SURF 2006

summer undergraduate research fellowship

Program and Activities

NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

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The Summer Undergraduate Research Fellowship (SURF) Program at NIST

Looking for a great opportunity for your undergraduate students to get hands-on research career experience during the summer? Submit a proposal to participate in the National Institute of Standards and Technology (NIST) - National Science Foundation (NSF) Summer Undergraduate Research Fellowship (SURF) program for students majoring in science, mathematics and engineering.

The National Institute of Standards (NIST) and the National Science Foundation (NSF) are committed to the development of undergraduate students interested in exploring research careers. The Summer Undergraduate Research Fellowship (SURF) program is a NIST-NSF partnership that provides opportunities for students to actively participate in NIST research programs. The SURF program, which began in 1993 in NIST's Physics Laboratory (PL), has now expanded to include all seven of the NIST laboratories, i.e., Building and Fire Research Laboratory (BFRL), Electronics and Electrical Engineering (EEEL), Chemical Science and Technology (CSTL), Information Technology (ITL), Manufacturing Engineering (MEL), and Materials Science and Engineering (MSEL). SURF is a part of the NSF Research Experiences for Undergraduates (REU) Program.

The SURF program is designed to increase NIST's role in the training of future generations of scientists and engineers and to increase the involvement of women and minorities in science, mathematics and engineering. The goal of this program is to expose students to applied research procedures in a unique environment. In addition to the laboratory experience, several additional components of the program are designed to enhance the students' experience.

Citizenship Requirements
The program is open to all United States citizens or permanent residents.

Student Eligibility
Students should be undergraduate students with a scientific major, a G.P.A. of 3.0/4.0 or better, intend to pursue a Ph.D., and must be covered by a health insurance plan (either through school or family). Students with physics, material science, chemistry, applied mathematics, computer science, or engineering majors are always encouraged to apply. However, there may be research opportunities for students with other majors.

Living Arrangements
SURF students participate in the SURF program at the headquarters site of the National Institute of Standards & Technology (NIST). NIST is located in Gaithersburg, Maryland, about 25 miles (40 kilometers) from the center of Washington, D.C. Housing arrangements have been made with two local apartment complexes for the SURF students to share fully furnished apartments (*no pets allowed*). Transportation from these apartments to and from the NIST campus will be provided.

The Washington Metropolitan area is rich in cultural and recreational opportunities. The apartments are just a short commute from the nation's capital, theaters, movies, restaurants, evening entertainment, historical and cultural sites, museums, shopping, and many local universities.

Research Programs Available to Students
All seven of NIST's measurement and standards laboratories are participating in the SURF programs: Physics, Material Science and Engineering, Building and Fire Research, Information Technology, Electronics and Electrical Engineering, Chemical Science and Technology, and Manufacturing Engineering. Please see the application packet, the SURF website (http://www.surf.nist.gov/surf2.htm) or the general NIST website (http://www.nist.gov) for summaries of current research opportunities.

Financial Support
SURFers receive Research Fellowships funded jointly by NIST, NSF, and their school. Students receive a $4,000 stipend for the 12 weeks ($3000 for a limited number of 9-week slots), in addition to travel and housing allowances. Universities are encouraged to share in the program in such ways as providing student credits, travel or housing allowances. This may change in 2007 so be sure to check out website for details.

This is a competitive program that ranks and reviews both the university and student portion of the application to determine the final list of SURF awardees. In the past, the NIST SURF program has been able to support approximately 100 students.

Deadline
The deadline for receipt of applications is in February. Visit http://www.surf.nist.gov/ surf2.htm for 2007 exact date.

Application
Applications must consist of two parts: the student's university must submit a grant proposal that provides details about its academic program and nominating one (or more students). ***The university should submit ONE application – regardless of the number or department from which the students are applying.*** Students must provide a copy of their transcripts, two letters of recommendation, and a letter of intent or personal statement. The letter should contain information that helps the review committee make an informed decision about the student such as why the student wants to participate in the NIST/NSF SURF program, and what areas of NIST research interest the student.

Specific program information and contact information for the Program Directors, and applications can be obtained from the NIST SURF website (http://www.surf.nist.gov/ surf2.htm). You can find ***university contacts under the FAQ section***. If your university would like to be added to the list, contact Anita Sweigert. To receive an application by mail, you may contact:

Anita Sweigert
National Institute of Standards and Technology
100 Bureau Dr.
Building 221, Room B160
Gaithersburg, MD 20899-8400
Telephone: 301-975-4200
Fax: 301-975-3038
E-mail: sweigert@nist.gov

http://www.surf.nist.gov/surf2.htm

2006 SURF Summer Seminars and Tours

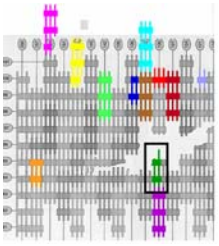
May 22 — First official work day and orientation for SURF Session I students.

May 31 — NIST Safety Orientation for Summer Students

The session provided an overview, including how to report emergencies, use of personal protective equipment, general safety, office ergonomics, laboratory safety, and radiation safety. A session was also given on June 14 for Session II SURF students.

June 1 — Dr. S. Shyam Sunder
Deputy Director, Building and Fire Research Laboratory
Lead Investigator for federal building and fire safety investigation into the World Trade Center disaster

The Federal Building and Fire Safety Investigation of the World Trade Center Disaster



A major scientifically-based investigation of the World Trade Center (WTC) disaster was completed recently by NIST. This study was carried out under the mandate of the National Construction Safety Team Act of 2002, which authorizes NIST to investigate major U.S. building failures. The purpose of such investigations is to establish the technical causes of building failures and evaluate the technical aspects of emergency response and evacuation procedures. Since NIST is not a regulatory agency and does not issue building standards or codes, the institute is viewed as a neutral investigator.

The talk described the NIST investigation and how it seeks to make buildings, occupants, and first responders safer in future disasters.

June 7 — Dr. Steve Banovic
NIST Materials Science & Engineering Laboratory, Metallurgy Division

Tour Stop: Metallurgical Studies on World Trade Center (WTC) Steel

Steve gave several tours throughout the summer in order for all interested SURF students to learn of this important NIST research. It was chilling to see the actual steel removed from the wreckage of the WTC.

In response to the events occurring on September 11, 2001, NIST conducted a 3 year, $16M investigation of the World Trade Center disaster. The main goal of the Metallurgy Division during this study was to characterize the microstructure and mechanical properties, failure modes, and temperature excursions seen by the

steel. The information obtained was used as inputs to the models simulating the behavior of each tower on that day. Steve's talk first described the construction of the towers and then focused on the recovery and identification of critical structural steel elements.

June 8 ***NIST Virtual Library (NVL) Demo and Research Library Tour***

The sessions provided an overview and tour that included demonstrations of the Library facilities, both manual and computer based. A repeat performance was held on June 19 for Session II SURFers.

June 8 Dr. Timothy J. Foecke
NIST Materials Science and Engineering Laboratory, Metallurgy Division

Preserving Historic Shipwrecks: Titanic, Arizona, Hunley and Monitor

A project was developed within the Metallurgy Division over the past 9 years wherein they gave technical advice to other agencies and outside organizations on the preservation and life prediction of historic shipwrecks. The talk reviewed the ongoing work with various wrecks: USS Arizona, CSS Hunley, USS Monitor, RMS Titanic and a few others. Finite element models were developed to predict mechanical stability under marine corrosion conditions, and once the models were reliable, remediation techniques were tried out virtually before any irreversible actions were taken on the actual sites. The techniques being developed will eventually be transferred to the public to be used in stewardship of hazardous shipwrecks in the littorals and on the continental shelf.

June 12 First official work day and orientation for SURF Session II students.

