineer Award. Candidates for this award are researchers employed by academic institutions who are in the first five years of their independent research careers. Individuals are nominated by directors of DP laboratories based on the candidate's contribution to the DP mission. Up to six winners are selected annually by the Office of Defense Programs from the nominations provided by the laboratory directors. Up to three of the winners of the DP Early Career Scientist and Engineer Award may also be designated annually by the laboratory directors as DP nominees for the PECASE. The nominating laboratory is responsible for funding the PECASE awardee for the next five years.

The PECASE embodies the high priority placed by the government on maintaining the leadership position of the United States in science by producing outstanding scientists and engineers and nurturing their continued development. The awards identify a cadre of outstanding scientists and engineers who will broadly advance science and the mission. Further, the awards foster innovative and far-reaching developments in science and technology, increase awareness of careers in science and engineering, give recognition to the scientific missions of participating agencies, enhance connections between fundamental research and national goals, and highlight the importance of science and technology for the nation's future.

The award is $250,000, given to the awardees through a $50,000 per year research contract. This provides the awardee an opportunity to continue research in the area for which he/she was nominated and for Sandia to benefit from the results of the developments.

Atomistic Modeling of Nanowires, Small-Scale Fatigue Damage in Cast Magnesium, and Materials for MEMS

Ken Gall
Georgia Institute of Technology

Jonathan Zimmerman (Org. 8776)
Sandia Principal Investigator

Project Purpose

Lightweight and miniaturized weapon systems are driving the use of new materials in design such as microscale materials and ultralow-density metallic materials. Reliable design of future weapon components and systems demands a thorough understanding of the deformation modes in these materials that comprise the components and a robust methodology to predict their performance during service or storage.

Traditional continuum models of material deformation and failure are not easily extended to these new materials unless microstructural characteristics are included in the formulation. For example, in LIGA (for the German term *Lithographie, Galvanformung, und Abformung,* for lithography, electroforming, and molding) Ni and Al-Si thin films, the physical size is on the order of microns, a scale approaching key microstructural features. For a new potential structural material, cast Mg offers a high stiffness-to-weight ratio, but the microstructural heterogeneity at various scales requires a structure-property continuum model. Processes occurring at the nanoscale and microscale develop certain structures that drive material behavior.

The purpose of this work, with PECASE recipient Ken Gall of Georgia Institute of Technology, was to understand material characteristics in relation to mechanical properties at the nanoscale and microscale in these promising new material systems. Research was conducted to employ tightly coupled experimentation and simulation to study damage at various material size scales under monotonic and cyclic loading conditions.

Experimental characterization of nano/microdamage was accomplished by novel techniques such as in situ environmental scanning electron microscopy, 1 MeV transmission electron microscopy, and atomic force microscopy. New simulations to support experimental efforts include modified embedded atom method (MEAM) atomistic simulations at the nanoscale and single crystal micromechanical finite element simulations.

Accomplishments

We focused on three topics:

Atomistic Simulations of Metallic Nanowires

We focused on the plastic properties of the nanowires and examined the effects of wire size, orientation, and structure on yielding of nanowires in a systematic manner. We examined slip, twinning, and reversibility in metal nanowires, and made a major discovery on shape memory and pseudoelasticity in metal nanowires.

Properties of Thin Films for Microelectromechanical Systems (MEMS)

We focused on thin Au film on Si microcantilevers, corrosion of Si structures, and material properties from SiO MUMPS™ designs. We began testing SiO MUMPS parts and the development of a miniature tensile frame.

Major findings include the ability of corrosion to influence device properties in the presence of a metal layer, evolution and intrinsic stress development in Au/Si thin films, and the mechanical properties of SIO materials.

Nanoindentation of NiTi Shape Memory Alloys

Nickel-titanium (NiTi) shape memory alloys undergo relatively large recoverable inelastic deformations via a stress-induced martensitic phase transformation. Although stress-induced phase transformations in shape memory alloys are well characterized and used at micrometer to meter length-scales, significant opportunity exists to understand and exploit martensitic transformations at nanometer scales.

Displacive stress-induced martensitic phase transformations may constitute an ideal nanometer-scale actuator, as evident in certain biological systems, such as the T4 bacteriophage. We used nanoindentation to study the fundamentals of stress-induced martensitic phase transformations in NiTi shape memory alloys. Results showed evidence of discrete forward and reverse stress-induced thermoelastic martensitic transformations in nanometer-scaled volumes of material.

We demonstrated shape recovery due to indentation, followed by subsequent heating, for indent depths in the sub-10 nm range. The indentation results revealed that stress-induced martensitic phase transformations nucleate at relatively low stresses at nanometer scales, suggesting a fundamental departure from traditional size scale effects observed in metals deforming by dislocation plasticity.

Our results revealed that the local material structure can be used to modify transformation behavior at nanometer scales, yielding an insight into the nature of stress-induced martensitic phase transformations at small scales and providing an opportunity for the design of nanometer-sized NiTi actuators.

Significance

The project created a large database of both experimental and computational results that link characteristics such as structure and defect content to a material's mechanical properties. This increase in knowledge is a huge boon as the trend in engineering systems has been to, and will continue to, take advantage of nanoscale and microscale structure to achieve desired materials properties.

In addition, the methods we employed can be applied to other materials of interest to existing Sandia technology, as well as future devices and technologies that would be of interest for Sandia mission needs. For example, the computational models and methods used to examine deformation and failure of nanowires can and will be applied to other nanowire materials, as well as nanoscale structures of other shapes, e.g., thin films, as the use of these materials becomes more commonplace in Sandia technology and the need for a predictive simulation tool becomes paramount.

Refereed Communications

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Generalized Continuum Models for Inelasticity in Solids: Formulation of Theories and Variational Methods for Computation

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Thao (Vicky) Nguyen (Org. 8776)
Sandia Principal Investigator

Project Purpose

The purpose of this project is to develop a generalized continuum theory, and numerical implementation of the theory, with embedded length-scales associated with microstructural defects to model inelastic behavior in solids. Classical continuum theories of inelasticity in solids break down when the deformation occurs at scales of a micron and below. In polycrystalline materials, for instance, microstructural features such as grain boundaries, dislocation clusters, microvoids, and microcracks introduce length-scale effects that are not represented in the classical theories.

However, length-scales embedded in additional degrees of freedom associated with generalized continua can be introduced on a physically and mathematically rigorous basis. Therefore, these theories are capable of modeling the influences of microstructure. Such models have gained prominence over the past decade and are being applied actively to model strain localization associated with material softening, large stresses ahead of atomically sharp cracks, grain size effects, grain rotation and breakage, and the influence of asperities in contact or friction. The most widely-used of such theories introduce length-scales via first and higher gradients of some inelastic strain measure.

There is a large range of these theories, and not all of them are equivalent. Fundamental physical, mathematical, and numerical questions remain on the order of strain gradients, the place of higher-order derivatives in governing equations, inelastic strain gradient dependence in yield functions and flow rules, and the application of additional boundary conditions.

In this project with PECASE recipient Krishna Garikapati at the University of Michigan, we are working with a class of generalized continuum inelasticity models of interest to Sandia researchers. The length-scales in these models arise from the density of geometrically necessary dislocations and the disclination density. They are represented by appropriately defined tensors. The models will be critically examined in context of the four issues raised above. Recourse will be taken to experimental data in addition to mathematical analysis.

In particular, we will draw heavily from dislocation theory. We will develop vector finite elements (VFE) and discontinuous Galerkin methods to solve initial and boundary value problems using these models.

Accomplishments

We continued development on VFE and discontinuous Galerkin methods for generalized continua. The VFE work was focused on a variant of the BCJ (Bammann–Chiesa–Johnson) plasticity model that includes the effect of plastic incompatibility-based strain gradients.

We successfully developed a two-dimensional VFE implementation of this theory and tested its numerical stability and convergence rate

Our discontinous Galerkin work focused on a strain gradient damage model. We proved stability and convergence and established rates of convergence for both these theories. For the Cahn-Hilliard equation we established results for time-discrete stability. These accomplishments have laid the groundwork to apply discontinuous Galerkin methods to incompatibility-based strain gradient plasticity theories.

Significance

We focused on developing a novel finite element approach for a variant of the BCJ plasticity model that includes the effect of plastic incompatibility-based strain gradients. The BCJ model is a physically based model for the plastic deformation of metals based on the evolution of microstructural defects such as dislocations and disclinations.

Variants of the model, with different levels of complexity, are currently being used to model the failure of components and systems critical to national security under realistic environmental conditions and situations. Successful completion of this project will result in a robust and more accurate finite element implementation of the BCJ model. Moreover, it will lead to improved numerical methods for modeling other material failure processes such as fracture. This will enhance Sandia's science-based modeling capabilities for safety and reliability.

Refereed Communications

G.N. Wells, E. Kuhl, and K. Garikipati, "A Discontinuous Galerkin Method for the Cahn-Hilliard Equation," *Journal of Computational Physics*, vol. 218, pp. 860-77, November 2006.

Developing Novel Scaffolds for Biological Molecules by Solving the I-QSAR Problem Using the Signature Molecular Descriptor

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Jean-Loup Faulon (Org. 8333)
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Project Purpose

This project is aimed at designing molecular compounds having specific biological activities and properties. This goal is accomplished in two steps. One creates a quantitative structure activity relationship (QSAR) between a set of known compound structures and their experimentally measured activities. In this first step, named forward QSAR, molecular structures are described using the signature molecular descriptor, which has previously been shown to give good accuracies in property and activity predictions.

The second step, named inverse-QSAR, consists of finding the structural elements (i.e., the signatures) that best match a given target activity and enumerating all the compounds matching these structural elements. This step comprises a set of Diophantine equations that are solved to find the signatures that match the targeted activities, and an algorithm that enumerates all molecular structures corresponding to a given signature.

In FY 2006, we benchmarked the technique and used it to design protein inhibitors as well as environmentally friendly foam-blowing compounds.

This work is being performed in collaboration with PECASE recipient Donald P. Visco, Jr. of Tennessee Technological University.

Accomplishments

We generated knowledge about what constitutes complicated inverse design problems using the signature molecular descriptor and potential solutions to the various bottlenecks that arise. We used template systems to develop inhibitors for g-secretase as well as inhibitors of Cdc25.

By working with these challenging systems (molecule size 50 – 100 atoms), we experienced a myriad of both computational and size-related issues, which forced us to refine the general inverse design algorithm. In particular, we will use a lower-signature height to generate a large pool of potential solutions (coarse-grained) and use a higher-signature height to refine that pool in order to identify the best candidate solutions to the problem.

Within this larger algorithm, we developed a modified brute-force solution technique to solve the system of Diophantine equations that result in the inverse design process with signature. This modified solution technique allows us to estimate the computational complexity of the problem and estimate the time required for solution using both the space and CPUs (central processing units) at hand. When problems become intractable, then larger, more robust approaches must be initiated.

Other work we accomplished:

- Incorporated multiple steps via multiple codes in the inverse solution algorithm into one, large script
- Generated post-processing scripts to filter nonphysical structures from structure generation code
- Developed parallel code to more efficiently implement the modified brute-force approach to solve the Diophantine equations.

Significance

The concept of designing compounds matching targeted properties and activities is novel and has not been successfully developed and applied prior to this work. We have filed a patent on the methodology developed in this project. While there are still bottlenecks we need to overcome, in particular to design compounds of high molecular weights (> 50 non hydrogen atoms), our technique can and has been used to design novel compounds.

There are many potential applications for this work, ranging from the design of novel materials having better physical properties (polymers for instance), to the design of environmentally friendly chemicals (foam-blowing agents), and the design of drugs that are more potent to a specific target (inhibitors of g-secretase, Cdc25, and cox-2).

Refereed Communications

D. Weis, J.L. Faulon, R.C. LeBorne, and D.P. Visco, "The Signature Molecular Descriptor 5: The Design of Hydrofluoroether Foam Blowing Agents Using Inverse-QSAR," *Industrial & Engineering Chemistry Research*, vol. 44, pp. 8883-8891, November 2005.

D. Visco, D. Weis, J.L. Faulon, S. Martin, and R.C. LeBorne, "Solving the Inverse-QSAR Problem with Signature Using a Reduced System," presented at the AIChE Annual Meeting, Cincinnati, OH, November 2005.

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Fundamentals of Embossing Nanoimprint Lithography in Polymer Substrates

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Blake Simmons (Org. 8755)
Sandia Principal Investigator

Project Purpose

Nanoimprint lithography (NIL) is a nanomanufacturing technique that uses a nanostructured master template to form features in a substrate with best resolution near 1 nm and areas as large as 100 cm^2. In embossing-based NIL, a nanostructured master is heated and pressed into a thermoplastic polymer film, forming a negative relief replica in the polymer film. Nearly all previous research on NIL has been for the purpose of nanoelectronics fabrication in which the polymer film acts as a mask layer. We seek to develop the embossed, nanostructured polymer film as the functional surface, rather than a mask layer.

The goal of the project is to develop a first principles understanding of polymer transport during printing such that any polymeric material could be employed for embossing-based NIL. This project is a joint collaboration with PECASE recipient William King of the Georgia Institute of Technology. The need for this research is particularly acute when polymer nanostructures are of size comparable to the polymer molecule radius of gyration, and when the nanoscale heat and mass transport properties of the polymer are not known.

The lack of fundamental materials science knowledge is the major limit to rational design of nanofabrication methods designed to produce specific feature sizes and shapes. This work aims to model and measure polymer properties during NIL for a large number of thermoplastic polymers. This link between material properties and processing parameters will enable rational NIL process design.

Accomplishments

This activity is investigating nanoscale polymer heat and mass transport that occurs during embossing-based nanoimprint lithography (NIL) and direct-write AFM nanoindentation. Master templates with features in the range 2 micron – 10 nm have been manufactured in silicon and electroplated into Ni metal. These Ni stamps were formed to accommodate many embossing trials with minimal deformation, as compared to other soft-lithography materials. A number of thermoplastic polymers have been investigated, with molecular weights in the range 10^4-10^7 kDa, corresponding to characteristic molecular lengthscales in the range 3 – 50 nm. These results have served as the initial training set to optimize design rules for advanced stamp designs.

Atomic force microscopy has been used to characterize the embossed substrates and correlate embossing conditions, polymer molecular properties, and manufactured feature sizes. Continuum and subcontinuum models of polymer transport and template deformation have proven beneficial in this analysis. The ultimate goal of this project is to establish design rules for the manufacture of polymer nano/microdevices, and we have succeeded in the initial stages of this project in developing the toolbox necessary to realize such designs in the next stage of this project.

In addition to developing these design rules for NIL, we have also investigated the interaction of patterned surfaces and cellular adhesion. The major goal of this aspect of the research is to determine the impact of topographical length-scales on the interaction between a cell and a surface. The results obtained from this research have been used to develop next generation tissue scaffolds and for mitigation of biofouling, and has been demonstrated by attaching osteoblasts in predetermined rational patterns.

Significance

Nanoimprint lithography is the ultraminiaturized version of the decades-old embossing process in which a master tool or mold is pressed into a soft material to create detailed patterns. Using a broad range of polymer materials, NIL produces structures on the micron or nanometer size scales, offering the potential for lowering production costs. However, quality issues caused by unpredictable polymer flow into the nonuniform features of embossing tools pose a major stumbling block. Earlier research into this complex process produced often conflicting recommendations, forcing manufacturers to pursue costly trial and error methods.

Using the results of experimental work, we examined every variable involved in the nanoimprinting process and recorded the outcome of each incremental change through the design space. We studied shear deformation of the polymer, elastic stress release, capillary flow, and viscous flow during the filling of imprinting tool cavities that had varying sizes and shapes. The results apply to any polymeric material that follows standard viscous flow rules and produces feature sizes larger than 50 nanometers. The next step in this research will be to modify the simulation software to account for physics changes that occur on smaller size scales.

These results will have applications in semiconductor manufacturing, where nanoimprinting offers a potential alternative to increasingly expensive lithography processes to produce circuitry. It could also help make high-volume production of nanoscale structures for optoelectronic, biomedical, and other applications more economically feasible.

Refereed Communications

J. Charest, M. Eliason, W. King, A. Talin, and B. Simmons, "Polymer Cell Culture Substrates with Combined Nanotopographical Patterns and Micropatterned Chemical Domains," *Journal of Vacuum Science and Technology B*, vol. 23(6), pp. 3011-3014, November 2005.

Rational Understanding and Control of the Magnetic Behavior of Nanoparticles

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Sandia Principal Investigator

Project Purpose

Magnetic spinel ferrite nanoparticles, MFe_2O_4 (M = Mn, Mg, Zn, Co, Fe, and so on), have great potential for biomedical diagnostics and targeted drug delivery. To realize biomedical applications of nanoparticles, the magnetic properties of the nanoparticles must be optimized and the surface of the nanoparticles must be modified with biocompatible ligands and/or polymer matrices that can also carry medicinal drugs. These two requirements are interconnected.

Nanoparticle coercivity is strongly dependent on the surface pinning of magnetic moments caused both by metal cation coupling and by magnetic surface anisotropy. Different surface metal cations possess different intrinsic coupling strength and will result in markedly different coercivities. For example, Co ion usually possesses a strong quantum coupling between electron spin and atomic orbital angular momentum. However, Mn ion has a weak coupling. Thus, Co terminated nanoparticles should display larger coercivity when compared to Mn terminated nanoparticles.

Surface modification of nanoparticles also profoundly alters the coercivity of nanoparticles. We hypothesize that the surface modification induced changes in coercivity are caused by missing coordinating oxygen atoms around surface metal cations. When the coordination of surface metal cations is similar to the coordination symmetry of the metal cations in the core of a nanocrystal, the surface magnetic anisotropy, the resulting surface pinning, and the coercivity should be low. Thus, the observed dependence of the coercivity on surface modification is likely due to changes on the coordination of surface metal cations caused by the chemical surface modification.

We will study the correlations between the coercivity of nanoparticles, the quantum couplings in surface metal atoms, and the surface modification. The research will be conducted at the Georgia Institute of Technology with PECASE recipient Z. John Zhang.

Accomplishments

We systematically investigated the superparamagnetic properties of $CoFe_2O_4$ and Fe_3O_4 nanocrystals. The observed blocking temperature of $CoFe_2O_4$ nanocrystals is at least 100 degrees higher than that of the same sized Fe_3O_4 nanocrystals. The coercivity of $CoFe_2O_4$ nanocrystals at 5 K is over 50 times higher than the same sized Fe_3O_4 nanocrystals.

We observed that the drastic difference in superparamagnetic properties between the similar sized spherical $CoFe_2O_4$ and Fe_3O_4 (or $FeFe_2O_4$) spinel ferrite nanocrystals was correlated to the coupling strength between electron spin and orbital angular momentum (L-S) in magnetic cations. Compared to Fe^{2+} ion, the effect of much stronger spin-orbital coupling at Co^{2+} lattice sites leads to a higher magnetic anisotropy and results in the dramatic discrepancy of superparamagnetic properties between $CoFe_2O_4$ and Fe_3O_4 nanocrystals.

Significance

This work provides insight to the fundamental understanding of the quantum origin of superparamagnetic properties. Furthermore, these results suggest that it is possible to control the superparamagnetic properties through magnetic coupling at atomic level in spinel ferrite nanocrystals for various applications. The ability to control magnetic properties is vital for the development of new magnetic materials for storage and sensing.

Refereed Communications

Q. Song and Z.J. Zhang, "Correlation Between Spin-Orbital Coupling and the Superparamagnetic Properties in Magnetite and Cobalt Ferrite Spinel Nanocrystals," *Journal of Phys. Chem. B*, vol. 110, pp. 11205-11209, June 2006.

E.L.H. Heintz, P. Rohatgi, D.F. Doyle, C.J. Fahrni, and Z.J. Zhang, "Magnetic $CoFe_2O_4$ Nanoparticle-Oligonucleotide Conjugates for Cellular Uptake and Magnetic Manipulation," to be published in the *Journal of American Chemical Society*.

Fabrication and Device Applications of Aligned Mesoporous Architectures

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Jeff Brinker (Org. 1002)
Sandia Principal Investigator

Project Purpose

A well-known problem in self-assembled silica/surfactant thin film mesophases and corresponding calcined mesoporous silica films is that two-dimensional hexagonal mesophases are oriented parallel to the substrate surface. Monosized pores oriented normal to the substrate surface are important for control of molecular and ion transport in synthetic membranes and for control of charge and energy transfer in photovoltaics and organic light-emitting diodes.

To date normally oriented channels have been formed by suction of sols through anodized alumina membranes, but drying and associated shrinkage lead to defects and irreproducibility. To overcome these issues, we will explore the capillary filling of preformed silica/block copolymer mesophases into alumina nanochannels.

The purpose of the project, a collaboration with PECASE recipient Yunfeng Lu at Tulane University, is to understand the mesophase transformation and/or reorientation under capillary force and to develop oriented mesochannels that are normal to the substrate surface. These materials are interesting for the applications of separation, highly sensitive sensing, and smart devices.

Accomplishments

In FY 2005, we demonstrated that self-assembled hexagonal mesophases can be aligned by capillary forces. By contacting a liquid crystalline hexagonal silicate/copolymer composite film with porous anodized alumina membranes, the liquid crystalline silicate/surfactant mesophases are gradually filled into the cylindrical alumina pores driven by the capillary force, resulting in oriented hexagonal mesophases normal to the substrate surface.

In FY 2006, we successfully captured the mesophase transformation at the interface between the preformed film and the alumina membrane by cross-sectional transmission electron microscopy (TEM). The parallel to normal reorientation of the cylindrical channels is well demonstrated by the cross-sectional TEM image.

Over a region 50-100 nm thick (depending on diameters of alumina nanochannels) the preformed hexagonal mesostructure is gradually reoriented by shearing force to a direction normal to the substrate. We systemically studied the effect of diameter variation of alumina nanochannels on the mesostructure orientation and identified the critical diameter for producing the oriented mesoporous silica nanowires.

Hexagonal mesophases are predominantly aligned along the silica nanowires using the alumina membranes with different channel diameters ranging from 200-30 nm. By tuning the diameter of the alumina nanochannels, the number of aligned mesopores within an oriented silica nanowire is therefore controllable. For example, a 30 nm sized silica nanowire only contains 2-3 straight oriented mesopores. When the diameter of the alumina nanochannels is reduced to 20-30 nm, the silica mesophase is no longer fully aligned. In the region where the diameter is 20 nm, a curved tubular mesophase is formed. However, in the region where the diameter is 30 nm, a short aligned tubular mesophase is formed indicating that 30 nm is the critical diameter of alumina nanochannels to produce oriented mesostructures by capillary filling.

Significance

Success of this work will provide new platforms for extensive use in water purification, separation, sensors, templated synthesis, microelectronics, optics, controlled release, and highly selective catalysts. For example, aligned mesoporous materials can be further functionalized with responsive or recognizable components, leading to the fabrication of smart devices, such as intelligent artificial membranes and highly sensitive sensors.

This work supports the DOE science strategic goal of maintaining a world-class research capability; e.g., advances in nanoscale science built around foundations in materials and chemistry that may lead to improved energy technologies and systems.

Other Communications

R. Kou, D. Wang, and Y. Lu, "Oriented Composite Mesostructures under Nanoscale Confinement," presented at the AIChE Annual Meeting, San Francisco, CA, November 2006.

On the Role of Numerical Error in Turbulence Simulations

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Auburn University

Matt Barone (Org. 1515)
Sandia Principal Investigator

Project Purpose

Because of the difficulties in isolating numerical and modeling errors in turbulence simulations, new approaches are needed to assess numerical errors. One promising approach is the Method of Nearby Problems (MNP) developed by our collaborator, PECASE recipient Christopher Roy at Auburn University, where exact solutions are generated via spline fitting of highly resolved numerical solutions. These exact solutions can then be operated on by the governing equations in order to generate small, distributed source terms.

We will focus on the extension of MNP from one dimension to multiple dimensions. Initial work will focus on two-dimensional (2D) problems such as unsteady Burgers equation, for which a number of exact solutions exist. Only general approaches will be investigated which can be extended to three- and four-dimensional problems in a straightforward manner. The chief difficulty that must be overcome is the development of spline fits which are continuous up to an arbitrary number of derivatives over the boundaries of each spline zone.

Successful implementation of multidimensional MNP will allow for the development of a unique test bed of realistic flow problems for evaluating different numerical discretization schemes used in unsteady turbulence simulations.

Furthermore, multidimensional MNP also has important applications in solution verification for the broader area of computational science and engineering.

In year two, we will focus on generating a realistic, multidimensional, unsteady exact solution for the Navier-Stokes equations (with small source terms). Subsequent effort will then focus on developing and evaluating new numerical schemes for unsteady turbulence simulations, methods for quantifying the dissipative and dispersive numerical errors of numerical schemes, and new subgrid turbulence models that account for the estimated numerical errors. Control of the dissipative numerical errors is especially important for compressible codes which often employ second-order numerics.

President Harry S. Truman Fellowship in National Security Science and Engineering

University Research, in partnership with Human Resources, established a distinguished postdoctoral program entitled the President Harry S. Truman Fellowship in National Security Science and Engineering (Truman Fellowship Program) in 2004. This program provides an opportunity each year for exceptional scholars to join Sandia National Laboratories (Sandia) in the continuation of Sandia's tradition of excellence.

The Truman Fellowship seeks to attract the best nationally recognized, new PhD scientists and engineers. It provides the opportunity for recipients to pursue independent research of their own choosing that supports Sandia's mission. The appointees are expected to foster creativity and to stimulate exploration of forefront science and technology and high-risk, potentially high-value R&D.

Truman Fellowship candidates are expected to have solved a major scientific or engineering problem in their thesis work or have provided a new approach or insight to a major problem, as evidenced by a recognized impact in their field. Funding for the Truman Fellowship projects is through Sandia's Laboratory Directed Research and Development (LDRD) Program.

In 2006, three additional Fellows were selected. They hailed from Stanford, University of California at Davis, and Pennsylvania State University. They joined two Fellows who had previously competed for the Truman Fellowship. Progress reports on all five independent research projects follow.

2006 Truman Fellows

Dr. Ilke Arslan received her bachelor's and master's degrees in physics from the University of Illinois-Chicago and her PhD degree in physics from the University of California at Davis. Her research focuses on the implementation and application of advanced techniques in the electron microscope to understand the structure-property relationships of semiconductor nanomaterials. She received numerous awards, among them the Royal Society Fellow at Cambridge University, where she worked in the world's leading group on electron tomography applied to materials science. Dr. Arslan is conducting her research project in the Materials Physics Department (8756).

Dr. Meeko Oishi's PhD and master's degrees in Mechanical Engineering are from Stanford University. Her bachelor's degree is from Princeton University. She was a National Science Foundation Graduate Research Fellow and received the John Bienkowski Memorial Prize in mechanical and aerospace engineering at Princeton. Meeko worked on creating new computational and analytical techniques to better understand the US electrical power grid, as pertains to development of techniques to provide insight to human-automation interaction in the grid. She was assigned to the National Systems Modeling and Analysis Department (6221).

Dr. David Scrymgeour obtained his PhD and BS degrees in materials science from Pennsylvania State University, where he was a National Science Foundation Graduate Research Fellow. David is measuring the piezoelectric and electrical properties of nanostructured zinc oxide (ZnO). The piezoelectric effect, the expansion and contraction of a material with the application of an electric field, is used in many sensing applications. Demonstration of this property in nanostructures could be used to create ultra-sensitive detectors. Dr. Scrymgeour is employed in the Surface and Interface Sciences Department (1114).

Ultrafast Low-Voltage MEMS Switches for Optics and RF Applications

Gregory N. Nielson (Org. 1749-2)
Truman Fellow

Project Purpose

The objective of this project is to develop and explore a completely new approach to microelectromechanical system (MEMS) switching that has the potential to dramatically increase the speed of MEMS devices while lowering both the voltage and energy required for actuation relative to current MEMS actuation techniques. The new actuation technique utilizes elastic potential energy stored in the MEMS structure to drive the mechanical switching. We are applying this switching technique to the optical domain to create high-speed optical switches.

Accomplishments

We spent time and effort on increasing the testing capabilities for our devices. We designed and assembled a control circuit that provides both resonant pull-in initialization and strain-energy switching control. We extended the capabilities of the vacuum chamber test setup to allow low-loss transmission of radio frequency (RF) signals into the chamber. We also assembled a test setup to couple light into and out of waveguides on chip for testing waveguide and future switch performance.

We fabricated and tested some parallel plate electrostatic MEMS devices. These devices were tested using the vacuum test setup. This device switched in less than 500 nanoseconds over a switching gap of 1.8 microns with an actuation voltage of 35 volts. This performance is about an order of magnitude better than any other MEMS device with comparable switching gap and actuation voltage.

Using these devices, we also investigated low-stress silicon nitride (silicon rich) and stoichiometric silicon nitride as isolation layers. The silicon-rich silicon nitride seemed to have some propensity for dielectric charging, even in vacuum. The stoichiometric silicon nitride caused the MEMS structures to fracture due to the high intrinsic stress in the film. We investigated the possibility of using high-permittivity dielectrics for isolation in place of the silicon nitride and designed a process to fabricate and test devices with zirconia, hafnia, alumina, and silica isolation layers. We initiated the fabrication of these devices for testing.

We designed, fabricated, and performed preliminary testing of torsional MEMS devices that are precursors to high-speed torsional MEMS mirror devices. These devices are designed to be significantly faster (~ 100X) than the torsional MEMS mirrors that we used last year to initially demonstrate the strain-energy switching and resonant pull-in. Some initial testing of these devices with the newly designed and assembled resonant pull-in circuit indicate that resonant pull-in was achieved at 15 volts, a 25 percent improvement over the quasistatic pull-in voltage that would otherwise be required to pull-in the device. While strain-energy switching tests are still pending, this device has a resonant frequency of 750 kHz, which should translate into a switching speed of at least 670 nanoseconds. We will continue testing these devices.

In anticipation of combining integrated optics with MEMS devices, we fabricated and tested waveguides to be integrated with MEMS devices to form high-speed integrated optical switches. We fabricated and tested single crystal silicon, polysilicon, and amorphous silicon waveguides. Based on the results of the waveguide investigation, we designed a fabrication process to integrate single crystal silicon waveguides with high-speed MEMS devices.

Significance

Switching is one of the key functionalities that MEMS have provided for a number of domains including RF, optical, fluidic, thermal, and direct current (DC) electrical. Within these domains, MEMS switches are used for a wide variety of switching applications. The dominant technique used for switching is electrostatic switching, although thermal, piezoelectric, and magnetic techniques are also used. Electrostatic switching has a number of appealing characteristics, such as ease of implementation, low power requirements, and fast switching (relative to the other switching techniques mentioned). One of the primary drawbacks to electrostatic switching is the high “pull-in” voltage required to achieve switching. The MEMS switching technique we are exploring takes advantage of the nonlinear dynamic behavior of electrostatic MEMS systems that allows a significant reduction in the voltage required for switching.

While the primary benefit of this switching approach is a reduction in the voltage required for operation, there are a number of other benefits that result from this technique. The reduction in voltage required allows stiffer structures to be switched at reasonable voltages, which leads to faster switching speeds.

The dynamic behavior is such that the velocity at impact is slower than it would be with the typical electrostatic switching technique where a high voltage is used. The reduction in the impact velocity may lead to improvements in reliability by reducing effects of the initial impact on the microstructure of the material as well as eliminating “bouncing” of the movable electrode on the mechanical stop. Reliability will also be increased as stiffer structures are used because that will help ameliorate the problem of stiction.

Since the device is positively held in both switch states, ringing (i.e., free oscillations) of the switch will be eliminated, which usually extends the switching time significantly. Also, for switching applications in the electrical domain, the positive holding of the device reduces the chance of self-actuation of the device.

Finally, the dynamic switching approach will use significantly less energy for switching. Much of the energy is recycled by converting it from stored potential energy to kinetic energy and then back into stored potential energy, ready to be used again in the next switching operation. The energy saved is reflected in the reduction in the applied voltage. If, for example, the dynamic switch operating voltage is one-quarter of the pull-in voltage, there is a 16X reduction in the energy used.

Since MEMS switching is very widely used in a variety of domains, the impact of these improvements in MEMS switching is significant.

Refereed Communications

G. N. Nielson and G. Barbastathis, “Dynamic Pull-In of Parallel-Plate and Torsional MEMS Actuators,” *Journal of Microelectromechanical Systems (JMEMS)*, vol. 15, pp. 811-821, August 2006.

Bayesian Inference for Inverse Problems, Model Structure, and Uncertainties

Youssef Marzouk (Org. 8351)
Truman Fellow

Project Purpose

Inverse problems are of great relevance to science and engineering. While progress in detailed, first-principles modeling of physical systems has been enormous, this progress has exposed a challenging and complementary task – inferring unknown model parameters, model inputs, and model structures from data in realistic problems. Several factors make these inference problems difficult to solve. Real-world observations are often sparse and are inevitably affected by noise and measurement error. Inversion is typically ill-conditioned; small errors in measurement can lead to enormous changes in the estimated model or model parameters. Moreover, multiple models may match a given data set, or no model may match the data.

This work develops a probabilistic setting for inverse problems, based on Bayesian inference. The Bayesian formulation provides a rigorous foundation for inference from parsimonious and noisy data, a natural mechanism for incorporating disparate prior sources of information, and a quantitative assessment of uncertainty in the inferred results. We also seek to develop efficient computational tools that surmount the cost of evaluating high-dimensional Bayesian integrals or probing posterior distributions, particularly for complex forward problems accessible only through expensive detailed simulations.

We consider two key applications: contaminant source inversion and gene regulatory network construction. Progress in algorithms for source inversion is important to homeland security, in response to current risks of bioagent or toxin release in public spaces. Efficient Bayesian inference from sparse and noisy data will provide well-founded estimates of confidence in threat characterizations, enabling better targeted and more effective responses. Robust inference of gene regulatory network structure may fundamentally enhance knowledge of crucial aspects of cellular function, from elucidating pathways between normal and diseased cellular states to clarifying and manipulating responses to pathogens and toxins. This work will thus impact Sandia’s portfolio in biotechnology and molecular biology. Principal investigator Youssef Marzouk is a Truman Fellowship Award recipient.

Accomplishments

Work in FY 2006 focused on stochastic spectral reformulations of the Bayesian approach to inverse problems. We first completed the theoretical foundation for these new approaches, then explored the accuracy and efficiency of the resulting methods by demonstrating them in practical applications. In time-dependent contaminant source inversion problems, we demonstrated that using polynomial chaos expansions to propagate a wide range of uncertainty, e.g., prior uncertainty, through the forward problem, and sampling the resulting spectral expansion, enables a substantially more efficient Bayesian solution of the inverse problem. This new formulation addresses a core computational challenge associated with the Bayesian formulation – the cost of evaluating high-dimensional integrals over the posterior, particularly when each sample or quadrature point requires solution of an expensive forward problem.

Next, we focused on the inference of continuous spatial-temporal fields. This class of problems includes source inversion where the source field is allowed to have an arbitrary space-time dependence; it also includes material property inversion, such as estimating the permeability or diffusivity of a material from sparse and/or remote measurements of scalar transport. Solving these problems in a Bayesian context required developing new methods for dimensionality reduction.

We appealed to the Karhunen-Loève (KL) expansion of stochastic processes, essentially using the prior to develop basis functions for the unknown field. This converts the full-dimensional inference problem to Markov chain Monte Carlo (MCMC) exploration of the joint posterior distribution of the KL mode strengths. Results on transient problems with spatially varying diffusivity show excellent agreement with the full-dimensional formulation and substantial speedup. Moreover, they allow polynomial chaos acceleration of Bayesian inversion in high-dimensional problems.

We implemented all of this work in a flexible and extensible code framework.

Significance

The first focus of this work, new algorithmic developments for Bayesian inference in complex inverse problems, should have a growing impact on both the inverse problems and the statistics communities. By introducing efficient spectral methods for uncertainty propagation into the realm of inverse problems, we are making Bayesian inference with detailed physical models far more computationally tractable. We expect that this will facilitate the adoption of Bayesian approaches, with their rigorous treatment of data noise and model uncertainty, by inverse problems practitioners. We also hope that these techniques will enable statisticians to employ more realistic, first-principles, physical models when analyzing data.

Impact on specific application areas begins with the prototypical source inversion problems we used to demonstrate our formulation. Contaminant source inversion is at the heart of pressing problems in homeland security, i.e., responding to bioagent or toxin releases in public spaces. Efficient Bayesian inference from sparse and noisy data will provide well-founded estimates of confidence in threat characterizations, enabling better targeted and more effective responses. Applications of inverse problems in Sandia's mission areas extend much further. Geophysical applications, e.g., characterizing subsurface properties from remote and indirect measurements, are fertile ground for considering uncertainties in physical models, measurements, and the resulting inverse solutions. We hope to leverage our work on Bayesian inference for continuous-field inverse problems into this area.

Experience with computational tools for Bayesian inference, developed in this project, has already begun to influence several other Sandia efforts, including:

- "Practical Reliability and Uncertainty Quantification for Complex Hierarchical Systems," LDRD Project 105814. Starting in FY 2007, this new project will use Bayesian techniques to estimate and extrapolate the reliability of complex systems from test data, with quantifiable credibility bounds.
- "Distributed Microreleases of Bioterror Pathogens: Threat Characterization and Epidemiology from Uncertain Patient Observables," LDRD project 93505. Started in FY 2006, this project uses Bayesian inference strategies to characterize an unfolding bioterror attack based solely on scarce patient data, in the earliest phases of an outbreak.
- A BES-funded Sandia project on analysis of experimental data in combustion chemistry, using Bayesian analysis and computational tools (e.g., MCMC) to construct uncertain chemical models.