June 15 Dr. Christopher Ekstrom
Leader, Clock Development Research Group
U.S. Naval Observatory

What Time is it Anyway?: Clocks, Timescales, and Atomic Fountains

Clocks range from the simple to the unbelievably complex. They are based on natural processes from celestial motions, to pendulums, to transitions in atoms. Each of these techniques has reigned supreme at different times in history, providing us with tools for applications from agriculture, to navigation, to basic science.

"What time is it anyway," covered the basic building blocks of a clock and how they were used to tell (and even vote) on the time. Dr. Ekstrom covered

timekeeping and timescales, including how the world decides what time it is. Finally, he covered a type of laser-cooled atomic clock called an atomic fountain, where he focused on the atomic fountains at the U.S. Naval Observatory. Both NIST and USNO have built atomic fountains, but with much different goals, both of which were discussed.

Dr. Ekstrom is the leader of the clock development research group at the U.S. Naval Observatory. His group develops advanced atomic clocks for use in the DoD Master Clock, which is housed in Washington, DC.

June 23 ***Norfolk REU Program Visits NIST***

Jordan Peck (SUNY Binghamton) and Jennifer Wiley (UMD, College Park) talked to a group of college students from a Norfolk REU about their experience in the NIST SURF program.

June 23 Dr. Kris Bertness
NIST Electronics & Electrical Engineering Laboratory,
Optoelectronics Division (Boulder)

Research Advisory Committee Summer Seminar: ***GaN Nanowires: Nanotechnology Goes Ultraviolet***

Wide-band-gap semiconductor nanowires combine optical and electronic properties of semiconductors to achieve new functionality with a multitude of applications. This is particularly important for the GaN-AlN-InN alloy system, where conventional epitomical semiconductor methods produce material with poor yield and strain-driven limitations to heteroepitaxy. The talk provided an overview of the variety of methods that exist to produce and process nanowires, including the vapor-liquid-solid (VLS) mechanism and catalyst-free molecular beam epitaxy. NIST researchers have shown that the catalyst-free methods produce material of exceptional crystalline quality, often better than the epitaxial films or bulk crystals. Although nitride semiconductors include materials with infrared band gaps, the most exciting applications are in the green, blue, and ultraviolet range of the spectrum. These materials have the potential to reduce the form factor and power consumption of UV light sources to revolutionize instrumentation in such diverse fields as biochemical analysis, water sterilization, and atomic ion traps. In addition to materials and application issues, the speaker addressed some of the interesting metrology challenges that was behind this work at NIST.

June 29 Dr. Laurie E. Locascio

NIST Chemical Science and Technology Laboratory,
Biochemical Science Division

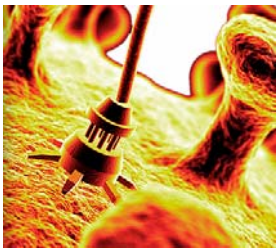
Microfluidics: Doing Chemistry in Nanoliters

Microfluidics and microarray technology, collectively called microanalytical systems, have been referred to as some of the great technological advances of the last decade. Research in these areas continue to thrive as researchers learn that by scaling down chemical processes, fundamental changes occur that can dramatically affect chemical separation, reaction and detection. Systems continue to shrink in size motivated by the desire to multiplex chemical reactions based on combinatorial methodology. Dr. Locascio's talk focused on designing and developing microfluidics systems for ultra-small volume analysis of biological systems including whole cells and model cell structures, DNA and proteins.

July 6 Dr. Curt A. Richter
NIST Electronics and Electrical Engineering Laboratory

Emerging Nanoelectronic Devices

Nanoelectronics, though its exact definition often varies, encompasses emerging technologies under development to supplement and/or supplant present-day CMOS technology which, with its ~30 nm channel lengths and sub-1.5 nm effective gate oxide thicknesses, is considered by many already to be "well into the world of nanoelectronics." Two specific emerging nanoelectronic device technologies, Si-nanowires and molecular electronics, were discussed in detail. Si-nanowire technologies fabricated by top-down approaches are the logical extrapolation of current CMOS while molecular electronics is based upon self-assembly, a radically different fabrication approach. These two technologies form a bridge between top-down nanoelectronics and bottom-up nanostructures with novel properties and functions, and they bracket the possible fabrication approaches for future information processing technologies.



July 10 ***NIST Center for Neutron Research Tour***

The NIST Center for Neutron Research (NCNR) annually invites the SURF students to tour its facilities and learn about some of the ways beams of neutrons are used in materials and other types of research. The tour was preceded by a lecture giving an overview of the Center

and principal areas of research, followed by stops at a number of experimental facilities where staff described ongoing research. The lecture and tour took about two hours to complete.

July 13

Dr. Daniel Sawyer
NIST Manufacturing Engineering Laboratory, Precision Engineering Division

Large Scale Metrology

Laser trackers are becoming the tool of choice for dimensional inspection of large manufactured parts and assemblies. HIST has contributed significantly to the development of tests and procedures for characterizing the performance of these measuring instruments. The results of this effort have been incorporated in a recently approved ASME standard, *B89.4.19 Performance Evaluation of Laser Based Spherical Coordinate Measurement Systems*. The presentation provided an overview of the principles and design of laser trackers, their use and the important elements of a well-constructed performance evaluation standard.

July 19

Annual Summer Horizons Program
Lisa Portis Morgan, Ph.D.
Events Coordinator
The Graduate School
University of Maryland Baltimore County

SURF students were invited to attend the annual Summer Horizons program at the University of Maryland, Baltimore County (UMBC). Summer Horizons presented a one-day introduction to Graduate School. The day included sessions on the benefits of a graduate degree, the application process, fellowship opportunities, an introduction to graduate programs at UMBC and a motivational speech by UMBC's President, Dr. Freeman Hrabowski.

Another important part of the program: a continental breakfast, hot buffet lunch, and afternoon snacks were provided *free* of charge.

July 20

Bettijoyce B. Lide
NIST Information Technology Laboratory

Toward an Electronic Health Record

Do you know where your medical records are? If you became sick while on vacation away from home and went to a distant emergency room, would your clinical information be available at the point of care? Do you still hand carry prescriptions, or does your healthcare provider send them electronically to the pharmacy, where they are automatically checked against your known allergies and medications?

Our nation enjoys the best medical care and the brightest medical personnel in the world, yet the enterprise is fraught with poor coordination, administrative inefficiencies, and avoidable medical errors. Also, healthcare costs impact us all. For example, healthcare expenses for auto workers add approximately $1,500 to the price of every new General Motors car.

The President has a Health Information Technology Plan and has created the Office of the National Coordinator for Health Information Technology within the Department of Health and Human Services to pursue technological opportunities to reduce costs, to greatly improve patient safety and quality of care, and to make healthcare more accessible. The seminar focused on the health information technology initiatives underway to fulfill the President's vision and, in particular, NIST's role in these path-breaking projects.

July 25 **Visit by University of Maryland Materials Research REU Program**

Sixteen students from the University of Maryland REU program (similar to our SURF program) toured a number of labs (metallurgical studies on WTC steel, trace explosive detection, and learning applied to ground robots) to learn of the research happening at NIST.

July 27 Mr. Donald Swenholt
Donald Swenholt Associates, Inc.

Giving Successful Presentations

An annual seminar provided to all SURF students, Mr. Swenholt gave techniques on making presentations more interesting to those in the audience, how to experience more pleasure and less anxiety in preparing and delivering your presentation. He also gave tips on making dry material come alive, how to make your long presentation seem short and the complex seem simple. If a SURFer wanted to learn how to gain and hold the attention of an audience, this class was not to be missed.

August 4 ***Tour of Pentagon***

The SURFers had the great opportunity of touring The Pentagon. The tour route was approximately 1 1/2 miles in length and lasted for about 90 minutes. The tour covered about 20 items of interest that included the mission of the Department of Defense and each of its branches of services, and numerous displays that highlighted and depicted significant moments in military history.