Refereed Communications

Y.M. Marzouk, H.N. Najm, and L.A. Rahn, "Stochastic Spectral Methods for Efficient Bayesian Solution of Inverse Problems," in *Proceedings of the Bayesian Inference and Maximum Entropy Methods in Science and Engineering*, pp. 104-110, August 2005.

J. Ray, Y.M. Marzouk, H.N. Najm, M. Kraus, and P. Fast, "Estimating Bioterror Attacks from Patient Data: A Bayesian Approach," submitted to *Proceedings of the RAND/ASA Conference on Quantitative Methods & Statistical Applications in Defense and National Security*.

Y.M. Marzouk, H.N. Najm, and L.A. Rahn, "Stochastic Spectral Methods for Efficient Bayesian Solution of Inverse Problems, *in Proceedings of American Institute of Physics,* pp. 104-110, February 2006.

Other Communications

H.N. Najm, T.B. Settersten, and Y.M. Marzouk, "Uncertainty Estimation from Experimental Data: Bayesian Analysis of NO Fluorescence Quenching," presented at the 31st International Symposium on Combustion, Heidelberg, Germany, August 2006.

Y.M. Marzouk, "Stochastic Spectral Methods to Accelerate Bayesian Solution of Inverse Problems," presented (invited) at LANL statistics seminar, Los Alamos, NM, June 2006.

Y.M. Marzouk and H.N. Najm, "Stochastic Spectral Methods for Efficient Bayesian Solution of Inverse Problems," presented at the 3rd World Conference on Computational Statistics and Data Analysis, Limassol, Cyprus, October 2005.

Y.M. Marzouk and H.N. Najm, "Polynomial Chaos Acceleration of Bayesian Methods for Inverse Problems," presented at the SIAM Conference on Parallel Processing for Scientific Computing, San Francisco, CA, February 2006.

Y.M. Marzouk and H.N. Najm, "Stochastic Spectral Methods to Accelerate Bayesian Solution of Inverse Problems," presented at the Valencia/ISBA 8th International Meeting on Bayesian Statistics, Benidorm, Spain, June 2006.

Y.M. Marzouk and H.N. Najm, "Stochastic Spectral Methods for Bayesian Inference in Inverse Problems," presented at Workshop on Statistical Inverse Problems, Gottingen, Germany, March 2006.

Human Interaction with Safety-Critical Interconnected Systems

Meeko Oishi (Org. 6326)
Truman Fellow

Project Purpose

The attentive driver of a car interacts with a control system that consists of a wheel, accelerator, brakes, gear shift, and so on. In spite of many advances, one can still find a way to turn a car onto its roof even without leaving a paved road. One of the active areas of research in control systems theory is the design of a control system that is guaranteed to operate within specified bounds. Even for purely automated systems, the problem is complicated, but it becomes even more so for hybrid systems, in which humans interact with automated systems.

This work is intended to develop first: general, formal one-step (in contrast to current multistep) methods to find hybrid control systems whose behavior is guaranteed bounded, and second: to develop formal methods for the recovery from error by a hybrid control system. It will turn out that both can be simultaneously achieved through a reachability analysis of hybrid control systems, which until recently was thought to be intractable for nontrivial systems.

Accomplishments

We obtained novel contributions in reachability analysis for human interaction with complex systems. We have presented a method to determine, through a Hamilton-Jacobi reachability computation, the set of states in safety-critical systems which will reach the desired equilibrium without saturating the input or violating the state constraints. Thus both envelope protection and stabilization under saturation are simultaneously achieved. This involves a reachability analysis on an extended state space that incorporates a parameter from the feedback linearizing input. By incorporating the input saturation, stability, and state constraints simultaneously in the initial cost function, the resultant invariant set will be the largest set of states, given bounded input, that will stabilize the system and always remain within a given constraint set.

The work contributes to the difficult problem of determining stabilizing controllers for safety-critical systems under nonlinear state and input constraints. We formulated the recovery problem for hybrid systems with flexibility in continuous inputs, discrete inputs, or state constraints. Standard reachability analysis will reveal those states from which failure is avoidable with the proper choice of control law. In the event that failure does occur, a new forward reachability calculation can identify those failure states from which recovery is possible, as well as the control input (both continuous and discrete) necessary for that recovery.

This new calculation exploits the flexibility inherent to the hybrid system – if this flexibility were not present, a recovery calculation would provide no new information from the initial backwards reachability calculation. The recovery calculation involves temporarily adjusting the system's constraints in order to recover to standard operation and standard constraints. The forward reachability calculation yields not only 1) the forward reachable set from error states, but also 2) the control law required to achieve that set.

Two real-world examples were presented to illustrate both methods: 1) longitudinal aircraft dynamics, and 2) two-aircraft lateral collision avoidance dynamics. The dynamics for both examples are derived from physical models of civil jet aircraft. These two case studies provide interesting motivation for further work in synthesizing recovery maneuvers. Future work will proceed in comparing the forward reachability result with a converse problem in which the standard operating region is propagated backwards in time under the new recovery dynamics.

Significance

These contributions were inspired by real-world problems in aircraft, but are likely to arise in other complex systems, including biomedical devices, driver-assistance programs, nuclear surety, the power grid, and other critical infrastructures. Many future directions of work are possible, including 1) minimization of the number of switched, nonsaturating controllers when multiple solutions to the control parameterization problem are possible, 2) alternative, less computationally exhaustive formulations to sample the parameter space, and 3) one-step synthesis of a minimal number and optimal selection of input parameters for switched, nonsaturating, feedback linearizing controllers.

Presentation and publication of some of this work in the 45th IEEE Conference on Decision and Control won a best paper award.

Refereed Communications

M. Oishi, I. Mitchell, C. Tomlin, and P. St. Pierre, "Computing Viable Sets and Reachable Sets to Design Feedback Linearizing Control Laws Under Saturation," in *Proceedings of the 45th IEEE Conference on Decision and Control*, February 2006.

M. Oishi, "Recovery in Flight Management Systems: Applications of Hybrid Reachability," in *Proceedings of the IEEE Advanced Process Controls Industrial Applications Workshop*, May 2006.

Piezoelectric Properties of Arrayed Nanostructures of Zinc Oxide for Sensor Applications

David Scrymgeour (Org. 1114)
Truman Fellow

Project Purpose

The drive toward smaller and more sensitive sensors for hazardous gas, explosive material, and biological agent detection is naturally leading toward the use of nanostructured materials and devices. The advantage of nanostructured sensors is that the small size leads to enhanced surface area to volume ratios ideal for ultrasensitivity. New semiconductor and oxide materials like zinc oxide (ZnO) that are now being grown at the nanoscale have many exciting cross-coupled properties like the piezoelectric effect that interlink various material states – elastic, optical, and electrical – and provide vast utility to these smart materials when compared to the traditional nanomaterials of silicon and carbon nanotubes. Using piezoelectric nanostructured ZnO, one can create electrically addressable nanoscale mechanical devices. Such structures can provide both actuation and sensing capabilities through the converse and direct piezoelectric responses, respectively.

In this Truman fellowship project, we are characterizing the piezoelectric and electrical properties of ZnO in nanoscale geometries using scanning force microscopy techniques and nanoscale electrical impedance measurements. The basic research provides the groundwork for creating ultrahigh sensitivity sensors that use piezoelectric effect and the resistive and capacitive properties. Piezoelectric sensors operate by measuring the frequency shift and resonant impedance change of the piezoelectrically generated acoustic waves. The propagation of these waves is strongly dependent upon the material/environment interface and can be shifted by surface-adsorbed species. Additionally, the resistive and capacitive properties of nanostructures are profoundly affected by interaction of the surface with gaseous species. The extremely high surface area to volume ratio, the inherently high resonant frequencies, and the surface-sensitive nature of the electrical properties of these nanostructures will enable the creation of small, accurate, sensors to target specific agents (gas, explosive, biological).

Accomplishments

Piezoelectric force microscope capabilities were constructed and added onto a current scanning force microscope. This technique is used to measure small piezoelectric distortions induced on the sample surface by AC voltage applied to a conductive tip in contact with the sample surface. This capability extends the capabilities of the scanning force setup to determine both the magnitude of the piezoelectric response and orientation of the piezoelectric crystal with resolutions down to tens of nanometers. We investigated various calibration schemes, and calibrated the instrument to allow for quantitative analysis of the piezoelectric effect at nanoscales.

We performed piezoelectric measurements on over 200 single nanorods, and compared results to single-crystal ZnO with known orientation. These results establish that the all the nanorods are [0001] oriented, which contrasts with preliminary morphological examinations of ZnO nanocrystals. We found that the amplitudes varied from rod to rod and are not strongly correlated to the physical dimensions like rod height or radius. The amplitude response was measured at 4.41 pm/V with a standard deviation of 1.73 pm/V, compared to only 2.97 ± 0.57 pm/V for the single crystal.

We performed measurements of the current-voltage characteristics on the nanostructures using conductive atomic force microscopy (C-AFM). Initial experiments show the nanorods create Schottky contacts with the tip. Modeling the response via thermionic emission theory, the ideality factors are in the range 1-4, with barrier heights of 0.70 ± 0.14 eV for diamond coated tips. Correlation of these properties to the measured piezoelectric properties is ongoing.

Significance

The demonstration of piezoelectricity in nanostructures of solution grown ZnO is an experimental first. The combination of this property along with the ease of growth on substrates at temperatures lower than 90 ºC and the previously established ability to pattern the zinc oxide nanocrystals can be used to create macroscale arrays of nanorods of piezoelectric material. This could be used in acoustic band gap crystals, nanoscale elastic wave generators, and nanoscale piezoelectric actuation and transduction.

The integration of nanoscale piezoelectric particles into polymer blends to create piezoelectric nanocomposites has not yet been explored. Ordered arrays of nanorods backfilled with polymer would be a nanoscale analog to 1-3 piezoelectric composites currently used in ultrasonic wave generation. Because the dimensions of the individual piezoelectric rods are very small, the resonant frequency of such an array would have a operating frequency much greater than the MHz regions typically found in traditional 1-3 composites.

Additionally, zinc oxide is a semiconductor with unintentionally carrier concentrations up to ~ 10^{20}. This could be exploited to create devices based on the interaction of piezoelectrically generated acoustic waves with conduction electrons. Similar work using bulk piezoelectrically active semiconductors investigated current oscillations and acoustic amplification in such materials and created acoustic delay lines and acoustic-wave amplifiers. Similar effects and devices have not yet been explored in nanostructured materials.

Refereed Communications

D.A. Scrymgeour and J.W.P. Hsu, "Piezoelectric Properties of Solution Grown ZnO Nanocrystals," presented at the Materials Research Society Fall 2005 Meeting, Boston, MA, December 2005.

D.A. Scrymgeour, T.L. Sounart, N.C. Simmons, Y.J. Lee, P.G. Clem, and J.W.P. Hsu, "Piezoelectric and Electrical Properties of Solution Grown ZnO Nanorods," presented at the Electronic Materials Conference 2006, State College, PA, June 2006.

D.A. Scrymgeour, T.L. Sounart, and J.W.P. Hsu, "Piezoelectric and Electrical Properties of Solution Grown Semiconductor ZnO Nanorods," presented at the Materials Research Society Spring 2006 Meeting, San Francisco, CA, April 2006.

Three-Dimensional Analysis for Nanoscale Materials Science

Ilke Arslan (Org. 8756)
Truman Fellow

Project Purpose

The major goal of this Truman fellowship project is to study the materials physics of nanomaterials through the development and application of state-of-the-art techniques in electron microscopy in order to understand their structure-property relationships. We focus on three materials systems: dislocations in thin film p- and n-type GaN, GaN and GaN/AlN core/shell nanowires, and ZnO nanorods interfaced with a polymer. The common theme of these three efforts is to understand how the structure and geometry impact the functionality of the three different semiconductor materials.

We want to understand why the solid-state lighting semiconductor GaN can be made into devices that function despite the high density of threading dislocations. To solve this, we need to characterize the dislocation on the atomic scale using imaging and spectroscopic techniques. Through a combination of experimental and theoretical work, we concluded that all of the dislocations are controlled by impurity segregation. Not all of the dislocations are deleterious, but if impurities have segregated to a particular dislocation, then the material's properties appear to be altered. Further work needs to be done, and a comparison between p- and n-doped thin films will be made.

We are working to understand the effect of constraining GaN and its alloys to one dimension and studying the quantum effects. We plan to measure the band gap of the nanowire at different diameters, as this is very important to precise device fabrication. We expect that the band gap will increase with decreasing nanowire diameter. Also, the material will now be dominated by surface effects, because the surface-to-bulk ratio is high. We want to understand what these effects are, and how they impact device functionality. We will use a combination of atomic, electronic, and three-dimensional (3D) measurements in the electron microscope, as well as conductivity measurements and theoretical calculations.

We also want to see how the interface affects the properties of the ZnO/polymer functionality. These materials are being developed for solar cell device applications. However, the bonding between the polymer and

ZnO is not understood, and the surface reconstruction of the ZnO is also not known. Using high-resolution electron microscope techniques, we will probe the atomic and electronic structure at the interfaces to try to answer some of these questions.

Accomplishments

We installed detectors, hardware, and software; performed preliminary experiments; and learned to operate the complex monochromator that allows the energy resolution (~ 0.1 eV) to measure band gaps. We performed the preliminary measurements of band gaps of GaN nanowires (NWs) at several different diameters. Also with monochromated electron energy loss spectroscopy, we made preliminary measurements of electronic states at the surface of the NWs that show a different signature than bulk.

For core/shell NWs, we analyzed GaN/AlN NWs using high-resolution scanning transmission electron microscopy (STEM) in 2D, and found that the GaN inside the AlN is not continuous everywhere, which was a great surprise. We also performed the first STEM tomography experiment to achieve a 3D tomogram of these NWs. While this provided useful information on the morphology of the outer AlN layer, we were unable to extract information on the inner GaN core. We will now use energy-filtered transmission electron microscopy (EFTEM) tomography to separate the core (Ga signal) and shell (Al signal). We expect EFTEM will allow us to reconstruct the two phases clearly. We performed the first experiment and reconstruction of a 90° tilt series on a test sample to demonstrate feasibility.

Finally, we performed the preliminary analysis of dislocation cores and found that point defects and intrinsic impurities are responsible for the change in electronic structure at dislocation cores. We will now perform the theoretical calculations to identify the responsible defects.

Significance

GaN and its alloys are an important class of semiconductors being developed for high-power electronics, light emitting diodes (LEDs), and laser diodes in the blue region of the spectrum. The combination of blue LEDs with the existing and optimized red and green LEDs will produce cheap and efficient white light with long lifetimes. The research described will contribute to realizing this goal. Also, ZnO interfaced with a semiconducting polymer has demonstrated potential as a solar cell device. Therefore, this project will impact the energy mission of DOE.

Two individuals were selected as distinguished postdoc Truman Fellows, beginning October 2006. Abstracts of their planned research project follow.

Passive & Active Electromagnetic Frequency Selective Surfaces for High-Power Beam Applications

Hung (Jacques) Loui (Org. 5345)
Truman Fellow

Dr. Hung (Jacques) Loui received his PhD in electrical engineering from University of Colorado at Boulder. He holds an undergraduate double major in electrical engineering and piano performance and won a number of prestigious piano competitions before focusing on engineering research. He received numerous scholarships and fellowships, including the Department of Education Graduate Assistance in Areas of National Need Fellowship. His research contributions include collaborations with NASA and the Universidad de Buenos Aires, Argentina. Jacques tackled an unsolved problem in quantitatively describing the radio frequency characteristics of thick metal surfaces with arbitrary inclusions. He developed, implemented, and tested an efficient computational method, which is a significant advance in the start-of-the-art for frequency-selective surface modeling. His research has immediate applications to antenna and radome structures, and his analysis method appears suitable and unique for a wide range of applications such as active switching and steering. Dr. Loui is conducting his research in the SAR Sensor Technologies Department (5345).

Abstract

Truman Fellow Hung (Jacques) Loui will study Frequency Selective Surfaces (FSSs) and their function as filters for electromagnetic radiation, passing desirable frequencies while reflecting others. An example is the door of a modern microwave oven, where a periodically perforated thin metal sheet embedded in dielectric (glass) passes light (high frequency) but confines the microwave (low frequency) used for cooking. Unlike conventional circuit filters, the transmission and reflection frequency responses of FSSs are functions of incident excitation profile, polarization, and direction.

FSS structures find application in radomes for radar antennas, and in shaping low-observable structures that hide complex internal structures that would otherwise be highly visible radar objects. Applications can include increased rejection of interference from nearby transmitters, stealth applications, covert applications, and even the construction of dichroic reflectors.

Thick, complex-geometry FSS structures and multilayer, electrically thin FSS structures are difficult to design and analyze with existing analysis codes. Truman fellow Jacques Loui brings to this effort a new and versatile Mode Matching Extended Generalized Scattering Matrix (MM-EGSM) engine for the analysis of EM radiation/scattering and Gaussian beam measurement methodology for the performance characterization of the proposed surfaces. The generality allows inclusion of dielectric fillings, coatings and metal-losses for multiple apertures inside a unit cell. In addition, both periodic and aperiodic structures under arbitrary excitation can be treated. This new method implements mode-matching using surface impedance boundary conditions across multiple coplanar boundaries and is significantly faster than brute-force numerical methods such as the Finite Element Method.

This study will include design and characterization of tightly coupled thin-metal complementary conformal FSSs using flexible dielectric, and passive thick-metal FSSs for use in high-power beam applications and low-observable radomes. A goal is to integrate active devices into thick-metal passive FSS plates. A compact thick-FSS implementing one of the following tasks: sensing, amplification, switching, mixing, focusing and shielding of EM beams will be demonstrated.

Network Design Optimization of Fuel Cell Systems and Distributed Energy Devices

Whitney Colella (Org. 8367)
Truman Fellow

Dr. Whitney Colella received her PhD in engineering science from Oxford University. She also holds a master's degree in science and public policy from Sussex, an MS in mechanical engineering from Stanford, and an MBA from Oxford. She has been recognized with British Marshall, Fulbright, National Science Foundation, and Overseas Research scholarships and fellowships. Whitney's research has been in experimental systems modeling of fuel cells that considered heating, cooling, and the use of by-product heat. She developed concepts and control strategies that challenge conventional analysis of fuel cells and show that, with imaginative design, they have more immediate commercial potential than generally thought. One of her recommendations was adopted by DaimlerChrysler's fuel cell subsidiary. She has also designed an integrated fuel cell power and heating system for the Stanford campus. As an undergraduate, she developed and built the world's first fuel cell-assisted bicycle. Dr. Colella is employed in the Hydrogen and Combustion Technology Department (8367).

Abstract

Work to be carried out by Truman Fellow Whitney Colella involves the modeling and testing of energy systems with the aim of designing them to achieve environmental, defense-related, and economic goals. Designs of alternative vehicles, power plants, and building thermal management systems, along with each technology's related energy supply chain will be evaluated. Assessment criteria for these energy systems and supply chains will include
1) their impact on the environment including a) greenhouse gas emissions, b) criteria air pollutants, c) solid waste production, d) human health, and e) energy efficiency;
2) their implications for national security including a) the security of the fuel and energy supplied, b) the diversity of the fuel supply, and c) the dependence on foreign oil; and
3) their costs to consumers, governments, and incumbent energy suppliers.

Both mobile and stationary energy systems, as well as different types of future transportation supply chains, such as those based on biofuels, hydrogen internal combustion engines, batteries, plug-in-hybrids, and fuel cells will be examined. Models of distributed energy networks that – on the supply side -- incorporate the details of fuel cell system operation and – on the demand side – incorporate the differing electricity, heating, and cooling demand patterns of American buildings will be constructed. Test data for key system components derived from other Laboratory programs will be incorporated.

Crucially, this project will combine Sandia's unique expertise in three main areas: 1) systems engineering applied to complex networks, 2) the design of renewable and efficient energy technologies, and 3) the design of national infrastructure to increase homeland security.

SANDIA-UNIVERSITY RESEARCH PROGRAM (SURP)

Since 1958, Sandia National Laboratories has provided research funding support to beginning faculty researchers at the University of New Mexico (UNM), the New Mexico Institute of Mining and Technology (NMT), and New Mexico State University (NMSU) through the Sandia-University Research Program (SURP). Each university researcher is partnered with a Sandia collaborator to satisfy the program's primary goals of obtaining needed scientific knowledge and technical expertise while strengthening the university laboratory technical community in mission-relevant areas. Investment in new faculty development helps create partnerships that build longterm strength for Sandia's Science and Technology foundations.

Funding for SURP comes from the U.S. Department of Energy/National Nuclear Security Administration's Office of Defense Programs through Sandia's Nuclear Weapons Strategic Business Unit. In order to ensure a close association between the faculty member and the Sandia technical collaborator, the SURP program has a matching-funds requirement for each funded research project. The Sandia collaborators view these investments as excellent leverage for their program's research dollars. Today, a new award is $40,000 per project, with $15,000 coming from the Sandia collaborator.

The SURP projects are selected for their high relevance to Sandia's research interests and mission needs. The projects are aligned with Sandia's Research Foundations: computational and information sciences, engineering sciences, materials and process sciences, microelectronics and photonics, and pulsed power sciences. New initiatives are usually in the energy and environment and biotechnology focus areas. Projects may include maturation and/or commercialization research support of technologies under development at Sandia. SURP benefits to Sandia include increased understanding in the subject matter explored by the projects, exposure to unique research areas, cost-effective research, and collaborative relationships between Sandia and New Mexico university faculty.

Universities and individual faculty members benefit from their participation in SURP through increased interaction with Sandia researchers, increases in faculty research production, faculty and student recruitment, grants from other institutions, experience in managing projects and student assistants, and awards, tenure, and fellowships. While Sandia selects SURP projects based on their value to Sandia's mission-relevant research needs, the Labs also tracks the significance of the SURP projects by their contribution to the broader scientific and technical communities. Two indicators of this significance are the additional funding and follow-on work obtained by the university researchers as a result of the SURP project and the number and breadth of conferences and publications that accept SURP project-related presentations and articles. A broad collection of national and international scientific and technical organizations and journals has accepted submissions related to the SURP projects by the university researchers. The diverse fields of these organizations represent Sandia's far-reaching interests and influence.

Variance Reduction for Monte Carlo Photon-Electron Coupled Transport Simulations

Taro Ueki
University of New Mexico

Leonard Lorence (Org. 1341)
Sandia Principal Investigator

We developed a variance reduction method for the Monte Carlo simulation of secondary electron emission. We evaluated the computation of the electron emission energy profile at the exit slab surface due to photon radiation for various materials and incident energy spectra of photons. Numerical results indicate that efficiency gain by an order of magnitude can be consistently obtained.

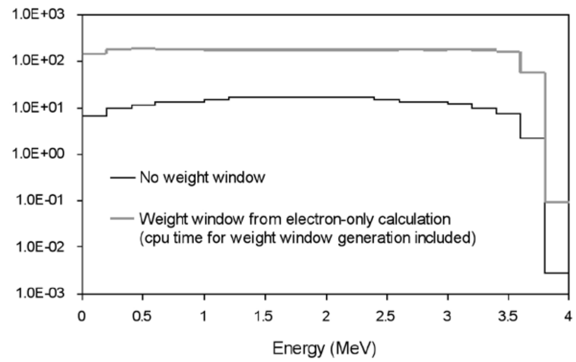

Figure 1: Performances of weight window methods (Al slab of 4 cm thickness: 4 MeV photon on one side; electron energy profile on other side)

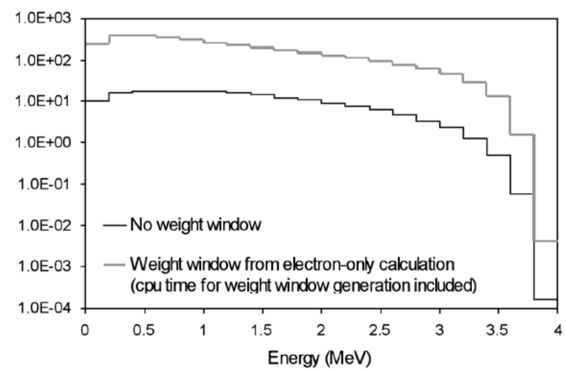

Figure 2: Performance weight window methods (Al slab of 4 cm thickness; photons of uniform spectrum over 0 –4 MeV on one side: electron energy profile on other side)

This variance reduction method can be applied to the electron range neighborhood at an electron detection surface independent of the photon penetration toward that neighborhood, except the information sharing of the maximum energy of incident photons.

We investigated the Monte Carlo simulation of photon and electron coupled-transport with the statistical weights of these particles as additional independent variables, and exclusively investigated the spatial control of weight.

We discovered that the photon weight in the electron range at an electron detection surface should be equated to the electron weight that is determined to be inversely proportional to the electron adjoint function [1]. We validated this discovery in a mathematically consistent manner based on the Boltzmann Monte Carlo equation approach [2].

In order to create a weight window common to photons and electrons, we conducted a preliminary Monte Carlo simulation of the forward electron-only problem, with the uniform source over the electron range at an electron detection surface, and over all solid angles and through the maximum energy of incident photons. Here, the weight window is a control device of weight, with the upper and lower bounds dependent on spatial cells. The photon weight window, which was more than the maximum electron range away from the electron detection surface, was constant.

We simulated photon and electron coupled-transport for slab materials, with photons normally incident on one side, and the electron emission energy profile to be evaluated on the other. We analyzed slabs of aluminum, carbon, silicon, germanium, lead, tungsten, and combined-lead-carbon of various thicknesses. In all problems, computing the reference case with no weight control took a long time. The computation of the 6 cm thick tungsten slab, for example, with incident photons of 15 MeV, took one and a half months to yield 10 percent standard deviation for the energy bin of 14-15 MeV.

We measured the simulation efficiency in terms of the figure of merit (FOM) available in the Monte Carlo N-Particle 5 particle transport code of Los Alamos National Laboratory [3]. Here, FOM is a measure of simulation efficiency that can be rigorously derived based on risk theory [4]. The efficiency gain with respect to the simulation with no weight control was an order of magnitude or more for these materials even when taking into account time spent on the preliminary Monte Carlo calculation of the forward electron-only problem. We observed that the efficiency gain is nearly the same for both the monoenergetic and uniform spectra of incident photons, as shown in Figures 1 and 2.

We had three breakthroughs:

1. Since the efficiency gain does not depend on the spectrum of incident photons, we can apply variance reduction techniques to the electron range neighborhood at an electron detection surface independent of photon penetration toward that neighborhood, except the information sharing of the maximum energy of incident photons. Therefore, once a weight window is created for the electron range neighborhood at an electron detection surface, it can be used for various experimental conditions that produce photon radiation fields of known maximum energy

2. Numerical results in Figures 1 and 2, and others not included in this report, show that the proposed weight window method is more efficient than simulation with no weight window, even when time spent on the weight window generation is taken into account.

3. The successful report of the variance reduction for the secondary particle simulation in the coupled-transport of radiation particles does not exist except for the multigroup forward-adjoint coupling simulation of neutron-photon coupled transport [5]. Our work has shown that in the continuous energy mode simulation of photon-electron coupled-transport, the developed variance reduction consistently raises simulation efficiency.

Further development of the variance reduction method investigated in this project became part of an LDRD project. The combination of methodologies in this project with maximum entropy methods is very promising and is under investigation.

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Intelligent Damage Detection for Structural Health Monitoring

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We looked at integrating artificial neural networks (ANN) with wavelet multiresolution analysis (WMRA) for intelligent detection and structural health monitoring of critical infrastructure. We conducted experimental investigations on a model bridge tested at the University of New Mexico (UNM), and used the resulting data, along with data from the American Society of Civil Engineers (ASCE) benchmark structure, to perform analytical investigations. (The ASCE benchmark structure is a four-story steel structure.) The analysis showed that the proposed module can detect damage in structures efficiently. We developed two new methodologies for damage-pattern recognition using Fuzzy set theory and the theory of possibility.

Experimental Investigations

We set up an experiment on a steel model bridge in the structural health monitoring (SHM) laboratory at UNM and constructed a test set up for a model bridge with model loading conditions. The model bridge is x m long and y m width and consists of two structural steel trusses and a composite bridge deck. We loaded the model bridge with random loading scenarios under standardized and repeatable loading conditions, and repeated the scenarios during different states of structural health conditions.

We selected three model (toy) vehicles for their sturdiness and their rubber tires, which would reduce the amount of high-frequency noise and more closely mimic the damping of real vehicles. To control the weight of each vehicle, we filled it with known weight of lead shot as cargo loads. We divided the bridge deck into three longitudinal lanes, each 250 mm wide. The model bridge and the loading vehicles are shown in Figure 1 (a) and (b) respectively.

Figure 1: Experimental investigation of a model bridge (a) Bridge configuration with three traffic lanes (b) Model trucks used to model bridge dynamic response

The vehicles crossed the bridge in set patterns of lane configuration and vehicle cargo loading. The variability in the system resulted in stochastic loading conditions that mimic realistic loading conditions on a bridge structure.

We tested the bridge under healthy and damaged conditions. We simulated the damaged conditions by loosening the bolts in one or two of the truss joints or by completely eliminating a structural element. We recorded accelerations at truss joints during the different loading scenarios and communicated it to an on-site server where damage diagnosis software was installed. Details about this experimental investigation were published in the SHM Workshop in Stanford, September 2005.

Innovative Methods for Intelligent Damage Diagnosis

1. An Integrated Neural-Wavelet Damage Feature

Our investigations lead to the development of a neural-wavelet module for intelligent damage detection in structure. We tested the module using the experimental data acquired from the model bridge and validated the model using data from the ASCE benchmark structure.

In both experiments (the model bridge and the ASCE benchmark structure), acceleration signals were decomposed using WMRA and were used to train an ANN to recognize the underlying patterns in the healthy structural dynamics. A damage feature was computed in the wavelet domain to represent the health state of the structure.

Figure 2 shows the integration method used for identifying damage in the ASCE benchmark structure and the results of quantifying the probability of damage. Some of the results were published in the SHM Workshop in Granada, Spain, in July 2006.

We are preparing a journal article describing our investigation.

2. Damage Pattern Recognition Using Fuzzy Systems

Most SHM approaches focused on statistical analysis for damage identification consider only random uncertainties. We introduced a method that accommodates other types of uncertainties due to ambiguity, vagueness, and fuzziness, which are statistically nondescribable. The proposed method, which primarily deals with epistemic uncertainty, improves damage identification by performing damage pattern recognition using fuzzy sets.

In this approach, we used the healthy observations to construct a fuzzy set representing healthy performance characteristics and prescribed the

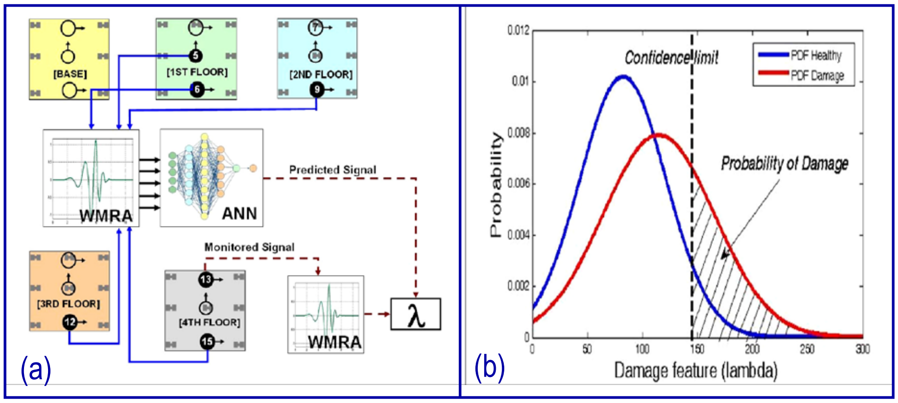

Figure 2: Identifying damage in the ASCE benchmark structure using the neural-wavelet module. (a) Module architecture in relation to the ASCE benchmark structure (b) probability of damage for damage case 6 where structural bracing was removed.

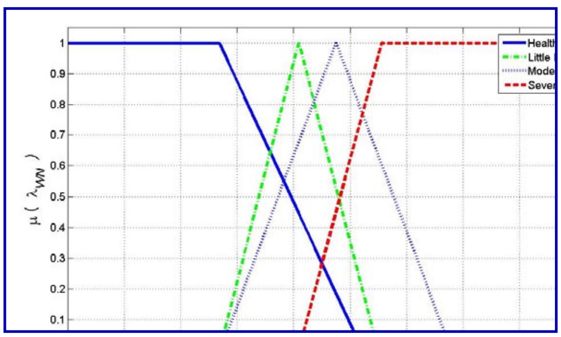

Figure 3: Fuzzy structural health patterns "Healthy," "Little Damage," "Moderate Damage," and "Severe Damage" as identified by the optimization method.

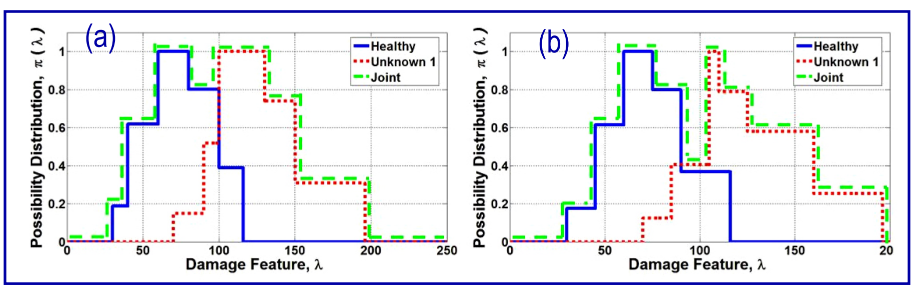

Figure 4: Individual and joint possibility distributions (of damage feature, λ_1) representing "Healthy" and a damage case (a) first overlapping scheme, (b) second overlapping scheme.

bounds on the similarities among the structural damage states. Thus an optimal group of fuzzy sets representing damage states, such as little, moderate, and severe damage, can be inferred as an inverse problem from healthy observations only. We used piecewise linear functions as fuzzy membership functions representing the states of healthy and damaged. We used the optimal group of damage fuzzy sets to classify a set of observations at any unknown state of damage using the principles of fuzzy pattern recognition based on maximum approaching degree.

Example results of the identified fuzzy sets representing damage cases are shown in Figure 3. Results of this research were published in the latest IEEE conference on Systems, Man, and Cybernetics and on Journal of Computer-Aided Civil and Infrastructure Engineering, September 2006.

3. Damage Pattern Recognition Using Theory of Possibility

We examined the process of SHM in the context of a nonstatistical damage detection paradigm. We particularly focused on applying the theory of possibility to the damage-detection problem. The basic idea behind the proposed approach is that the application of possibility theory does not require probabilistic knowledge or assumptions on the damage feature and thus encompasses aleatoric and epistemic types of uncertainties. The approach is not damage-feature dependent and thus is generic for use in many SHM systems. Additionally, we introduce two new damage metrics that extract damage evidence information from observations performed at unknown health states of structures.

Some of the results of the possibility distribution of healthy and damage cases are shown in Figure 4. Results of this research were published in the Arab Structural Engineering Conference, Kuwait, November 2006, and in an article submitted for publication (in review) in ASCE Journal of Structural Engineering.

A new proposal is under way to submit intelligent damage detection of car components to the United States Council for Automotive Research. We will use the results of the collaborative research performed in the last two years under the SURP program to acquire this funding opportunity.

Refereed Communications

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Other Communications

S. Horton*, "A Neural-Wavelet Damage Detection Module for Structural Health Monitoring," International Workshop on Structural Health Monitoring, Stanford, CA September 2005.

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* indicates a student coauthor/ presenter.

Task-driven Multiformation Control for Coordinated UAV/UGV ISR Missions

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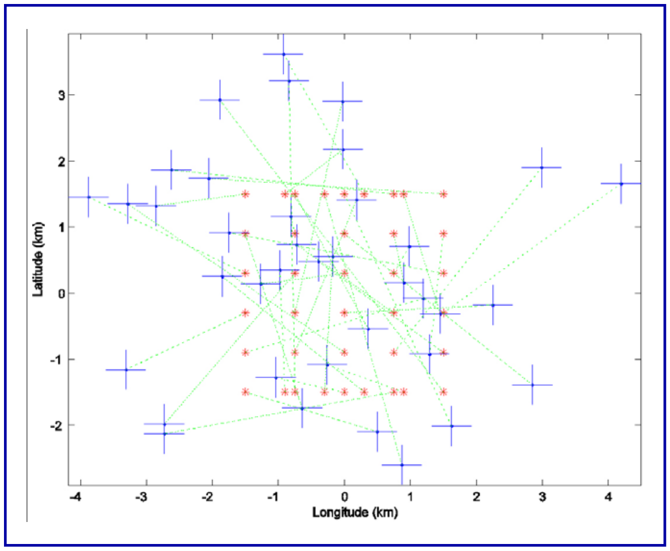

Figure 1: Ground vehicles stabilize to given desired locations, each selecting the location that minimizes total distance traveled. Ground vehicles have limited, directed motion sensors (searchlights of limited range) and they need to fall into formation in order to establish a virtual fence that partitions the search area into cells.