August 8 Final presentations by SURF students moderated by invited guests.

August 8 Lunch: SURF Directors and special invited guests.

August 9	Final presentations by SURF students moderated by invited guests.
August 10	Final presentations by SURF students moderated by invited guests.
August 11	Last day for SURF students and farewell pizza party.

2006 SURF Summer Activities

It's always difficult when you're in a new city, with a new job -- unless you're a SURF student. SURFers find themselves in the same boat and thus forge bonds that may last a lifetime. They work together AND play together; they've found the magic bullet for balancing the two. In fact, to make life easier they can get it all scheduled using their own forum for social and work-related chatting.

NIST SURF Forum

For NIST SURF-related chat & info (this is not a US Government website)

NIST Research and Other Opportunities
Important Meetings & Dates
    Seminars, socials & more
Working at NIST
    Guidelines to the workplace
Please help…
    Solve a problem or find something I need for my project
Complaints
    Log out and post as a guest if you want to be anonymous
After NIST
    Graduate school options and other career opportunities
SURF Chat
Chat Central
    Off topic chat, forum games and everything else
Nature
    Hiking, camping, biking
Baltimore & Washington, DC
    Museums and the arts
Sports
    Organize a group to play a sport
Music
    Listen or play together
Apartment Life
    Organize activities at Summerfield
After Work
    Organize activities outside of Summerfield
Take a Trip
    Get a group together for weekend travel (e.g., New York City)
Religion
    Find friends with the same interests
Film
    Organize a movie night at your apartment or the theatre
Apartment Assignments
    Chat with your new apartment mates
Before You Arrive
Info on travel, apartments & $$$
What will happen on the first day

SURF BBQ – NIST Picnic Grove

To welcome the SURFers to NIST, the SURF Directors provided burgers, salads, desserts, and sodas. It doesn't take a "rocket scientist" to know that if food is mentioned you'll find the SURF students there.

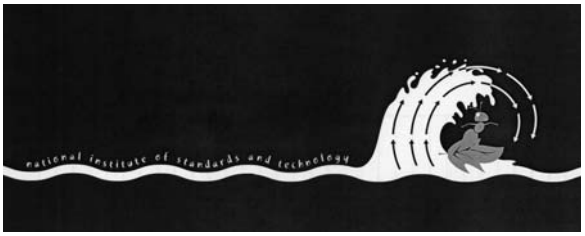
Cooking for students – better have plenty

SURF Directors Marc Desrosiers and Larry Reeker at the grills

SURF students enjoying the fruits of the SURF Directors labor

2006 SURF T-Shirt Design

Each year the group has the task of designing a t-shirt during their stay at NIST, our own version of *Project Runway (PR)*. See below the design that was this summer's winner – and unlike *PR*, the creators of the design(s) not chosen don't get booted out for the summer.



t-shirt front

t-shirt back

The Washington Metropolitan area is rich in cultural and recreational opportunities. NIST is just a short commute from the nation's capital, theaters, movies, restaurants, historical and cultural sites, museums, shopping, and many local universities. The students didn't have to wait until after work either since NIST has a fitness center, soccer, volleyball, softball, and many other activities to participate in during lunch break. You didn't have to spend a lot of cash to have fun, since there were always movie nights, poker parties, pool parties, basketball games and karaoke. Also, a number of students live in the area and invited out-of-the-area students to their homes for activities.

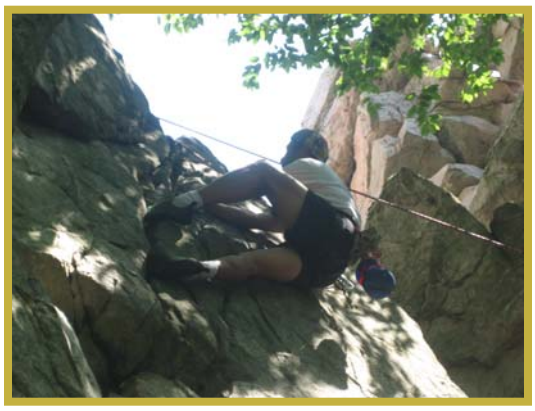
Celebrating the Fourth of July in the Nation's Capital (and elsewhere)

Congress established Independence Day as a holiday in 1870 and in 1938 Congress reaffirmed it as holiday, but with full pay for federal employees. Today, communities across the nation mark this major midsummer holiday with parades, fireworks, picnics and the playing of the "Star Spangled Banner" and marches by John Philip Sousa.

The SURFers marked the holiday on the National Mall with half a million of their nearest and dearest friends. Ann Swain, an Einstein Fellow from Woodinville, Washington who was at NIST for the 2005-2006 school year, sang in the choir – I'm sure all the SURFers waved to her.

Rock Climbing – Natural and Manmade

Ken Inn, a Physics Lab SURF Advisor, has taken SURFers rock climbing at Sugar Loaf Mountain for the past several years. Several SURFers tried their luck at the indoor rock climbing wall. Check out those brave enough to try the "real" thing.

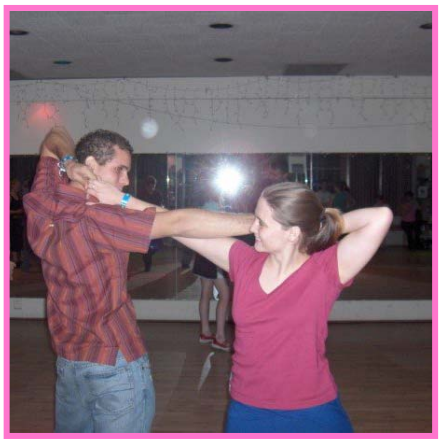


NIST Softball Team

A couple SURFers played on the NIST Computer Science Division softball team. They didn't win a single game (0-11, oh well they had an awesome time anyway). Their team did 'win' the title 'most fun team to play.' Hmmm… I wonder if it had anything to do with dressing up like pirates for one of the games. The guys had one slight problem; they found out that eyeliner runs right into your eyes when you're sweating out in right field (bet Johnny Depp didn't have that problem in *Pirates of the Caribbean*).

Dancing with the Stars (or in this case SURFers)

The NIST Standards Employee Benefits Association (SEBA) offered free dance lessons during the summer. Check out this move.…



Golf Anyone??

Tiger Woods may not have been on this golf course, but you didn't have to worry about whispering here, just having a good time.

Student Abstracts
2006 SURF Program

Appalachian State University

Modeling a Medical Particle Accelerator Using Monte Carlo Simulation Methods
L. Bailee Christopher

The Monte Carlo method for simulating particle transport was used to develop a model of the Ionizing Radiation Division's Varian Clinac 2100C particle accelerator as a source of photons. In order to relate measurements to the dose-to-water standard used for radiation therapy calibrations, computations are required. Increasingly detailed calculations generally provide for a more accurate realization of the standard. Using the details of the accelerator provided by Varian and other information available in related literature, the BEAM/egsNRC code, which has been widely applied to modeling similar systems, was used to develop a source model to compare with measured data at both 6MV and 18MV energies. The transport in water was accomplished using the dosxyz code, also derived from egsNRC. It is expected that utilizing a coupled approach comparing measurement to calculation and adjusting calculational details (e.g. beam energy) will lead to a much more accurate source model than is currently available for other NIST photon sources (e.g. Co-60 and Cs-137 heads).

Plasma Oxidation of Ultra-Thin Aluminum Layers for Magnetic Tunnel Junctions
Eric D. Peterson

This talk focuses on plasma oxidation of thin aluminum films used as tunneling barriers in Magnetic Tunnel Junction (MTJ) devices. We investigated different plasmas triggered with positive and negative bias, focusing specifically on oxidation time, plasma composition (NO_2 and O_2), and plasma geometry. The characteristics of the plasma, potential difference, current, and gas pressure were correlated with the impedances of the MTJ devices created. MTJs have applications in various technologies such as magnetic memory and magnetic field detectors.

An MTJ is a type of tunnel barrier device that uses magnetic material so that the relative spin state of these layers can be flipped by an external magnetic field. The magnetic spin of one layer, called the "hard" layer is aligned in one direction. The other layer, called the "soft" layer is not aligned in any specific direction. The resistivity of the MTJ depends on whether the spin states of the hard and soft layer are aligned or anti-aligned. When they are aligned, the resistivity of the MTJ is low, if they are anti-aligned, the resistivity is high.

The tunnel barrier is a critical component of any tunnel junction, including the MTJ. When oxidized, aluminum preferentially forms alumina (Al_2O_3) which is an excellent MTJ barrier material. Plasma oxidation has qualities that make it ideal for forming these barriers. The reactive species, O* and O^+, present in the plasma are more reactive than O_2. This helps to create a stoichiometric alumina film that is deeper than a thermally oxidized film.

Our group is studying the interaction between this alumina barrier and highly charged ions (HCI) of Xenon with a charge state of 44^{+}. The alumina barrier is formed from an aluminum film on the order of 1 nm thick. The oxidation of the aluminum film is a critical step to forming an alumina barrier that is both a good MTJ barrier and also sensitive to HCIs. The RA product is an important metric for determining the characteristics of a device. We studied how the characteristics of the plasma and its interactions with the materials of the device affected the RA product of devices. These measurements can help us to improve the consistency and predictability of the oxidation process.

Boston University

Polyelectrolyte Deep Eutectic Solvents

Sam Hong

Deep eutectic solvents (DES) are low-cost, green alternatives to room temperature ionic liquids. A typical DES is a binary mixture of a quaternary ammonium salt and a hydrogen bond donor. The ammonium salt is dissociated, resulting in a highly polar liquid mixture that can dissolve a diverse array of materials including metal salts and cellulose. All DES systems reported thus far have been composed of small molecules.

We explore the formation of a new DES using poly(acrylic acid) (PAA) as the hydrogen bond donor and chlorine chloride as the ammonium salt. Including a polyelectrolyte component adds rigidity to the DES, and the binary mixture might be considered a plastic rather than a liquid. A polymer DES with the conductivity of an ionic liquid could be applied as a polymer electrolyte in batteries, supercapacitors, or fuel cells, where its ease of processing, mechanical strength, and low volatility would be key advantages. Both components of our polymer DES are inexpensive and nontoxic; poly(acrylic acid) is used in diapers and chlorine chloride is added to chicken feed.

The formation of our polyelectrolyte DES was studied by constructing a binary phase diagram using a combinatorial temperature gradient. A single phase dominated the PAA-rich compositions; no phase separation was observed at accessible temperatures. Phase behavior was observed in the chlorine chloride-rich compositions, with a two-phase region at lower temperatures and a single-phase region at higher temperatures. The phase transition temperature was clearly dependent on composition. The eutectic critical point appears at the equimolar mixture of chlorine chloride and acrylic acid residues, indicating that a hydrogen bonding interaction with specific stoichiometry may be responsible for eutectic formation.

To evaluate the application potential of the polyelectrolyte DES, its ionic conductivity was measured using impedance spectroscopy. Our preliminary results indicate a maximum ionic conductivity of $\approx 10^{-7}$ S/cm, far below that of a small molecule DES. We will discuss possible reasons for the low conductivity and indicate potential routes to improvement. Plans to further elaborate the structure and properties of the polyelectrolyte DES will also be described.

California Institute of Technology

Investigation of Hot Particles in Rocky Flats Soil Material
John Shen

The Rocky Flats Soil-II material is a natural-matrix radionuclide Standard Reference Material (SRM) used to evaluate different analytical methods of measuring radioactivity. Discrepant reported values of plutonium and uranium in the SRM from different metrology laboratories point to the presence of hot particles of unknown composition in the material. The objective of this study was to isolate and characterize the hot particles. Chemical techniques such as attack with acids, EDTA dissolution, pyrosulfate fusion, and gravity separation are used to isolate the hot particles. Also, soil particles are collected on collodion film and identified via Fuji autoradiography. After hot particles are isolated, they are characterized by secondary ion mass spectrometry, chemical microscopy, and x-ray diffraction. It can be found that the particles are mainly composed of plutonium oxides and other resistate minerals.

College of Holy Cross

The Development of a Raman Standard for 633 nm Excitation Source
Kathryn Noonan

Theoretically when using Raman spectroscopy the true Raman spectrum of a particular sample should look the same no matter what instrument it is taken on. Unfortunately instrumental bias prevents this from occurring, creating the need for calibration. Typically the x-axis in Raman spectra is calibrated with a pen lamp or standard with sharp peaks. The y-axis however is slightly more difficult.

Intensity calibrations in Raman spectroscopy are normally done with a broadly emitting white light source. Unfortunately these lamps are very expensive for the typical Raman user and thus a method of calibration using a glass standard has been developed. Widely fluorescing glasses with minimal features are ideal standards of intensity calibration because they are relatively inexpensive and can go just about anywhere a portable Raman system would be used.

Although SRMs exist for excitation at 488 nm, 514 nm, 532 nm, and 785 nm, there is currently no standard at 633 nm. 633 nm is a very popular wavelength in academics making cost an important factor in the creation of a standard. It is therefore important to find an SRM or other material currently in existence that would allow for calibration at 633 nm. SRM 2241 was found to be too far red shifted while SRM 2242 did not fluoresce enough to be used as a standard. Other materials tested include ti:sapphire, U_3O_8 glass, yellow plate unknown polyimide sample, GP-7, GP-8 (calibration slides for axon microarray scanner), cy5 dye, alexafluor633, and an assortment of red filters. The dyes, each tested on multiple gratings with multiple objectives, were found to be in good agreement with each other, unfortunately they are both prone to decay. It was found that GP-7 made from polymethyl methacralate produced the most ideal fluorescence spectra.

College of William and Mary

Measurements of Radon Diffusion Coefficient with NIST Radon Standards as a Source
William Ames

We measured radon diffusion coefficient with a new method, using a NIST radon standard as a radon source. The cylindrical polyethylene capsule with radium solution inside (NIST standards SRM 4973) was placed inside the hollow cylinder made from the tested material. Radon diffused through a polyethylene wall and then through the tested material and was collected inside the diffusion chamber for some time interval (accumulation time). Then radon was transferred into the NIST pulse ionization chambers (PIC) for its activity measurement.

In the case of thin films as samples, the time dependence of an emanation fraction $f = A_{Rn}/A_{Ra}$ allows us to determine only the radon permeability $D_x K_p^x$ (D_x is the diffusion coefficient of tested material, while K_p^x is the ratio of radon solubility in tested material with respect to that of in polyethylene). However, for thick samples both D_x and K_p^x can be determined separately.

Results of our diffusion coefficient measurements are in reasonable agreement with previous results by other authors.

Interfacial Molecular Charge Transport in Monolayer Films
Sarah Cotts

Currently, many groups are studying ways to implement organic molecules into existing device technologies for creating smaller, faster devices. By understanding charge transport in molecular thin films, more effective molecular based device structures can be developed. Film structure and molecular orientation were manipulated to optimize charge transport. Films of organic self-assembled monolayers (SAMs) were tethered to SiO_2 surfaces by multi-step reaction chemistry. Their structure and charge-transport properties were characterized using spectroscopic ellipsometry, atomic force microscopy (AFM), FT-IR spectroscopy, and contact angle measurement. UV patterned films were imaged using AFM as well as electrostatic force microscopy. Ultimately, mixed hole and electron transport films will be made to maximize charge transport at the interface of hole transport and electron transport regions. This device will have applications in technologies such as organic light emitting diodes (OLEDs) in flat or flexible displays.