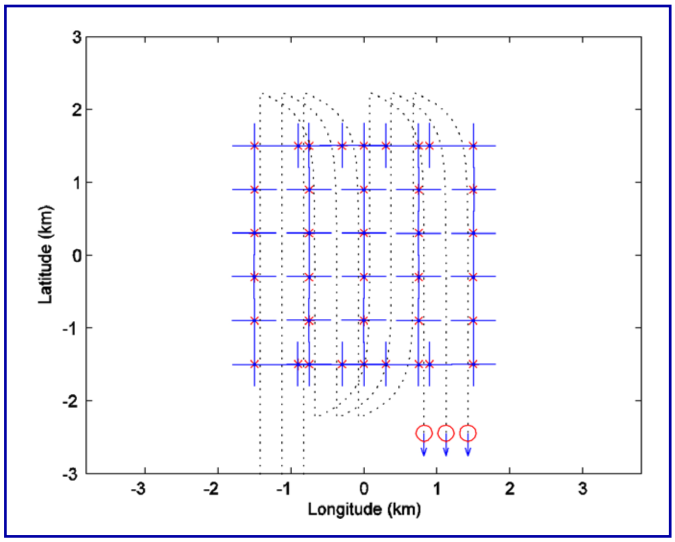

Figure 2: Once the ground formation has stabilized, a formation of aerial vehicles scans the secured area cells in search of the target.

We developed a switched cooperative control scheme to coordinate groups of ground and aerial vehicles for the purpose of locating a moving target in a given area. To do this, we stabilized the ground group into a guarding formation using a navigation function and then steered the aerial group along a trajectory that uniformly scans the enclosed regions (Figure 2). The approach is novel in that it combines decentralized flocking algorithms with navigation functions for obstacle avoidance, convergence to designated position, and direction control.

We developed a hybrid coordination scheme for coordinating heterogeneous autonomous vehicles (aerial and ground) into ordered sequences of subtasks that culminate in a global objective, which is to locate a moving target within a given area. The approach is modular in the sense that the problem is decomposed into subtasks and assigned to different vehicle groups according to their specific motion and sensing capabilities. The approach exploits team diversity by having ground vehicles in roles that involve guarding and securing the area, taking advantage of their mobility, while fast-moving aerial vehicles clear sections of the secured area until the target is located or a false alarm is reported.

In our hybrid control architecture, vehicles switch between different controllers according to the phase in the executed plan they are in. Controller transitions can be state or time dependent, based on communication constraints. Each controller is designed with formal guarantees of convergence and performance, obtained within a Lyapunov stability framework.

These multivehicle cooperative controllers combine decentralized flocking with steering using navigation functions. In this way, we achieve distributed motion synchronization within a vehicle team and direct control over the group's motion direction and formation shape. We extend our earlier navigation function construction methodology by relaxing the assumption of point-robots; the vehicles are assumed to be surrounded by a visco-elastic "shell" that enables them to keep reasonably large distances without compromising convergence.

Combining low-level, fairly stable cooperative motion controllers with a switching strategy, enables us to efficiently use the different motion and sensing modalities of ground and aerial autonomous vehicle groups and perform cooperative tasks in a way that we can guarantee task completion within finite, computable final time.

In the process of developing the hybrid cooperative search strategy, we abandoned the originally proposed idea of changing the ground vehicles' locations based on aerial group motion. The modification will improve efficiency; the time for converging ground vehicles to desired destinations would be much longer than the time needed by aerial assets to clear a region, thus slowing down the search task.

In the modified approach, ground vehicles stabilize once at the initial phase of the plan, secure the area, and guard partitioned regions while aerial vehicles quickly sweep them. In the proposed framework, partitioned regions are scanned sequentially, but there is no restriction in the order of scanning; the latter can be freely designed so that regions with increased probability of containing the target are searched first.

Refereed Communications

H.G. Tanner, "Switched UAV-UGV Cooperation Scheme for Target Detection," submitted to IEEE International Conference on Robotics and Automation, 2006.

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Multiplexed Fiber Optic Sensors for Simultaneous Measurements of Temperature and Strain in Geothermal Wells

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Real-time and remote measurement of the key parameters of geothermal wells, as well as their temporal and spatial variations, can provide critical information to improve plant efficiency and optimize plant operation to accommodate a resource that is declining with time.

This research focused on developing thermal, long period, fiber grating-based sensors and multiplexing methods for in situ geothermal well logging. Its successful completion will result in cost-effective and reliable fiber optic sensors for real-time and in situ measurement and monitoring of the temperature, strain, and pressure in geothermal wells.

Thermal Long Period Fiber Grating and Fabrication

A long period fiber grating (LPFG) is an in-line fiber device with a core refractive index that changes periodically in the range of 100 µm to 1 mm, which promotes coupling between the core mode and the copropagating cladding modes. This mode coupling condition is very sensitive to the period of the refractive index change; therefore, it can be used as a sensor to measure physical quantities such as the strain, temperature, and pressure.

Traditionally, LPFGs are fabricated by periodic ultraviolet (UV) irradiations to the fiber, which introduces a permanent modification of the refractive index of the fiber core. However, the UV-induced refractive index changes can only survive relatively low temperatures (~150 ºC).We investigated the method of fabricating LPFGs using CO_2 lasers periodic irradiations, which resulted in thermal long period fiber gratings (TLPFGs) that survived very high temperatures.

As shown in Figure 1, we fabricated LPFG by exposing a section of optical fiber to high-power CO_2 laser

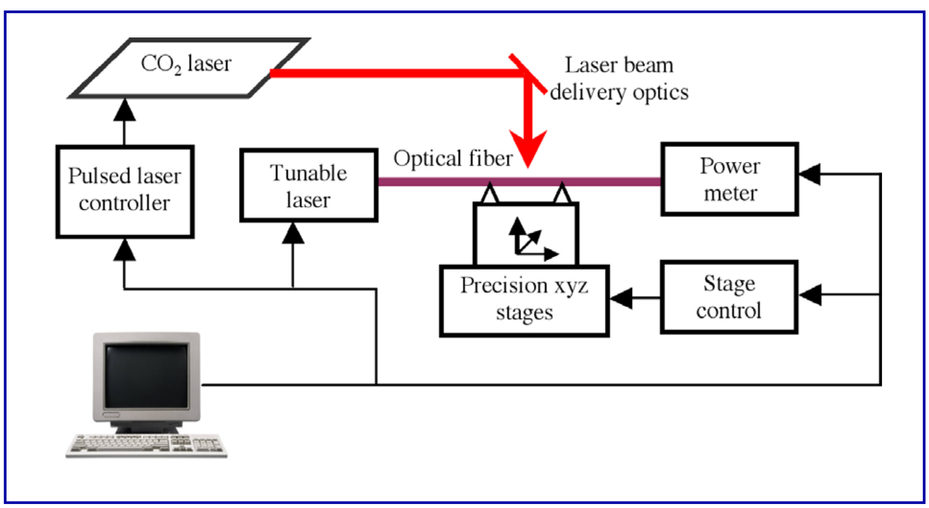


Figure 1. Schematic illustration of the CO_2 laser based LPFG fabrication system.

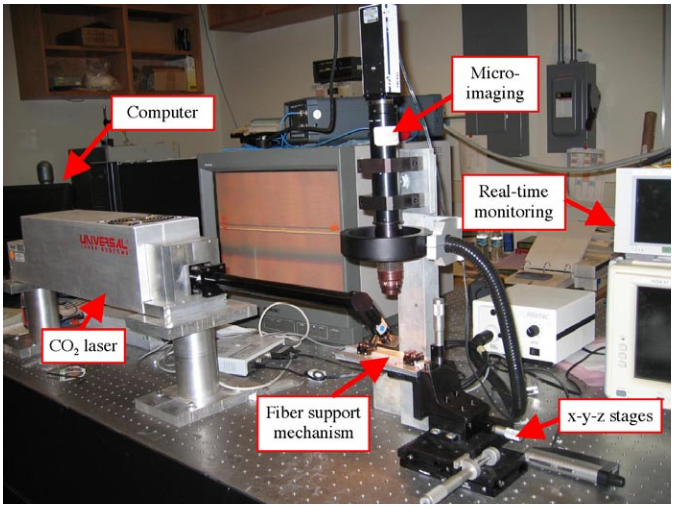
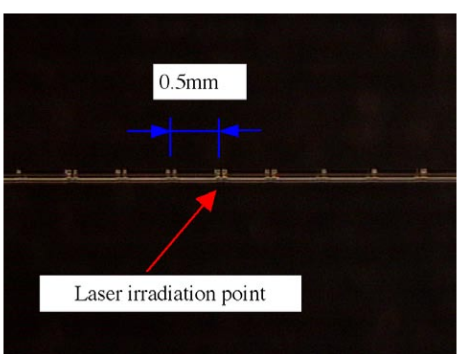


Figure 2. Photograph of the CO_2 laser based LPFG fabrication system.

irradiation at the wavelength of 10.6 µm to introduce periodic refractive index changes inside the optical fiber. The photograph of the CO_2 laser based LPFG fabrication system is shown in Figure 2. The system included a high-power CO_2 laser, computer-controlled precision three-dimensional translation stages, fiber support mechanisms; an on-line signal monitoring system; and the computer program to coordinate the entire fabrication process.

The CO_2 laser power was controlled by a computer program to step through a pre-designed power-time trajectory. The x-y-z stage allowed accurate positioning of the optical fiber toward the laser beam. The on-line monitoring system provided real-time scan of the resonance spectrum of the fabricated TLPFG.

Figure 3(a) shows the microimage of a typical TLPFG, where the laser irradiation marks can be clearly identified on the fiber. The corresponding transmission spectrum of this TLPFG is shown in Figure 3(b). High-quality TLPFGs can now be fabricated using the system with very good repeatability. With a period of about 0.5 mm and about 50 points of irradiation, the fabricated TLPFGs had a typical low loss (typically 2 dB), a resonance wavelength around 1550 nm, and a resonance peak of above 12 dB. If the number of exposure points increased to about 100, the resonance peak could reach 20 dB. The resonance wavelength could also be tuned in the range from 1510 nm to 1640 nm by slightly changing the period.



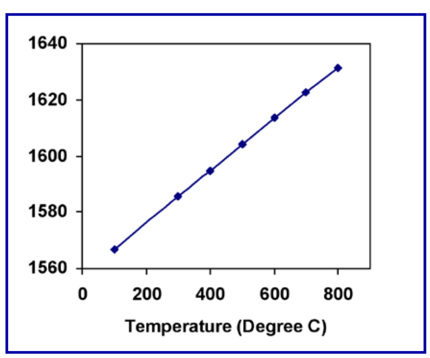


Figure 3. TLPFG, (a) microimage of a fabricated TLPFG, (b) typical transmission spectrum of a TLPFG.

Performance Evaluation of TLPFGs

We tested the TLPFGs in our lab to evaluate their temperature sensitivity, strain sensitivity, and high temperature stability and annealing effects.

Temperature Sensitivity

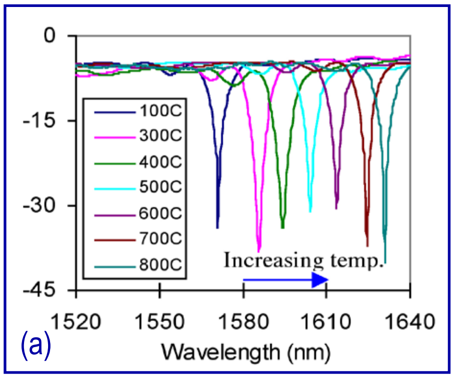
We placed a TLPFG in an electric furnace side by side with a thermocouple. The transmission spectra of the TLPFG at the temperatures of 100, 300, 400, 500, 600, 700, and 800 degrees Celsius are shown in Figure 4(a). The TLPFG resonance wavelength shifted toward the long wavelength as the temperature increased, indicating that the grating mainly coupled the core mode to low-order cladding modes. Figure 4(b) shows the resonance wavelength of the TLPFG calculated at different temperatures. The resonance wavelength had an almost linear relation with temperature, proving that the TLPFG can be used as a temperature sensor by monitoring the resonance spectrum shifts.

Sensitivity to Strain/Fiber Bending

As the fiber stretches or bends, the period of the TLPFG changes correspondingly, causing the resonance wavelength to shift. To verify this, we mounted a TLPFG on a steel plate so that it would bend following the deformation of the steel plate. Figure 5 shows the fiber bending effects on the TLPFG transmission spectrum. The fiber bending shifted the resonance wavelength toward the long wavelength, and we noticed that a reduction in the loss and a broadening of the spectral dropout accompanied the shift in the resonance wavelength. was fabricated using Corning SMF-28 single mode fibers.

High-Temperature Stability and Annealing Effects

We investigated the stability of TLPFGs at high temperatures and found that thermally induced



(a) Transmission spectra at various temperatures (b) Change of the resonance wavelength with temperature

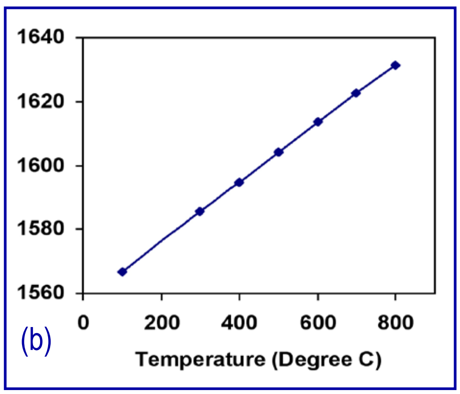


Figure 4. Temperature sensitivity evaluation of TLPFG. The LPFG had a period of 500 µm and was fabricated using Corning SMF-28 single mode fibers.

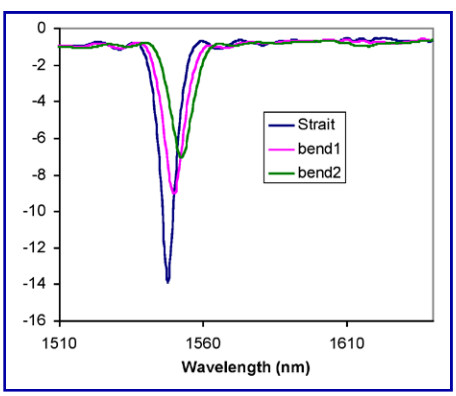


Figure 5. Shift of the resonance wavelength caused by bending. The LPFG has a period of 515 µm and

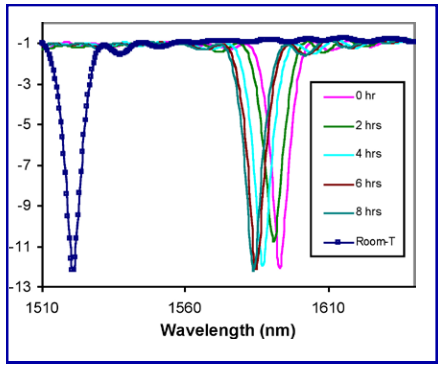


Figure 6. Shift of the TLPFG transmission spectrum in response to annealing at 650 °C for eight hours. The LPFG had a period of 500 µm and was fabricated using Corning SMF-28 single mode fibers.

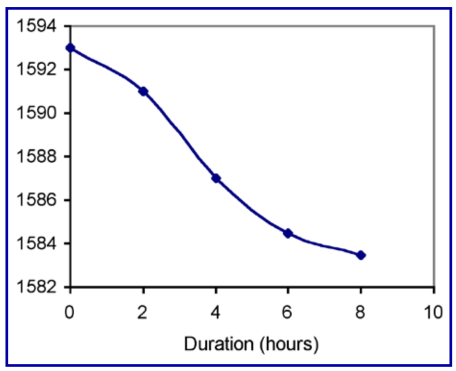


Figure 7. Drift of the TLPFG resonance wavelength caused by annealing at 650 °C.

refractive index modulations tend to decrease when the grating is subject to very high temperatures. This is mainly caused by the annealing process, as the built-in thermal stresses tend to release under long-time exposure to very high temperatures. The potential decrease of the refractive index modulation during the annealing process could be a major practical constraint in such applications.

We studied the gratings' thermal stability experimentally by placing the TLPFG in high-temperature environments. At temperatures below 500 °C, we observed no obvious drift of the transmission spectrum in eight hours' time. However, as the temperature increased to 650 °C, the whole transmission spectrum began to drift toward the short wavelength, as shown in Figure 6. The resonance wavelength as a function of the duration is plotted in Figure 7.

Although there was about a 9 nm drift in the resonance wavelength drifted for the entire eight hours, the drifting slowed as the exposure time increased. We also found that the peaks position changed about 1 nm after cooling to room temperature. We attributed this irreversible change to the stress relief and the plastic deformation of the fiber after annealing at such high temperatures. It is worth noting that there was no obvious degradation of the TLPFG quality after eight hours' exposure to 650 °C because the TLPFG attenuation band maintained the same strength and shape compared with what it was before.

Partially based on the research findings of this work, the Office of Naval Research funded one research project, called "Understanding the Optical Behavior of Zeolite Thin Films and Nanoparticles to Develop Micro Chemical Sensors: Bridging the Nanoscale and the Microscale." The project received one of seven ONR Young Investigator Program (YIP) Awards in 2006.

We are preparing one journal article.

Development of Nanoparticles/ Nanocomposites as Efficient Surface-Enhanced Raman Spectroscopy (SERS) Substrates

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From an analytical viewpoint, Raman spectroscopy offers several important advantages: non-destructive, highly specific, multiplexing capabilities, and little sample preparation. Still, it has been used more frequently for structural analysis than for trace detection, because of the small cross section for Raman scattering resulting in low sensitivity.

Discovery of surface-enhanced Raman spectroscopy (SERS) suggests that low concentrations of analytes are detectable. A major barrier for analytical applications is that the preparation of SERS substrates is far from "standardized" or reproducible. Few of the many methods reported to prepare the substrates could generate substrates with good efficiency consistently. We proposed to develop nanomaterials as efficient SERS-active substrates.

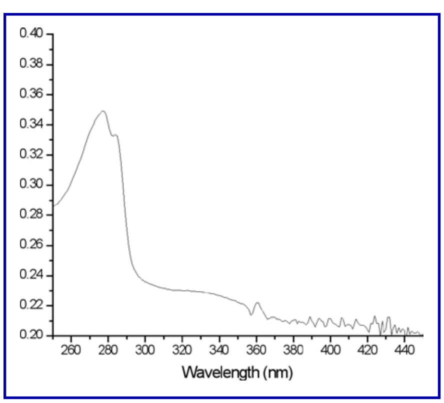

Figure 1. UV-vis absorption spectrum of silver nanoparticles-based SERS substrates.

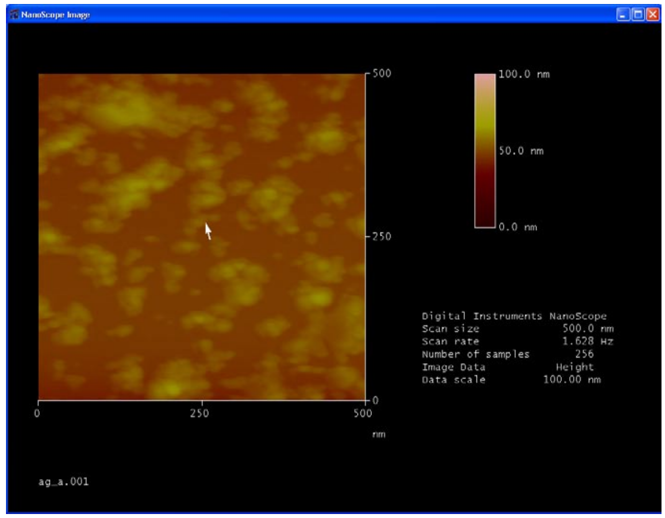

Figure 2. AFM image of silver nanoparticles-based SERS substrates.

We demonstrated a simple and reproducible method to produce silver nanoparticles-based nanomaterial as efficient substrates for SERS. We synthesized silver nanoparticles-based substrates in a reverse microemulsion system consisting of sodium dodecacyl (SDS), cyclohexane, hexanol, and H_2O. We collected the nanoparticles and washed them several times with methanol through sonication and centrifugation. he final product, which we dispersed in deionized water, remained stable and SERS-active for weeks when stored in the dark. For the purpose of comparison, we also prepared silver colloids in the same manner and followed the well-practiced procedures.

The silver nanoparticles were characterized in a couple of ways. The ultraviolet (UV) absorption spectra of the silver nanoparticles, both in the microemulsion and after several washings, are shown in Figure 1. Figure 2 is an AFM image of the final Ag nanoparticle-based material after several washes and redispersion in water and being dried on a mica surface.

We performed the SERS measurements on a home-built setup based on an inverted microscope. The laser source for all SERS measurements was an Argon ion laser radiated at 488 nm. We focused the incident laser beam by an objective (either 40× or 10×) onto the sample. Typical excitation power at the sample was ~2mW. Raman signals, which we collected by the same objective, passed through a notch holographic filter and coupled into a spectrometer equipped with an air-cooled (CCD) detector. We used Rhodamine 6G (R6G) as the probe molecule.

In a typical measurement, silver nanoparticles were isolated, by centrifugation, from the solution where they were dispersed. We then sonicated and incubated them in a small amount of 0.2 µM R6G solution for several minutes, applied the mixed solution onto a cover slide, and measured its SERS signals.

A typical SERS spectrum of R6G obtained with silver nanoparticles-based substrate is shown in Figure 3. As a comparison, we collected SERS spectrum of R6G using conventional silver colloids, with R6G concentration at 1 µM. Although we took these two spectra under the same conditions, i.e., same laser power, exposure time, and number of accumulations, the difference between them is clearly

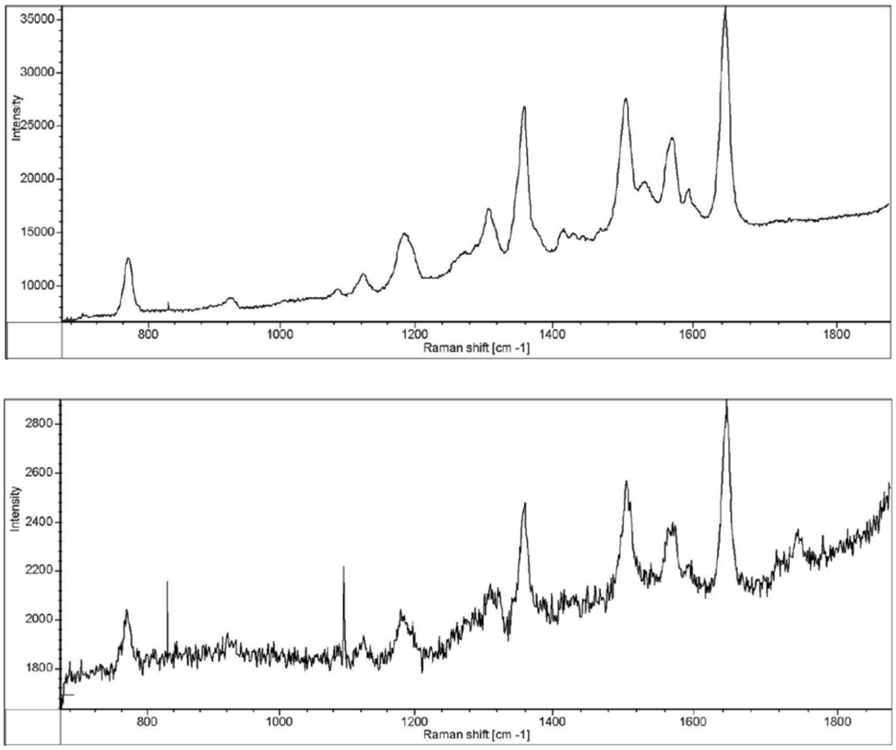

Figure 3. SERS spectra of R6G on the silver nanoparticles-based substrates (top) and conventional silver colloid substrates (bottom). All experimental conditions were the same for the two measurements.

noticeable. The silver nanoparticles-based substrate has a much better signal-to-noise ratio, and the intensity is about 10 times greater than the one with the silver colloids, even at five-fold lower concentration of the analyte.

We demonstrated a simple method to produce silver nanoparticles-based nanomaterial as efficient substrates for SERS. The method can prepare SERS substrates in a reproducible way. Compared to the SERS substrates of the conventional silver colloids, the silver nanoparticles-based substrate has a much better signal-to-noise ratio. The Raman signal intensity from our silver nanoparticles-based substrate is about 10 times greater than the one with the silver colloids, even at five-fold lower concentration of the analyte. The prepared substrates could be dispersed in water, and they remained stable and SERS-active for weeks when stored in the dark.

A proposal based on the results of this project is planned for submittal to either National Science Foundation or Department of Energy.

Refereed Communications

"Preparation of Ag Particle-based Nanomaterial as Efficient Substrates for Surface-enhanced Raman Spectroscopy" submitted to Chemical Communications, November 2006.

Characterization of the Plasma Source in the Magnetically Controlled Triggered Plasma Opening Switch

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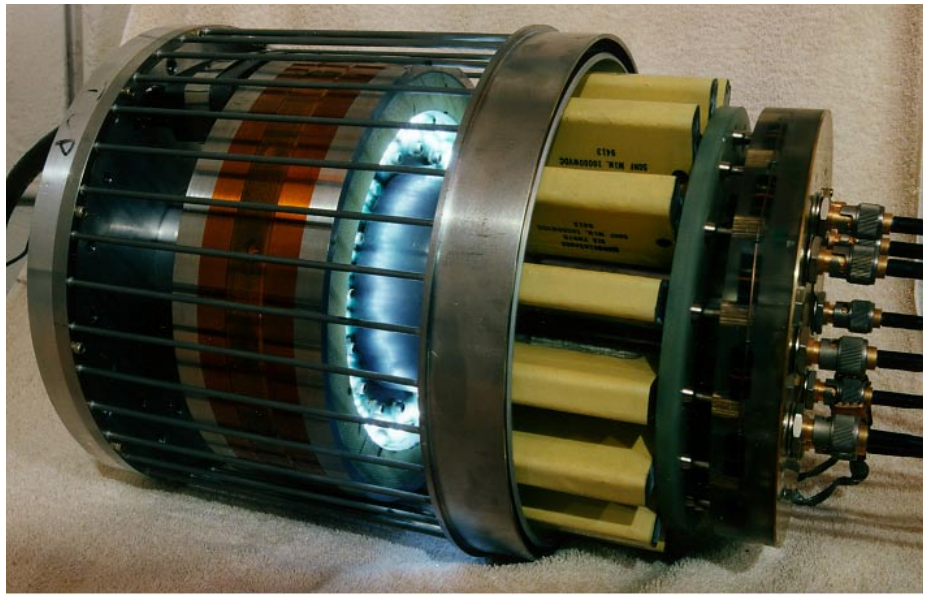
Sandia Principal Investigator



Plasma opening switches are an established technology for pulse compression and voltage multiplication in pulsed power applications [1]. To improve the opening speed and timing of traditional self-opening switches, Sandia initiated the magnetically controlled triggered plasma opening switch (TPOS) experiment. The focus of this work has been to characterize basic plasma parameters of the TPOS source using interferometry and electrostatic probes.

We completed a characterization of axial density profiles versus switch operating parameters, and our initial measurements suggest that the axial plasma density gradients are weak, and that energetic ions (> 800 eV) are produced by the source.

We performed measurements in the vacuum test stand, shown in Figure 1, that was assembled last year during the first-year SURP project. This year our efforts focused on three areas:
1) construction and application of a radially viewing millimeter wave (120 GHz) interferometer, 2) construction and application of electrostatic probes, and 3) development of a tangentially viewing $\lambda = 10.6$ µm (CO_2) interferometer.

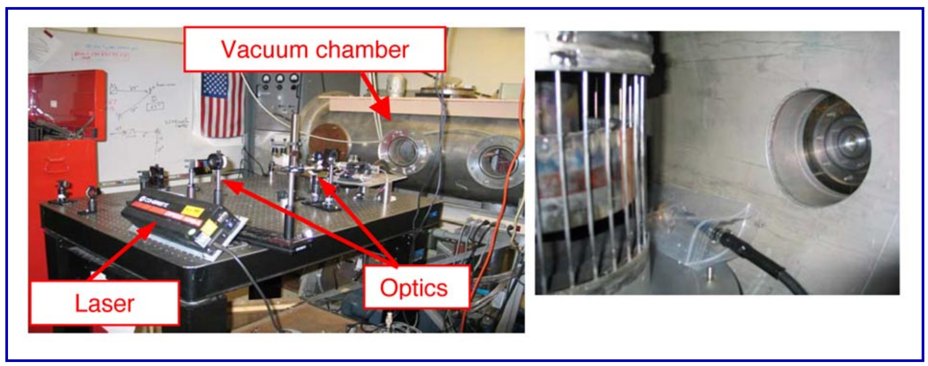


Figure. 1. Left: TPOS source test stand. Vacuum chamber in rear, interferometer optical table in foreground. Right: Switch source mounted vertically inside the vacuum chamber.

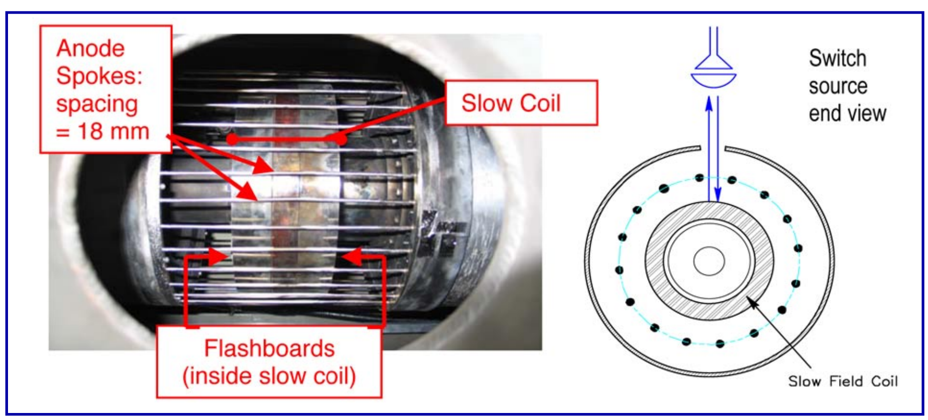


Figure 2. Left: Side view of the TPOS source. The radially viewing mm wave interferometer reflects from the slow coil. As such, the beam must pass unimpeded between the anode spokes, which have spacing not much larger than the diffraction limit. Right: end view showing interferometer beam path.

We developed the 120 GHz interferometer, installed the system, and obtained density measurements. Though the interferometer circuit design was relatively straightforward, the optical design (or, more correctly, quasioptical design) was challenging due to the geometrical constraints. In particular, the mm wave beam was reflected from the "slow" coil for the radial view. This required the beam to pass between two anode spokes, which are spaced 18 mm apart – close to the diffraction limit in this case, as shown in Figure 2.

In order to accomplish the required focusing, we built two cylindrical planar-convex HDPE lenses to focus the radiation from a rectangular horn antenna to the right spot size at the desired location (beam waist located at the slow coil). We designed the lenses using a modified ray tracing technique developed as part of this work (see *breakthrough research* below). The mm wave interferometer, together with the measured antenna pattern, is shown in Figure. 3.

When installed, the mm wave system performed very well, and we measured plasma density versus time for varying sysem parameters (flashboard voltage and "slow coil" capacitor bank voltage). Data are shown in Figures 4 and 5. The significance of these data is that the density vs. source parameters has been quantified, and that the data suggest that the axial density gradient is weak, which was not expected. The weak axail gradient may impact the understanding of the TPOS plasma dynamics.

We also made electrostatic (double Langmuir) probe measurements. After several iterations, we found a working probe design that avoided unipolar arcing; see Figure 6. Example ion saturation current data is shown in Figure 7. Though the signal-to-noise ratio is poor in this case, the measured

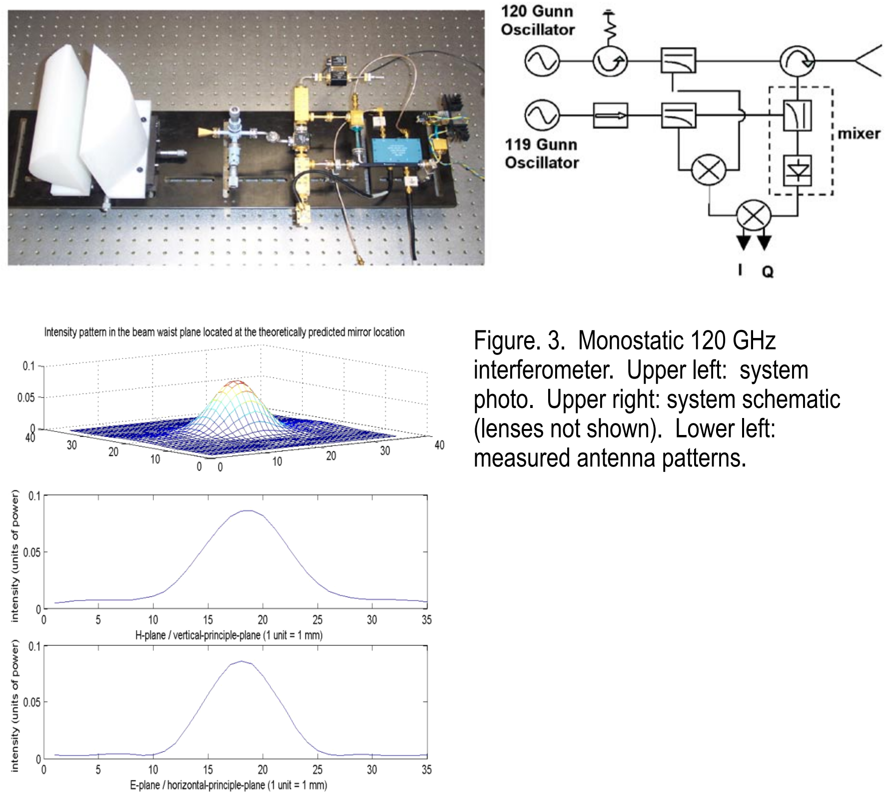


Figure. 3. Monostatic 120 GHz interferometer. Upper left: system photo. Upper right: system schematic (lenses not shown). Lower left: measured antenna patterns.

Figure 4. Measured plasma density on the axial midplane from the 120 GHz radially viewing interferometer for two flashboard voltages and various "slow coil" capacitor bank voltages. An 18 cm path length was assumed. Half radius magnetic fields corresponding to these bank voltages are 212 Guass (1 kV), 466 Guass (2 kV), 724 Guass (3 kV), and 954 Guass (4 kV).

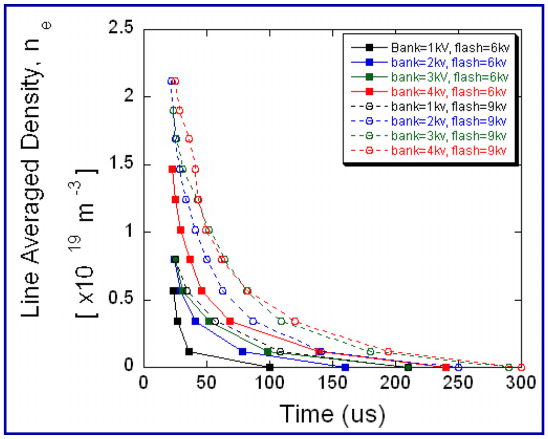
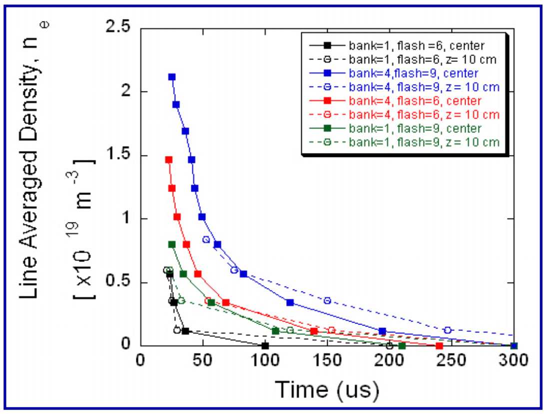


Figure 5. Measured plasma density at two axial positions from the 120 GHz radially viewing interferometer. Axial positions are: z = 0 cm (axial midplane), and z = 10 cm. An 18 cm path length, and O-mode propagation were assumed. Half radius magnetic fields corresponding to these bank voltages are: 212 Guass (1 kV), 466 Guass (2 kV), 724 Guass (3 kV), and 954 Guass (4 kV).



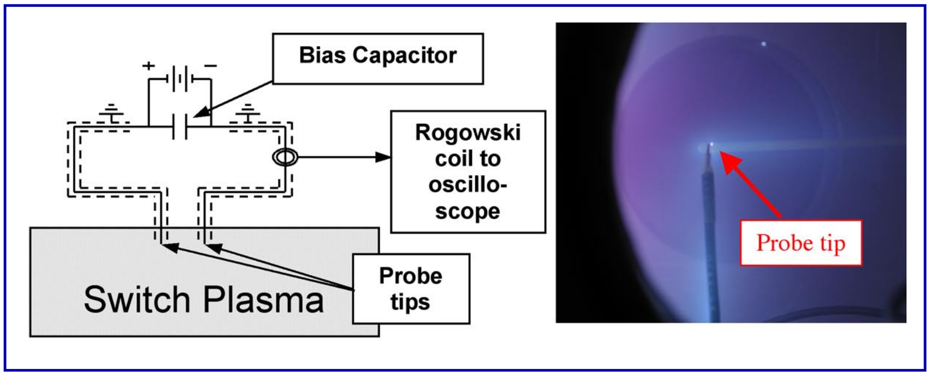


Figure 6. Double electrostatic probe circuit (left), and photo of the probe in the plasma (right).