NIST Conformance Testing Framework Promotes HL7 Compliance
Justin Manweiler

According to the Institute of Medicine (IOM), there are approximately 98,000 deaths in the U.S. each year attributable to medical errors. In an effort to reduce the risk of human mistakes, strong informatics standards are necessary for improved communication between diverse healthcare systems.

In the U.S., Health Level Seven (HL7) is the prevailing standard. When fully employed, it allows disparate systems to exchange key sets of clinical and administrative data. Widespread compliance would lead to superior quality of care, improved patient safety, and reduction of costs. The expansion of its use is vital to the realization of a National Health Information Infrastructure, connecting distributed health data nationwide.

Due to its universal nature, designed to accommodate the whole of the healthcare industry, the HL7 standard is overwhelmingly large in its entirety. Increasingly, message communication profiles are desirably used to limit the scope of the specification to the individual needs of a particular implementation. This necessitates extensive profile-specific conformance testing to ensure interoperability and correct behavior. Mere validation against only the HL7 specification itself is far too lenient to provide any reasonable level of assurance. Currently, this testing must be performed manually, as each particular profile requires a customized testing suite. Additionally, it must be verified that the profiles themselves are fully compliant with the overall HL7 specification.

At NIST, under lead scientist Rob Snelick (Division 897), work is being done to simplify the process of validation for HL7 systems. During the past two summers, my personal work has been aimed at the development of an automated system of validation for messages against profiles as well as messages and profiles against the HL7 standard itself.

With the further completion of the HL7 conformance-testing framework being developed here at NIST, the difficulty associated with system implementation and subsequent debugging will be reduced. HL7 compliance will be thereby promoted, further realizing the potential of healthcare IT.

Quantum Mechanics of a Magnetic Field Generated by Non-Abelian Vector Potential

Ashwin Rastogi

Modern quantum mechanical treatments of electromagnetism have adopted the general principle that the vector potential is a more physically fundamental structure than the magnetic field itself. The quantum mechanical Hamiltonian and resulting differential equations depend on the vector potential only; the idea has been further confirmed by experimental observation of the Aharanov-Bohm effect, wherein the effect of a non-zero vector potential is observed in a region with no magnetic field. This concept is somewhat at odds with classical electrodynamics, which relies almost exclusively upon the magnetic field. The quantum theory however remains consistent with the principle of gauge invariance, which requires that all physical observables remain invariant under certain types of gauge transformations. In this project we consider the quantum mechanics of a charged particle in the magnetic field generated a non-Abelian vector potential.

Standard considerations of magnetic field assume that the vector potential (and thus the field itself) are Abelian, that is, that its components commute with each other. For a non-Abelian system, this assumption is dropped, and components of the vector potential must be represented by non-commuting matrices instead of scalars. In considering the physics of a non-Abelian vector potential, many fundamental principles of electromagnetism must be reconsidered and generalized from the standard Abelian cases. We have been particularly concerned with the

relationship between the vector potential and magnetic field, and the form of allowable gauge transformations in the non-Abelian case. The nature of several of these generalized non-Abelian relationships imply that there is no classical analog for non-Abelian fields. The problem is therefore considered quantum mechanically using the canonical Hamiltonian and Schrodinger equation. By application of the Heisenberg picture of quantum mechanics, we can also derive an Ehrenfest theorem-analog for the non-Abelian problem, and solve the resulting differential equations to obtain a pseudo-classical treatment.

Recent developments with Bose-Einstein condensation (BEC) have indicated that the quantum mechanics of exotic fields, including non-Abelian fields, can be mimicked by a BEC in particular types of laser-generated lattice structures. Furthermore, from a theoretical approach, non-Abelian fields are of major concern in various aspects of particle physics and high energy physics. Consequently, we are interested in deriving the mechanics associated with non-Abelian vector potentials and comparing these results with empirical data from BEC experiments. The development and results of this project could allow for further experimentation with non-Abelian fields to be carried out in cold-physics laboratories, as opposed to the traditional high energy accelerators used in particle physics.

Colorado School of Mines

Quantum Phase Transitions in the Hubbard Model

Roger Brown

The goal of our research is to predict quantum phase transitions of cold fermionic gases in one dimensional systems. These systems of ultra cold atoms are experimentally relevant because they can be very accurately generated and manipulated using sets of counter propagating laser beams to create a one dimensional optical lattice. This research is also of interest to condensed matter physics because the behavior of these systems is well described by the Hubbard Hamiltonian and variations of it.

We investigated the two and three site cases of the Hubbard, Bose Hubbard or Fermi-Bose Hubbard models, which lead to relatively small diagonalizable Hamiltonians. From these we were able to plot phase diagrams for the systems as a function of scaled chemical potential and tunneling parameters. The computation time to diagonalize the exact Hamiltonians scales exponentially with the number of wells so, to investigate larger systems we employ an algorithm created by Vidal [G. Vidal, Phys. Rev. Lett. 91, 147902 (2003)], which uses the Schmidt decomposition to truncate the Hilbert space. J.E. Williams at NIST has created an implementation of this algorithm in Mathematica which is called the Matrix Product Decomposition Toolbox (MPD Toolbox). Using the MPD Toolbox, we were able to study the Hubbard Hamiltonian for a relatively large number of sites, and also treat an effectively infinite system. In the case of the Hubbard Hamiltonian we calculated the components of spin along the x and z axes as a function of scaled chemical potential and tunneling in order to generate a phase diagram appropriate for spin 1/2 fermions.

Phases of Ultra Cold Gases in the Fermi-Bose Hubbard Model
Daniel Schirmer

The experimental realization of a BEC has stimulated the interest in theoretical models of zero-temperature quantum phase transitions. Ultra cold gases confined in optical lattices can demonstrate a wide range of different phases by varying controllable system parameters, such as optical lattice intensity, particle number, spin composition and the inter-atomic interaction. This project aims to unveil phases in a one dimensional system of fermions coupled to a bosonic molecular state, in the limit of an infinite number of lattice sites. This is accomplished by solving the Fermi-Bose Hubbard model using a numerical method developed by G. Vidal [G. Vidal, Phys. Rev. Lett. 91, 147902 (2003)], and implemented into a Mathematica package by J. E. Williams at NIST, which was used extensively in my research.

This research focuses on calculating diagrams of the homogeneous system as functions of nearest neighbor hopping energies, onsite fermion chemical potential, onsite fermi-bose coupling strength, and a detuning factor, determining relative boson chemical potential. For most calculations, onsite interactions are not considered.

Because ultra cold gases are relatively easy to create, manipulate, and observe, they function as a future test bed for studies in solid-state physics and quantum computation. Theoretical tools such as phase diagrams are especially important to the development of these fields.

Cornell College

Human Computer Interfaces of Tomorrow: How Science Fiction Has Become Reality
Cody Dunne

Technologies straight out of movies like *Minority Report* are now becoming a reality with gestural interfaces, wall sized touch sensitive displays, multi-user interactive media tables, and incredibly scalable user collaboration software now on the market. Traditional presentation technologies revolve around standard keyboards and mouse emulation devices, but many emerging and exciting technologies allow for more intuitive interaction and efficient demonstrations and meetings. To support Virtual Manufacturing Enterprise (VME) pilot implementations and demonstrations, intensive research has been performed on currently available large-scale presentation and collaborative human interfaces.

Many of these systems use computer vision techniques for hand, glove or laser pointer tracking, and some allow for multiple simultaneous users with software that allows for the analyzing and sharing of images, videos and other interactive remote content. A few of the most promising of these technologies may be implemented in the Advanced Manufacturing Systems and Networking Testbed (AMSANT) Facility to interface with projected screens displaying complex and detailed VME simulations.

Cornell University

In Search of Anisotropy in Cobalt Nanoparticles

Kevin Baler

Magnetic nanoparticles offer a novel means to remove tumor cells in the body. Cobalt nanoparticles show promise for this application due to their anisotropic and super-paramagnetic nature. The anisotropy produces a magnetic moment along an easy axis of magnetization which can be rotated. Rotation of this moment requires a transfer of energy to the particle thus raising its temperature. High enough temperatures induce a localized hyperthermia whereby the tumor cells are destroyed.

Anisotropy was measured using the following technique: field cooling in a Vibrating Sample Magnetometer (VSM), then measuring the hysteresis at 0˚ and 90˚ degrees from the axis of magnetization; the integrated difference between the two loops is the total anisotropy energy (Fig. 1). Torque measurements on the VSM of the field cooled sample confirmed the anisotropy and suggested a simple uniaxial anisotropy (Fig. 2). To find a resonance frequency where the particles change magnetization easily, the susceptibility as a function of frequency was carried out on an AC Susceptometer (ACS) in three temperature regimes of the particles; below the Néel temperature, between the Néel and blocking temperatures, and finally above both the blocking temperature and the Néel temperature.

We found strong anisotropy in the particles, which may come from the intrinsic anisotropy of the particles or the formation of long particle chains. Further experiments are needed to separate these two components. If the particles have a strong intrinsic anisotropy, we would expect a well defined resonance frequency that will maximize energy absorption. Continuation of these experiments will determine which frequencies resonate with the particles. With further experimentation, the potential of Cobalt nanoparticles for advances in biomedicine and cancer treatments can be realized

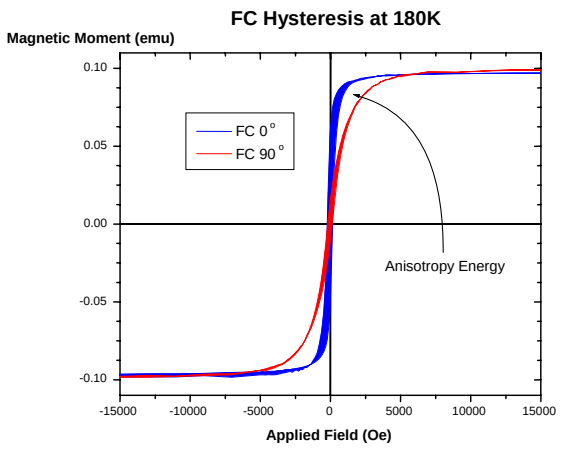


Fig. 1

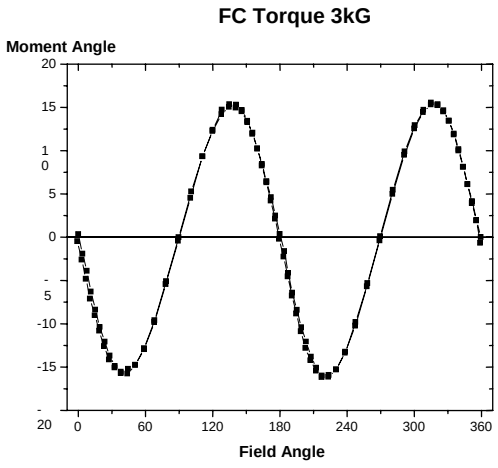


Fig. 2

Spatial Statistics for Carbon Nanotubes
Jarred Ramo

Polymer composites, where nanoparticles are used as filler in polymers, are a class of materials that have been extensively studied during the last two decades because of their exceptional physical properties. They are valued for their light weight, durability, mechanical properties, electrical properties, and heat resistance. Since the discovery of carbon nanotubes in 1991, research on polymer carbon nanotube nanocomposites has indicated that the dispersion of the tubes is critical for obtaining better physical properties. BFRL and MSEL researchers at NIST are studying the heat resistance of a carbon nanotube in PMMA polymer composite. Interest focuses on the fabrication of composite exhibiting a distribution of carbon prepared to be as uniform (dispersed) as possible. Researchers also seek to quantify the correlation between measures of uniformity of the composite and its resultant physical properties.

Previous results indicate that the dispersion of the tubes is critical for obtaining better physical properties of the nanocomposites. However, these studies describe only qualitative levels of dispersion with high magnification images determined by TEM or SEM. In order to be able to predict physical properties of polymer carbon nanocomposites, quantitative determination of the dispersion of the carbon nanotubes in polymers is needed. This study is a first attempt to characterize the dispersion of the nanotubes in PMMA quantitatively and the relationship between the quantified dispersion level and selected physical properties of the PMMA nanocomposites.

We quantify uniformity, across composites of different densities, using chi-squared statistics, probability plot correlations, and variational distance. We then examine the relationships between the resulting uniformity indices and light absorbance, storage modulus, peak mass loss under burning, and electrical conductivity.

Davidson College

Optimization, Quality Assurance, and Quality Control in Neutron Detector Development
Daniel Clayton

Neutron detectors constructed of thin metal tubes sputter coated on the interior walls with boron carbide were recently developed by Proportional Technologies, Inc*. Neutrons entering the detector are converted by the $^{10}B(n,\alpha)^{7}Li$ reaction. The resultant energetic charged particles escape through the boron carbide coating and then ionize a gas contained within the tube. In turn, the ionized gas creates an electrical pulse along a center wire. If the boron carbide layer is too thick a proportional number of the reaction events are lost. Thus, the neutron conversion efficiency is primarily dependent upon the mass of boron carbide coating the wall, the ^{10}B isotopic loading of the carbide, and the stoichiometry of the coating.

Neutron depth profiling (NDP), a non-destructive isotope specific analytical method at the end of cold neutron guide NG1 at the NIST Center for Neutron Research (NCNR), was used to quantify the concentration versus depth of boron in the coating. The same nuclear reaction important in the neutron detector sensitivity, $^{10}B(n,\alpha)^{7}Li$, is also used for NDP analysis. A well-defined

neutron beam is used to probe sample coupons taken from boron carbide coated tubes. NDP enables the determination of the coating mass thickness so that the probability of particle escape can be calculated and the neutron detection efficiency maximized.

Samples taken from the manufacturing process were analyzed for ^{10}B mass, temporal, positional, and stoichiometric variability. All sample measurements were corrected for variability in neutron flux (<1%) and electronic dead time (<1%). A well-characterized boron standard was used to determine ^{10}B content in the unknown samples, and background spectra were acquired by analyzing the reverse side of several samples.
Film thicknesses were found to range from 0.58 μm to 0.99 μm and densities were found to range from 2.72×10^{15} ^{10}B-atoms/cm^2 to 3.19×10^{15} ^{10}B-atoms/cm^2. One sample, not included in the above statistics, showed a density about 18% less than the average. The overall temporal variance was ±4% for thickness and ±8% for density. The positional variance was dependent on the date of the manufacture, with a minimum thickness variability of ±2% and a maximum of ±18%. The minimum average mass density variability was ±3.4% and the maximum was ±12.2%. The data shows that the sputter coating process has the greatest source of variability with respect to the date of manufacture.

Drexel University

Developing a Robot Classification System for Urban Search and Rescue

Iris Howley

After the initial usage of robots for victim recovery on September 11, 2001, the urban search and rescue (US&R) field experienced a tremendous increase in technology. Robots, no longer bound to manufacturing and bomb disposal purposes, appeared on the market with capabilities covering a wide spectrum of uses. For the average US&R responder, the options can be overwhelming. Technical robot information is numerous, difficult to obtain, disorganized, and presented in incomparable formats. Choosing which robot for what disaster can be a formidable task.