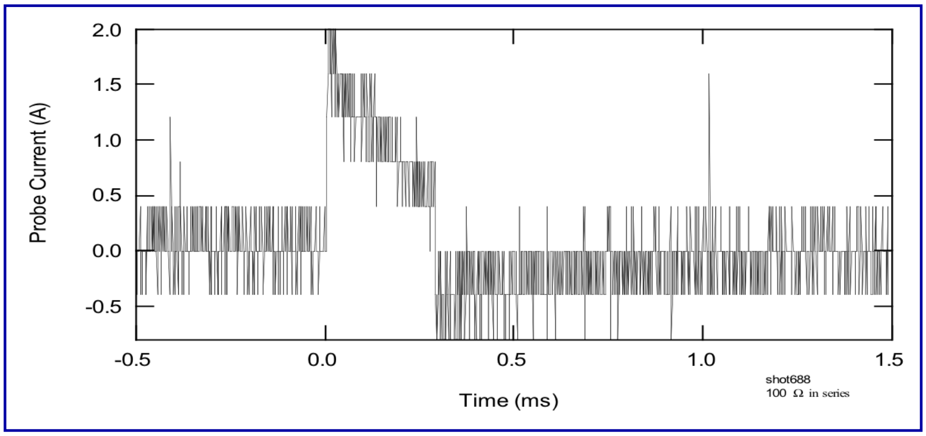


Figure 7. Probe ion saturation current signal. The very large probe current at relatively low plasma density (n ~ 10^{19} m^{-3}) suggests very energetic ions, with drift energies > 800 eV.

current is rather large, I ~ 1.5 A. Our present interpretation is that the ions have a high drift energy, > 800 eV (limited space does not allow for a detailed justification of this tentative conclusion). We are setting up a visible Doppler spectrometer in order to verify the high ion velocity.

Breakthrough Research

Progress has been slow, but we are continuting to develop the λ = 10.6 µm (CO_2) interferometer. Implementation of the 120 GHz interferometer with near-diffraction-limited focusing required us to develop new quasioptical design tools. Quasioptics is, of course, the appropriate limit of optics in this case, where the usual ray optics assumption that λ << L is not valid, and where L is the typical dimension of the optical components [2]. In order to design the cylindrical planar-convex lenses used, we developed a modified ray tracing technique that tracks rays through the optical system, correcting for the fact that the propagating beams are significantly nonGuassian. We implemented this method in a MATLAB code.

As far as we are aware, this modified ray tracing technique has not been published elsewhere and is the subject of Naga Devarapalli's masters thesis, as well as a journal paper currently in preparation. Again, limited space does not allow for a detailed description of the method. We refer the interested reader to the forthcoming thesis and paper, referenced below.

Electrostatic probe measurements suggest the existence of high-energy ions, accelerated by the flashboard sources. Visible spectroscopy is currently being set up in order to confirm the fast ion drift velocity via Doppler shift measurements of carbon line emission.

Follow-on research is continuing with anticipated financial support from Organization 1644 to complete the characterization of the TPOS source. The CO_2 interferometer will be completed and installed, and visible spectroscopy will be deployed. These new systems will be used with the existing mm wave interferometer and electrostatic probe to finish characterizing two existing versions of the TPOS source.

References

[1] See, for example, T.J. Rank (1989). J. *Applied Physics* 65(7), 2652; M.E. Savage, D.B. Seidel, and C.W. Mendel, Jr. (2000). *IEEE Trans. Plasma Sci.* 28(5), 1533; and references therein.

[2] P.F. Goldsmith. *Quasioptical Systems*. Piscataway, NJ: IEEE Press, 1998.

Refereed Communications

N. Deverapalli, "120 GHz Tracking Interferometer for Characterization of the Plasma Density in the SNL Triggered Plasma Opening Switch," Masters Thesis, Electrical and Computer Engineering, University of New Mexico, December 2006.

D.P. Jackson, et al., "Ion Collection Current Diagnostic for Exploring Plasma Opening Switch Performance," *IEEE Trans. Plasma Sci.* 34(5), 1900, 2006 (from first year SURP work).

N. Deverapalli, et al., "Diffraction Limited 120 GHz Tracking Interferometer," to be submitted to *Review of Scientific Instruments*.

Other Communications

N. Devarapalli, A.G. Lynn, and M. Gilmore, "120 GHz Tracking Interferometer for Characterization of the Plasma Density in the SNL Triggered Plasma Opening Switch," poster presented at the 16th Topical Conference on High-Temperature Plasma Diagnostics, Williamsburg, VA, May 2006.

A.G. Lynn, W.T. Clark, M. Gilmore, N. Devarapalli, M.E. Savage, and R.A. Sharpe, "Preliminary Interferometric and Probe Measurements on a Triggered Plasma Opening Switch Source," poster #2P16, *Proceedings of the IEEE International Conference on Plasma Science,* Traverse City, MI, 2006.

W.T. Clark, N. Deverapalli, A.G. Lynn, M. Gilmore, M.E. Savage, B. Stoltzfus, and R.A. Sharpe, "Characterization of a Plasma Opening Switch Source by Interferometry and Probe Measurements," poster presentation at the 48th American Physical Society Division of Plasma Physics Annual Meeting, Philadelphia, PA, October 2006.

Inorganic Carbon Usage by the Marine Cyanobacterium Synechococcus WH8102

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Synechococcus WH8102 is a dominant oceanic photosynthetic cyanobacterium with a genome that encode for a type of carboxysome (prokaryotic microcompartment) previously only found in chemolithoautotrophic proteobacteria. Many of the genes thought to be critical for proper functioning of a carboxysome-based CO_2-concentrating mechanism (CCM) are not identifiable in the genome.

A new class of bicarbonate transporter was recently discovered, and analyses of its function and expression, along with the kinetic properties of the CO_2 capturing enzyme Rubisco, will elucidate the photosynthetic function of this species. These data will provide critical physiological information needed for understanding carbon sequestration by *Synechococcus.*

This year was plagued by critical errors in substrate syntheses for studying the CO_2 capturing enzyme Rubisco. However, we trained an undergraduate student who presented our work at the national meeting of the American Society of Plant Biologists. In the process of troubleshooting and testing, she made a significant discovery in the activation properties of a Red algal form of Rubisco.

Surprisingly, the enzyme from the coastal macroalga *Ploclamium cartilagineum* is similar to that of cyanobacteria with carbon dioxide and magnesium binding properties orders of magnitude different from the well-characterized spinach enzyme. This raises significant questions about the origin, evolution, and regulation of Rubisco in photosynthetic organisms.

Interestingly, Red algae also have light harvesting complexes like those found in cyanobacteria, and our data are the first kinetic studies to suggest that a more cyanobacterial like (in function) Rubisco is present in some eukaryotes. We plan to submit a grant proposal in July 2007 to pursue this discovery.

We also demonstrated that our membrane inlet mass spectrometry system is functional. We hope to conduct additional measurements this year with support from the University of New Mexico (UNM) and other agencies.

Our breakthrough research was discovering that activation of Red algal Rubisco is more like cyanobacterial Rubisco than land plant or Green algal Rubisco. We discovered mid-year that an unacceptably high concentration of inhibitors existed in the substrates we had generated for proposed Rubisco assays, so we resynthesized and tested new batches of compounds.

We had difficulty extracting sufficient amounts of Rubisco from WH8102, so we tested new synthesized compounds on the well-studied enzyme from spinach and an unstudied but successfully purified enzyme from the Red algal *Plocamium cartelagineum.* These efforts consumed nearly all of our resources but generated significant discoveries.

We will continue with our original plans using funds from the Biology Department at UNM in an effort to acquire enough data for resubmitting a National Science Foundation (NSF) grant written in the first year of funding. We will also pursue our SURP-supported discoveries in Red algal Rubisco funding with the intent of a July 2007 NSF submission.

Refereed Communications

S. Sanchez Monzon and D.T. Hanson, "Activation of Red Form I Algal Rubisco from *Plocamium Cartilagineum*," *Plant Biology* 2006, American Society of Plant Biologists, Boston, MA, July 2006.

Storage Optimization in a Microgrid

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John Boyes (Org. 6251)
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A microgrid is an electrical network containing distributed energy resources such that the network can provide reliable service to its loads under grid-connected or islanded conditions. A surety microgrid adds additional requirements to ensure continued operation of critical systems under the most adverse of conditions.

This project consisted of developing a method to determine optimal storage deployment within a surety microgrid, given the system resources, demand pattern, and operating conditions and constraints. This work is part of the research that will enable the realization of reliable and secure power systems. We demonstrated the method on a Sandia-provided surety microgrid test system resembling a military base.

The purpose of the project was to develop a method to determine the location and amount of storage that must be deployed in a surety microgrid, such as a military base, in order to increase its reliability by a predetermined amount. For the purpose of demonstrating the method developed, the Sandia team provided the New Mexico State University (NMSU) team with a test system that resembled a military base and named it Base Alpha. The system data made available to the NMSU team was also typical of the kind of data generally available for military bases.

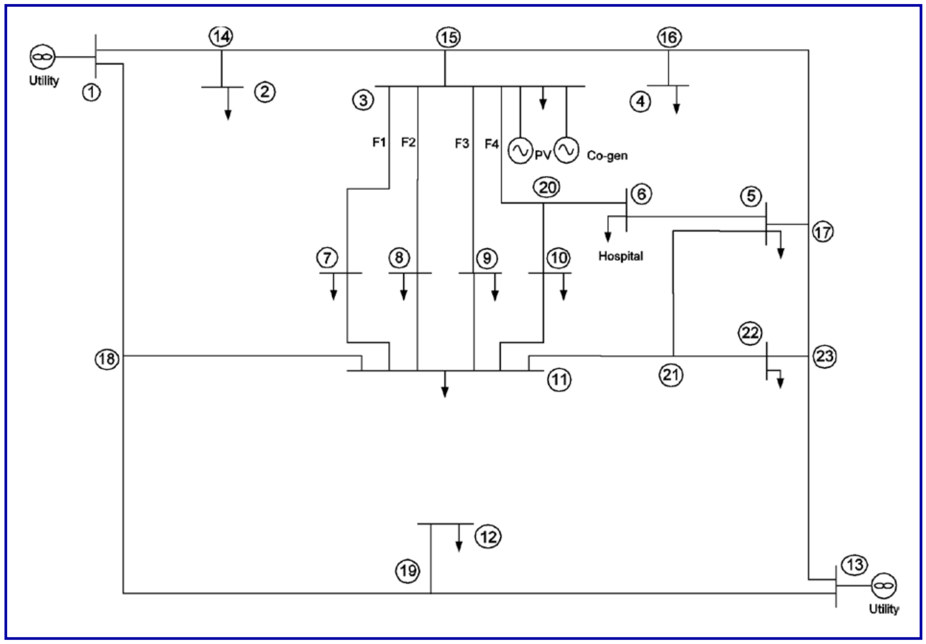

Figure 1. Equivalent network for Base Alpha system.

After examining the system configuration and the data, we developed the following strategy:
1. We would equivalence the system, i.e., build a simpler system that retained the functional elements of the original system that were relevant from a reliability analysis perspective and that was amenable to reliability analysis.
2. We would conduct a needs assessment, using a suitable method, to determine the amount of storage required at the important locations within Base Alpha.
3. We would perform an analysis to verify whether the recommended deployment strategy provided the expected reliability benefits.

From the recommended storage deployment, the Sandia team could decide, based on the storage alternatives available to them, how much of each type of storage (such as batteries, fuel, etc.) they wanted to deploy. In the following paragraphs, the methods applied in each of the four steps, and their outcomes, are briefly reported.

System Equivalencing
The drawing of the Base Alpha system, as provided by Sandia, is shown in Figure A1, in the Appendix. This was equivalenced to a 23-bus system, of the form shown in Figure 1, above. The data was also equivalenced appropriately. Peak load data was provided by Sandia. Load shape data was obtained from FERC 714 filings for the PNM service area. Some data for component reliability was provided by Sandia; the rest was obtained from the IEEE Gold Book [1].

Reliability, Need and Benefit Assessment
The capacity of a storage device must be specified in terms of both the amount of energy (in J or Wh) it can store and the rate (in W) at which it can release the energy, i.e., the power capability. This implies determination of system down times. In order to obtain a good indication of system

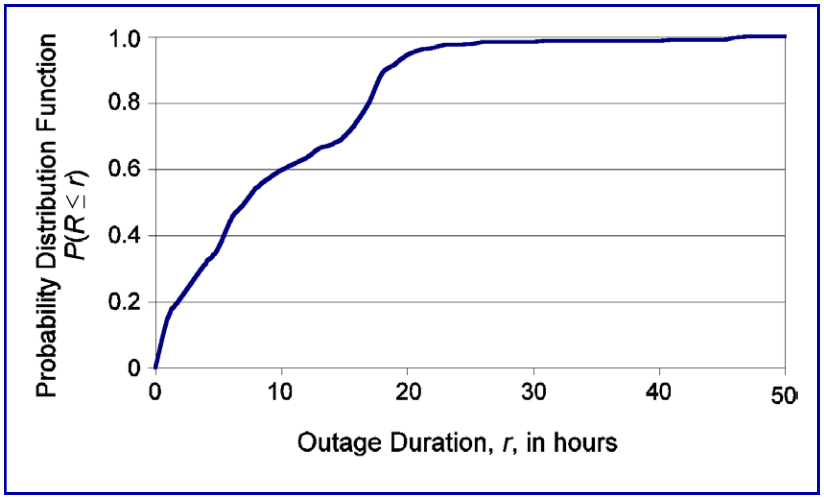

Figure 2. Interruption duration distribution at Bus 6.

down times, we decided to generate probability distributions of down times not only system-wide but also at every load point. We accomplished this using a detailed, sequential, asynchronous Monte Carlo simulation [2, 3] taking into account all system and component dependencies.

Since self-dependence was important, we performed the simulations for islanded (disconnected from utility) conditions. The distributions thus generated resembled that shown in Figure 2, which represents the probability distribution function of the outage durations at bus 6 (which was designated a critical load bus). From these distributions, it is possible to make decisions regarding how much total storage should be augmented at each critical node.

The original contribution of the research comprised the development of a method that would enable determination of the quantity of storage required to be augmented at important locations in the system to produce a desired amount of reliability improvement. The method can be summarized as follows.

Accurate system modeling and detailed Monte Carlo simulation produces an "artificial history" of the system. Data can be extracted from this history to provide accurate estimates of reliability indices and the probability distributions of these estimates.

Consider the following: At a given system bus, unavailability (or loss of load probability), P_F, may be estimated from the ratio of total down time r_T encountered at that bus during the simulation, to the total time t_T over which the system operation was simulated:

$$\hat{P}_F = \frac{r_T}{t_T}$$

Supposing one desires to "add a 9 of reliability" at that bus, this amounts to reducing P_F by 90 percent. This can be achieved by adding storage at that bus that can serve the load at that bus for a period of time t_S, which is given by

$$t_S = \frac{t_A}{A_S}$$

where A_S is the overall availability of the storage devices deployed at the given bus, and t_A is determined from

$$\int_0^{t_A} r f_R(r) dr = 0.9\overline{r}$$

where R is the random variable representing the down time at the bus, $f_R(r)$ is the probability density function of R, and $\overline{r}$ is the mean duration of the outage at the given bus, i.e., , n_F being $\overline{r} = r_T / n_F$ the number of outages experienced at the given bus over the period of simulation. The value of t_S can be determined from the data collected from the simulation. The derivation of these relationships, and the development of a means of solving this, constitute the original contribution of this research.

Before the decision was made to use the Base Alpha system, we had made some progress in developing an integrated method to optimally deploy storage resources in any microgrid. Our goal was to determine the optimal sizing and location of storage resources in a microgrid given the network configuration, the heat and power requirements at various load points, and the stipulated reliability at the load points. After examining the Base Alpha system, the nature of data available for such systems, and the requirements of such systems, the Sandia and NMSU teams agreed that a change of direction would better enable them to accomplish this work.

We resumed the work the NMSU team initially started and built a framework for integrated optimization of the deployment of all forms of DER generation and storage — such as microturbines, fuel cells, solar panels, wind turbines, backup generators, batteries, superconducting magnetic storage, super/ultra-capacitors, flywheels, and fuels. In other words, we decided to expand it into a broader, more flexible and universally applicable methodology. This was the basis of the SURP proposal for FY2007. We are also working on identifying a suitable federal agency that will continue to fund this significant work. We are preparing articles on the described work.

Refereed Communications:
M.R. Vallem, D. Jensen, and J. Mitra, "Reliability Evaluation and Need-Based Storage Assessment for Optimal Microgrid Architecture," Proceedings of the 38th Annual North American Power Symposium, Carbondale, IL, September 2006.

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[1] *IEEE Recommended Practice for Design of Reliable Industrial and Commercial Power Systems.* (Also known as the IEEE Gold Book or the IEEE Standard 493-1997.) Published by the Institute of Electrical and Electronics Engineers, NY, 1997.

[2] A.M.L. da Silva, W.F. Schmitt, A.M. Cassula, and C.E. Sacramento, "Analytical and Monte Carlo Approaches to Evaluate Probability Distributions of Interruption Duration," *IEEE Trans. Power Systems*, vol. 20, no. 3, August 2005.

[3] C. Singh and J. Mitra, "Reliability Analysis of Emergency and Standby Power Systems," *IEEE Industry Applications Society Magazine*, vol. 3, no. 5, pp. 41–47, September/October 1997.