Developing robot ontology organizes the relevant information about robots and their capabilities, so urban search and rescue responders may select a robotic tool to fit their needs more precisely and efficiently. Results from testing methods for robotic technologies developed by the National Institute of Standards and Technology can be used in combination with the ontology to make better comparisons of robots full capabilities. Using ontology to define these concepts rather than a taxonomy or a database adds increased functionality and flexibility, allowing for the usage of class properties, relationships between concepts, multiple inheritance, and even integration into the Semantic Web.

This proof of concept system demonstrates the basic functionality of the Robot Ontology and forms the basis for further knowledge representation challenges. While various attributes of an urban search and rescue robot are simple to define, such as height and weight, modeling the robot's range of motion and the operating environment are more involved. Additionally,

knowledge base queries must be carefully formed to extract the correct information. This project uses the Java Expert System Shell (JESS) to reason over robot facts represented in the Web Ontology Language (OWL) and delivers the urban search and rescue responder's best-fitting robot matches.

Elizabethtown College

Suppression of Coherence in Electron Microscopy

Robyn M. Dunstan

A prerequisite for electron tomography (as currently practiced) is that the signal be a monotonic function of the mass thickness of a line of material in the sample. This is known as the "projection requirement". However, crystalline samples show significant diffraction effects, so electron tomography has been limited to amorphous samples or to High-Angle Annular Dark-Field Imaging. The latter achieves an incoherent signal of about 1% of the original beam. Recently, Levine and Anderson of NIST proposed scanning full-field Transmission Electron Microscopy images to achieve an incoherent probe on the sample, a procedure they term "Synthetic Incoherence". In principle, for samples of moderate thickness, this will satisfy the projection requirement.

In the present work, an analytic form is given for hollow cone illumination and numerical results are given for the square scan scheme proposed by Anderson, including the practical effect of the electron dwell time at the start of the scan.

Georgetown University

Simulating Heat Transfer in a Water Calorimeter for Use in Radiation Dose Standardization

Stephanie Cope

Absorbed dose, the amount of energy transferred into matter by ionizing radiation, is measured in the unit **gray**, Gy [J/kg]. A sealed water calorimeter has been developed to establish the current standard in radiation dosimetry. Once the calorimeter is irradiated, changes in temperature are measured. From these temperature changes, one can find the absorbed dose rate through dimensional analysis. The temperature change in water generated by a standard dose of 1 Gy is 0.24 mK. This poses experimental challenges which we attempt to address through finite element analysis.

Systematic errors exist in all calorimeters of a similar design. Probes (composed of mostly glass, air, metal and epoxy) extend from either end of the vessel to assure accurate temperature readings. Experimental data are higher than expected values because of excess heat produced by these non-water materials. Two dimensional axially symmetric models, created in FemLab, were used to simulate these findings. FemLab is a finite element analysis and solver program; it allows us to reproduce the conduction occurring experimentally throughout all regions of the phantom. By manipulating the model, we can produce calculated results closely resembling experimental data. Finally, we can explore alternative designs and understand irregularities in the data.

A stable radiation dose standard is essential to advancements being made in the medical field, industry and ionizing radiation research as a whole.

Gettysburg College

Effects of Surface Roughness on Instrumented Indentation
Brian Morgan

Instrumented Indentation (IIT) is used to characterize the mechanical properties of various metal and polymer films. The elastic modulus of the material is calculated as a function of the material's stiffness and the area of contact with the indenter tip. The stiffness is a function of load divided by displacement. The contact area is inferred through a tip shape function that relates the area to contact depth. In order to calibrate the tip shape function, a standard of a known modulus, such as single crystal fused silica, must be analyzed. The fused silica, however, is an ideal indentation material because it is a stiff, smooth substance. Many samples have an inherent roughness that cannot be polished because the process would destroy the surface of interest. Polymers subjected to UV degradation or filled with nanometer size particles are perfect examples of such fragile surfaces. Sample roughness poses a problem for IIT because it essentially results in variations in the actual contact being made during the first few hundred nanometers of indentation. The purpose of this research was to produce and study samples of different materials with varying but quantified amounts of surface roughness. Using IIT, the modulus and hardness of each sample was determined, and, through comparison, a qualitative model was developed to describe the effect of surface roughness on mechanical property measurements.

Temperature Corrections in Industrial Irradiation Processing
Tanya Ostapenko

In the routine operation of a radiation processing facility, dose measurements of the product made at regular intervals document the dosimetric quality control of the process for the facility operator and regulatory authorities. It is important that this dosimetry be suitably accurate and traceable to a national primary standard. The most widely recognized and best available method for high-dose measurements is the alanine – Electron Paramagnetic Resonance (EPR) dosimetry technique. This technique is based on relative EPR measurements of stable free radical concentrations induced by radiation, where the concentration is proportional to the absorbed dose. Subsequently, this is compared to a calibration curve created from the same batch of dosimeters irradiated to precisely known doses with a standard source.

At present, the procedure of calibrating a source for a customer comprises sending unirradiated alanine from NIST to the customer, who irradiates them with the industrial source to be calibrated. The irradiated dosimeters are returned to NIST, the EPR signals are measured and compared with aforementioned calibration curve and the dose values are calculated. The only unknown factor is the temperature during irradiation; this is not controlled and can vary greatly during an irradiation. The dosimeter response has a dependence on temperature; this dependence is compensated by applying a correction factor to the dosimeter response in order to compute the

absorbed dose. Moreover, there is no standard protocol on how to estimate the irradiation temperature and apply this correction.

Several methods have been proposed for calculating a correction factor which compensates for temperature variations. This work involved experimentally simulating industrial temperature profiles using a Co-60 source to evaluate these methods. The formula proposed by Peter Sharpe and Arne Miller yielded the lowest uncertainty in profiles where the temperature oscillated during irradiation. However, for profiles whose temperature increase or decrease is gradual, even the Sharpe-Miller formula does not provide an accurate correction factor. Temperature correction uncertainty estimates were computed for all the temperature profiles studied. These data will prove useful to industrial irradiation facilities in computing the overall uncertainties for their process.

Gustavus Adolphus College

Towards Protein Resistance of Silicon
Sarah Hackenmueller

Protein resistant surfaces are highly desirable when working with biomedical devices, such as in situ medical implants and ex situ diagnostic sensors. Silicon is an ideal substrate for working in bioelectronics due to its semiconductor properties offering the potential of advanced functionality not available in metal and glass substrates typically used. A crucial step in utilizing silicon substrates for bioelectronic applications is to achieve a surface that inhibits non-specific attachment of biological molecules. Typically polymeric ethylene oxide has been used to resist non-specific attachment of biological layers to the surface. In this work, small ethylene oxide molecules (EO_6) were specially synthesized and used to understand the protein resistance of monolayers formed on silicon from starting thiol, alcohol, alkene, and disulfide functionalities. These EO6 molecules were tethered to the hydrogen-terminated silicon(111) surface using both ultraviolet and thermal reaction conditions. Contact angle, infrared spectroscopy and spectroscopic ellipsometry measurements were used to characterize the surface layer before and after protein adsorption. Molecules with differing functionality were examined to compare the impact of functionality on layer formation and, ultimately, the properties of the monolayer. Studies with octadecyl molecules were performed to understand and compare the reactivity and quality of layer formation of thiol, alcohol, alkene, and aldehyde functionalities.