Appendix

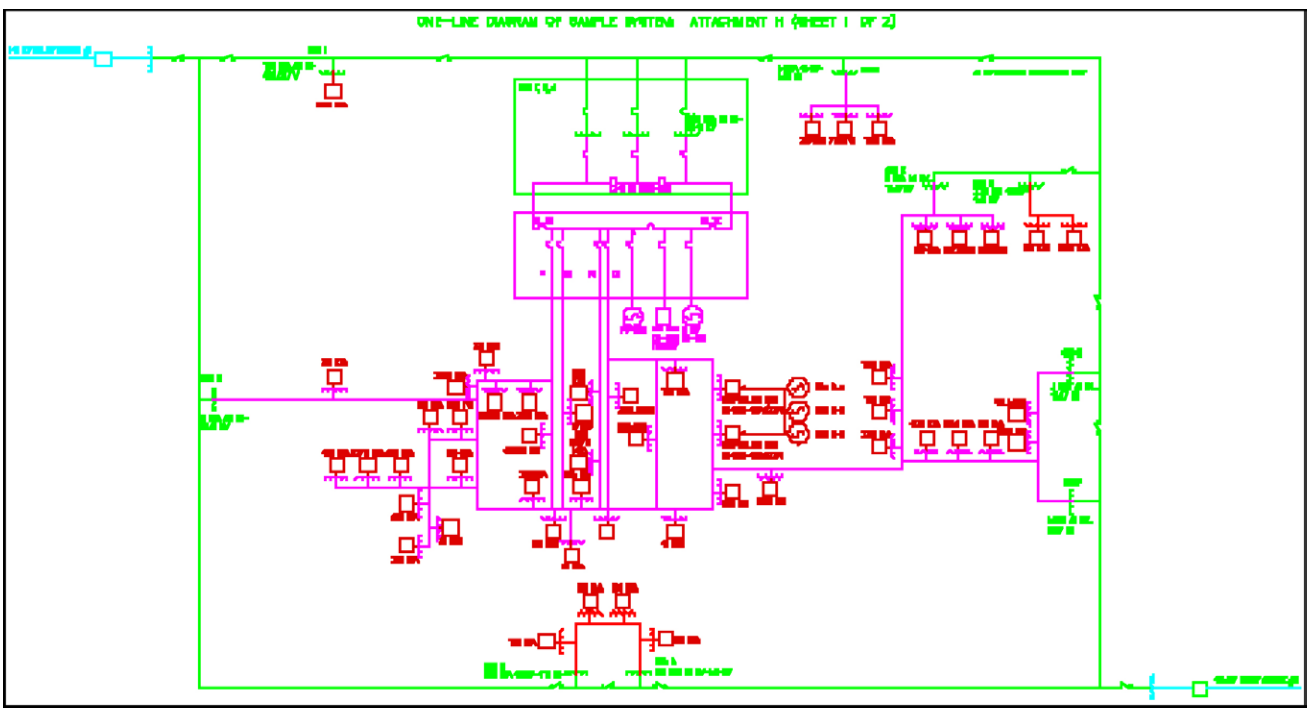

Figure A1. Original schematic for Base Alpha

GIS-Based System Dynamics Modeling of Watershed Processes for Water Resources Management in the Rio Grande, New Mexico

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New Mexico Institute of Mining and Technology

Vince Tidwell (Org. 6313)
Sandia Principal Investigator

In the Western United States, an imbalance between water supply and demand is prompting water conflicts between multiple water stakeholders (e.g., farmers, conservationists, developers) even during recent wet winters. This project will result in a new decision support system that integrates watershed hydrology with ecologic, economic, policy, and institutional aspects of the water resources problem. It will also provide detailed watershed modeling for flood and drought forecasting, estimation of the spatial distribution of runoff, evaporation and aquifer recharge, and the simulation of basin water storage and supply throughout a variety of basins feeding the Rio Grande.

Accomplishments this year consisted of updates to the semi-distributed watershed model formulated within Powersim that have improved performance and helped build confidence in the model ability to simulate historical events. By increasing the use of VB-script within the Powersim environment, the model is able to operate at storm-event scale, using both synthetic and historic input data, and calculate monthly outputs to be used by the Sandia LDRD System Dynamics Toolbox for the Middle Rio Grande. We met our general goal of providing a model to simulate tributary inflows from precipitation records to the Sandia model.

While rainfall generation and evapotranspiration are separate Powersim modules, the remaining water balance components (interception, infiltration, runoff, and drainage) are embedded in a single hydrologic response unit (HRU) module taking advantage of the VB-script capabilities of Powersim. The variable infiltration capacity (VIC) module is now able to properly partition soil moisture, thus increasing the accuracy of runoff generation within the model.

In addition, we made model developments to account for water losses in ephemeral channels, groundwater redistribution of deep percolation from the unsaturated zone, and snow accumulation and melt dynamics within a partially covered HRU element. We are continually testing various model components and improving simulation output. In essence, however, the model development has been completed and is ready, after more thorough testing, to be delivered to Sandia.

We completed the GIS processing of the watersheds in the Middle Rio Grande basin, which consisted of delineating watersheds along the river reach, subdividing these watersheds into HRUs, and determining unique properties for each HRU. In addition, we synthesized the data sets into model parameters based on topographic, vegetation, and soils characteristics within each delineated sub-basin. As a result, the model setup for the Middle Rio Grande is essentially ready for model applications after more thorough tests are performed.

Initial runs of the model on the Rio Salado produced encouraging results and provided preliminary output data sets that will be used to calibrate the model. Model output in the form of spatial runoff, soil moisture, and evaporation maps are under preparation for publication. In addition, we are analyzing historical and prospective time series output as part of the material in preparation for publication. We are making progress toward incorporating spatially distributed PRISM rainfall radar datasets as model input, in addition to the current use of the stochastic rainfall model and historical rain gauge records. We are also using digital orthophotos and field reconnaissance when available to improve HRU classification.

Our progress has been significant over this past period. We developed a simple, yet physically meaningful, watershed model for use in the Sandia decision support system. The applications of this model to the Rio Grande and other basins worldwide will be an integral part of the water resources decision support activities at Sandia.

Over the past year, no major changes were necessary to the research direction. We completed the model development and are conducting model testing exercises in the Rio Salado that will result in publication-quality simulations for a series of papers and a masters thesis (under preparation).

We anticipate publishing the major results from this project over the next year, including a masters thesis at New Mexico Tech and at least one journal publication on the work.

Additional work for this research project will be funded by a new project from the New Mexico Water Resources Research Institute and a contract with Sandia for watershed modeling in the Gila River Basin. Using these sources, we will conduct short- and long-term simulations to reproduce observations of hydrologic state in the watersheds that contribute to the Rio Grande and to explore sensitivity of the parameters that feed the model. We will also determine water supply sensitivity to climate change, land-use change, and interannual variability in rainfall as future scenarios. Finally, the watershed model will be linked with a GIS software package to test the coupling of semi-distributed modeling with system dynamics modeling.

Refereed Communications

C.A. Aragón, L.A. Malczynski, E.R. Vivoni, and V.C. Tidwell, "Modeling Ungauged Tributaries Using GIS and System Dynamics," presented at the 26th Annual ESRI International User Conference, San Diego, CA, August 2006.

Poster presentation

C.A. Aragón, E.R. Vivoni, L.A. Malczynski, V.C. Tidwell, and S. Gonzales, "Modeling the Contributions of Ungauged Tributaries to the Rio Grande: A System Dynamics Approach," presented at the American Geophysical Union, Fall Conference, San Francisco, CA, 2006.

C.A. Aragón, "Modeling the Contributions of Ungauged Tributaries to the Rio Grande Using a System Dynamics Approach. New Mexico Institute of Mining and Technology, Socorro, NM, (master's thesis in preparation).

C.A. Aragón, E.R. Vivoni, L.A. Malczynski, V.C. Tidwell, and S. Gonzales, "Modeling the Contributions of Ungauged Tributaries Using a System Dynamics Approach," to Environmental Modelling and Software (journal manuscript in preparation).

EXPLORATORY PROGRAMS

As a means to assist Sandia in achieving its mission-related needs, the University Research Office supports interactions with some universities that do not have “key” or “regional” status. Such interactions are meant to explore niche technical areas of interest and forge new strategic relationships in critical skills areas. Programs include, but are not limited to, such areas as senior research clinics, educational and research institutes, student internships, and joint research in specific areas of interest. These programs are evaluated regularly to determine their value toward achievement of Sandia’s mission objectives.

EXPLORATORY PROGRAMS: Harvey Mudd College Clinic

In order to strengthen the pipeline for student interns, Sandia extended its university research partnerships to include an undergraduate university in 2004. Typically, Sandia’s university partnerships are with those universities having graduate research programs. Harvey Mudd College was selected because of the high rating of its undergraduate engineering programs. In the past, the University Research Office worked with Harvey Mudd College to identify the appropriate means of tapping their brightest undergraduate talent. Activities included sponsoring research clinics, identifying students as candidates for internships, and considering Harvey Mudd College graduates as full-time employees. In 2006, Sandia line organizations sponsored two Harvey Mudd College Clinics—one Engineering and one Physics Clinic—at $40,000 each.

The Harvey Mudd College Clinic Program engages students in the solving of real-world, technical problems for corporate clients. Engineering, mathematics, physics, and computer science departments each conduct clinic projects that draw upon the unique talents of students and faculty advisors. Since the Clinic program was developed at Harvey Mudd College nearly 40 years ago, over 250 organizations have participated. The College has completed over 1,000 projects.

Students work in groups of four or five under the guidance of a student project manager, a faculty advisor, and a liaison from the Sandia sponsoring organization. Projects begin in September, involve about 1,200 work hours and are completed the following May. The liaison outlines the project requirements, approves the team’s proposal for accomplishing the work, and receives weekly progress reports. In most cases, the student team visits the sponsoring company for a mid-year project review and typically provides a summary presentation to senior officials at the end of the project. Clinic teams present their research during public forums held on campus and submit final written reports to the customer upon completion of the project. Sponsors retain full rights to all intellectual property developed by the team.

Funding for the Clinics comes from the Sandia organization that has a need for the particular research. Sandia selects Clinic projects based on the value to mission-relevant research. The value of the Harvey Mudd College Clinic program in helping Sandia achieve its mission objectives continues to be evaluated.

Simulation of an Object-Based Filesystem

Harvey Mudd Student Research Team:
Mark Kegel (Project Manager), David Coyne, Esteban Molina-Estolano, Selene Tan

Faculty Advisor
Professor Geoff Keunning
Computer Science

Sandia Principal Investigator
Ron Oldfield
(Org. 1423)

Abstract

A significant challenge facing I/O researchers for future-generation systems is how to evaluate the scalability of an experimental I/O system in the absence of a physical machine. Analytic modeling is one solution, but it is requires approximations that may hide subtle effects that have a potentially large impact on accuracy when scaled to thousands of processors. A second approach approximates performance by implementing I/O system protocols on top of a composition of simulated devices for storage, network, and processing. It is the second approach that we have chosen for this project.

The long-term goal of this project is to develop a complete simulation framework to evaluate the scalability of experimental I/O systems and protocols. The first step toward that goal (the main work of this HMC clinic) is to design and develop an accurate simulator for object-based storage devices.

Background

A significant amount of the first semester focused on background reading and design of the basic architecture for I/O node simulation.

The general goal is to model a typical, in-practice, object-based storage device (OSD). The OSDs used in practice today simply provide an object-interface layered on top of a Unix file system. For example, the Lustre OSD uses the ext3 file system at the lowest layer. Therefore, the first version of the HMC simulator should model the following components:

- the OSD library that provides an object-based interface to the client,
- the underlying file system, and
- the disk device that is accessed by the file system.

Accurate simulation requires an in-depth knowledge of the inter-workings and specific implementations of each of the components. Since an intimate knowledge of the disk device and file system are impractical for a part-time research project, we chose to simplify our requirements and try to leverage existing software to make an initial implementation feasible. In particular, we chose to use OMNET++ simulation framework, a simple Omnet++ File System Simulator (FSS) for the file system, and the DiskSim software for accurate modeling of the disk device. Despite the existence of this software, integrating them to form a coherent and complete I/O node simulator is a non-trivial task and became the primary goal of the first year.

Goals and Accomplishments

To help drive the development, we established a deadline of March 1, 2006 for completing development on the I/O-node simulator-allowing all of March and April for debugging, testing, and documentation. Along the way, we also set intermediate development goals to keep the project focused. The complete list of goals and approximate completion dates follow (details are in the HMC mid-year report):

GOAL	COMPLETED
Complete basic architectural design of the simulator	October, 2005
Make DiskSim work as a stand-alone simulator.	October, 2005
Run and examine the OMNeT++ FSS simulator.	October, 2005
Select message format for communication between OMNeT++ components.	December, 2005
Create stubs for OMNeT++ modules.	December, 2005
Drive DiskSim as a slave to a C++ stub.	February, 2006
Select and configure representative DiskSim model.	February, 2006
Complete implementation of an OMNeT++ component to generate OSD commands.	February, 2006
Complete implementation of a basic file system module for OMNeT++	February, 2006
Complete implementation of an OMNeT++ component that interfaces with the DiskSim driver.	February, 2006
Integrate and test all components. Make sure at least one OSD command gets processed from end-to-end.	February, 2006 (expected)
Run and test the I/O node simulator on a partial set of OSD commands.	March, 2006 (expected)
Finish implementation (the rest is debugging, testing, and writing)	March, 2006 (expected)

Although incomplete, the results of this work and the FY'07 clinic team are now being applied toward two current efforts at Sandia. We are working with Rolf Riesen to incorporate the I/O node simulator as part of the I/O component of his supercomputer simulation project. We are also trying to develop a simple I/O node simulator (based on the HMC prototype) that can run on a compute node of Red Storm. This will simplify the effort of testing I/O software at scale without dedicated system time.

The progress of the project and the abilities and enthusiasm of the team have been very satisfactory. The project is expected to continue to completion and lead to useful software for the Sandia Scalable Computing Systems Group.

Optical Characterization of Soot Aerosols

Harvey Mudd Student Research Team: Mark Dansson, Rachel Kirby, Mike Martin, Tristan Sharp, Shannon Woods

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Abstract

Coated soot aerosols pose cardiovascular and pulmonary health risks and are one of the least understood contributors to climate change. A better understanding of the optical properties of soot will lead to a better understanding of the effects of soot on climate and allow for superior monitoring of its presence in the atmosphere. The goal of this project is to measure the total extinction and polarization-resolved differential scattering cross section of uncoated and coated soot particles at red wavelengths (633-660 nm) and to study how these optical properties depend on the coating thickness. The total extinction cross section of uncoated and coated soot particles are measured using the cavity ringdown technique. The polarization- and angle-resolved scattering from uncoated and coated soot particles are measured using a lock-in technique.

Accomplishments

The Cavity Ringdown Spectroscopy (CRDS) setup has been successfully used to detect soot extinction times. A HeNe at 632.8 nm is used for the CRDS experiment. To avoid multi-mode buildup, a spatial filter has been placed after the cavity to block off-axis light, transmitting only the TEM_{00} mode. The output is simultaneously observed by PMT and verified by CCD imaging by use of a beam splitter. The ringdown timing data shows less than 0.1% drift over the course of one hour, indicating stable and reproducible data. The electronics were tested to ensure sufficiently fast detector response to measure expected signal decays. It has been verified, through testing, that the decay time of the soot filled cavity was due to laser extinction by the soot. The CRDS setup is considered complete with only operating procedure details to be worked out.

The scattering setup has been aligned on the rotational axis and is ready for calibration. A high power laser diode of 100 mW at 658 nm, passed through a polarization filter, is used for the scattering signal. The signal was successfully processed and amplified using a lock-in amplifier, while sinusoidally modulating the diode current for intensity control. Polarized light scatter has been collected from 500-nm polystyrene spheres. The scattering signal off 100-nm spheres was prohibitively weak for use. The signal from the 500 nm spheres is adequate for calibration purposes and provides qualitative agreement with Mie theory over a large range of angles when the solid angle of the pickup lens is taken into account.

The soot flow down the sample flow tube can be controlled using a butterfly valve at the end of the three-inch-diameter cooling pipe section in combination with a second filter box used to provide suction down the sample path. Changing the flow conditions can vary the soot size distribution. The coating system has been set up with two 2-liter Erlenmeyer flasks in water baths for temperature control. We will use them for preliminary demonstration of the effect of coating on soot optical properties. A more uniform coating arrangement will require a narrow dwell-time distribution for particles in the organic coating vapor. Various designs are being considered, including aerodynamic lenses and a co-flow of filtered air surrounding the soot stream through a cylindrical vapor chamber.

EXPLORATORY PROGRAMS: University Of Texas System

One of the university partnerships that is establishing new and exciting ways to collaborate is with the University of Texas System. In 2004, the University of Texas System (UT System) was identified as a possible partner with which to achieve some of our mission-related goals. For purposes of the original exploratory program, the UT System schools consisted of UT Austin, UT El Paso, UT Arlington, UT Dallas, and UT Southwestern Medical Center.

An MOU was signed in March 2004 to formalize the relationship between Sandia and UT Arlington, Dallas, and UT Southwestern. Relationships had already existed for about six years with UT Austin and UT El Paso. The MOU allows for the conduct of cooperative Homeland Security research in the areas of biotechnology, nanotechnology, microsystems, and engineering sciences. The agreement allows researchers to share facilities in Albuquerque and at UT campuses in Dallas and Arlington. Biotech research will be conducted at UT Southwestern Medical Institute in Dallas.

In April 2005, a second Memorandum of Understanding (MOU) with UT System was signed. This MOU further enhanced the already established agreement signed in 2004 by encompassing all UT System schools. Its purpose is to provide peer review for Sandia's research programs, to participate with Sandia scientists on collaborative research projects, and to provide specialized courses taught by UT professors to increase educational opportunities for Sandians.

In FY 2006, Sandia and the University of Texas System renewed their commitment to the joint Memorandum of Understanding established in 2005, charging their institutions with strengthening Research Program Interfaces and Collaborations, Peer Review and Scientific Accountability, and Education and Transformation. Their overarching goal is to achieve a greater mutual impact on national security issues.

In particular, UTS is providing independent oversight to assess and enhance Sandia's Science, Technology & Engineering excellence through the Peer Review process.

One outcome of the partnership in Education has already caught the attention of and will directly benefit Sandians. The Texas State legislature granted the UT System permission to charge in-state tuition and fees to employees and dependents of organizations working with UT in science and technology development. This means that Sandians and their dependents can pay in-state rates when enrolled at a University of Texas System institution. This benefit also extends to those taking distance-learning classes.

Another outcome of the commitment by SNL and UTS is a joint post doctoral fellowship program across Sandia's Bioscience Research Foundation and UT Medical Branch. This program is rapidly growing the Research Program Interfaces across the two institutions and will serve as the springboard for building future programs.

Sandia has had similar memoranda of understanding with UT Austin for about five years and with UT El Paso for about seven years. Various research projects have been ongoing as a result. As a result of the emphasis on new collaborations, at least twenty-three research projects exist, up from twelve research projects last year.

In FY06, Sandia had research contracts totaling $3.5 million with UT Austin and UT El Paso, up from $1.5 million in 2005. There were no contracts placed with UT Arlington, Dallas, Southwestern, or Galveston Medical Branch. Approximately 198 UT System graduates are currently employed at Sandia. In addition, 13 students in the UT System currently work for Sandia.

The value to Sandia of this exploratory program and the results of the research investment will continue to be evaluated.