Hamilton College

Neutron Beam Collimation Using Monte Carlo Simulation Techniques
Daniel Campbell

Radiative emission during beta decay of the neutron into a proton, electron and antineutrino occurs as a result of the inner bremsstrahlung of the electron. Photons released in neutron beta decay are difficult to detect due to the long lifetime (885 seconds) of free neutrons and the weak branching ratio for the radiative decay mode. An experiment is underway at the NIST Center for Neutron Research to measure the branching ratio and determine the spectrum of photons emitted in radiative decay. In the apparatus, the proton and electron are guided to a silicon surface

barrier detector by a 4.6 T magnetic field. Photons are detected by a scintillator that is viewed by an avalanche photodiode. For an event to be included in the data set, these photons must be coincident with the electron and followed by a delayed proton. If neutrons collide with the apparatus background gamma rays can also be produced. A Monte Carlo simulation of the guide tubes and collimator preceding the detector was used to improve the neutron beam collimation, so as to minimize this background. Monte Carlo simulations follow particles through the series of events which they undergo and compute both the position and survival probability of all particles. A program was developed to convert raw flux and position data output from the Monte Carlo into a flux histogram plotted against radius. The Monte Carlo simulated beam distribution was found to have very good agreement with that of experimentally determined beam images. Small changes in Monte Carlo parameters such as aperture sizes, collimator length, guide tube length and guide tube coating were found to dramatically alter simulated neutron beam collimation, distribution and flux. In the experiment, neutrons may diverge no more than 1.4 cm from the center of the apparatus to be detected by the silicon surface barrier detector. This desired collimation was achieved for several guide tube and collimator arrangements with less than 20% loss of the incident neutron flux.

Illinois Institute of Technology

Examining Lipid Bilayer Molecular Dynamics by Neutron Scattering and Molecular Dynamics Simulations

Edwin J. Schwalbach

The molecular dynamics of lipid bilayers play a significant role in many systems of biological importance. For instance, lipid bilayers are a model of cell membranes, the dynamics of which are critical to many cellular activities. This study aims to understand the molecular motions of dimyristoyl phosphatidylcholine (DMPC) lipid bilayers through a combination of neutron scattering and molecular dynamics simulations. Experimental analysis included the measurement of molecular dynamics in DMPC bilayers using the High Flux Backscattering Spectrometer at the NIST Center for Neutron Research. The measurement of quasi-elastic neutron scattering from DMPC bilayers at both 295K and 315K hydrated at a relative humidity of 75% with D_2O allowed computation of molecular relaxation times. Elastic scattering measurements between 320K and 10K verified phase transition temperatures. Small angle neutron scattering measured beam transmission as well as bilayer thickness for comparison with computer simulations.

Two types of molecular dynamics simulations were performed and compared with the experiments; an all atom simulation was run in NAMD, and a less detailed but computationally faster coarse grain model was run with GROMACS. Each simulation trajectory spanned 100 ns at conditions mimicking those of the experiments, and began from the same set of 72 equilibrated lipid molecules. Calculation of the intermediate scattering functions and subsequent curve fitting led to the determination of relaxation times for the simulated trajectories. The values from each model were compared with each other as well as with the experimentally determined relaxation times. Calculation of the mean squared displacements allowed another direct comparison to experimentally measured values. Simulation data that compare favorably to

experiments give insight into the atomic scale motions that neutron scattering cannot easily access.

Indiana University, Bloomington

Surface Barrier Detector Properties for the Precise Neutron Flux Measurement

Craig Huffer

The characterization of surface barrier detector's was preformed. Pulse height spectra for alpha particles were taken from a Np-237 source and fitted to the expected spectra to determine the resolution of our surface barrier detectors. The resolution of the detectors was taken as a function of the bias voltage to determine the ideal operating bias voltage for each detector. The best resolution was compared for each detector to determine which detectors should be used in the Absolute Neutron Flux Measurement. The detector of highest resolution, which will be used in the alpha-gamma device, was measured to have a FWHM of 23.4 keV at a bias voltage of 45 V. This detector's resolution will be sufficient for our experiment. Efforts were also taken to setup the alpha gamma device and to reduce the noise of the barrier detectors in the alpha gamma device through grounding loops, electrical isolation, electrical shielding, and mechanical isolation.

Johns Hopkins University

Wind Load Factors for Tall Buildings

Amelia Wright

For a structure to function safely, the strength or capacity must be greater than the demand induced by the loads acting on the structure. The probability that a structure will fail is the probability that the demand exceeds the capacity. Although the probability of failure of a structure can never be zero (e.g., the structure can be hit by a meteorite), it can be reduced enough to ensure a safety level acceptable by society in a cost-effective manner. The load and resistance values are defined in statistical terms, rather than being deterministic. To assure that the design is safe, nominal design values of the loads must be multiplied by load factors larger than unity, and nominal resistance values must be multiplied by resistance factors smaller than unity.

The ASCE 7-05 Standard specifies the same load factor for all buildings, regardless of whether they are rigid or flexible. Tall buildings are flexible, so their response to the randomly varying aerodynamic loads they experience under wind is dynamic and depends upon the damping inherent in their motion. Because damping values are affected by large uncertainties, the actual value of the damping as experienced during the building motion can differ significantly from the nominal damping value used in design. The safety margin inherent in the load factor must therefore account for these uncertainties. It follows that load factors must be larger for tall buildings than for rigid buildings, since the latter's response is not a function of damping.

The goal of this project is to develop wind load factors appropriate for tall building design, and to compare them with load factors specified in the ASCE Standard on the basis of estimates of rigid building response. The development of load factors entails the use of information on uncertainties inherent in the various parameters that determine structural response. The talk will include a description of the dynamic and statistical elements of the methodology used to estimate load factors for tall buildings. It is anticipated that this work will provide a basis for recommendations to the ASCE 7 Wind Loads Committee on load factor values for tall building design.

Kansas State University

Thermophoretic Sampling of Soot from a Diffusion Spray Flame
Nelson Green

Light absorption and scattering by aerosol particles (i.e. soot) in the atmosphere has been shown to play a prominent role in climate change. Quantifying its effect requires accurate optical property measurements of aerosol particles. The optical properties of soot are related directly to its morphology. Soot particles levitated by ultrasonic waves were imaged using a high-speed camera. Analysis of soot particles using a transmission electron microscope (TEM) will give useful information on the soot's morphology. Soot is collected from a diffusion spray flame onto a grid for TEM analysis using a thermophorectic sampling probe. Unlike previous probes, when moving in and out of the flame, the grid is protected inside an aluminum rod. A small hole in the rod allows the grid to be exposed using a pneumatic actuator. The transit time of the grid during actuation allows us to measure the length of the exposure by reflecting laser light off the surface and into a photodiode. A pressure regulator and flow restrictor set the speed of the actuator and allows different transit times. This exposure technique should allow better spatial recognition and reduce streaking from high sooting regions within the flame.

Kennesaw State University

Using Small Angle Neutron Scattering to Investigate the Phase Behaviors of Mixed Lipid Systems
Gina Polimeni

Membrane proteins, which ensure the functioning of many vital biological processes, have been poorly characterized due to their inherent adversity to being crystallized. In particular, their removal from the phospholipid membranes in which they are embedded disrupts their folding patterns. However, once a suitable platform for membrane protein crystallization has been engineered, the structures of these fragile proteins can be determined. Biomimetic environments such as those having similar properties to actual phospholipid bilayers have been the preferred choice in attempts at membrane protein crystallization. A wide variety of self-assembled amphiphilic systems are currently being investigated in order to understand the mechanics of their interactions with membrane proteins and to explore their utility as processing phases for membrane protein crystallization.

One of the most promising biomimetic environments is the so-called bicelle phase, which has been shown to occur in mixed lipid systems. Bicelles are relatively small, disc-like structures intermediate between bilayers and micelles that self-assemble in mixed solutions of short- and long-chain lipids. Membrane proteins can be solubilized in these phases without being denatured, since they incorporate easily into the central lipid bilayer region of the bicellar disc. The characteristic sizes and thermodynamic behavior of the bicelles can be manipulated by changing the length and molar ratios of the lipids as well as their overall concentration. Therefore, these systems can be tuned to accommodate membrane proteins over a range of folding temperatures and geometries.

To explore bicellar phase behavior, we have examined a variety of mixtures containing different short- and long-chain phospholipids. Viscosity, birefringence, and transparency were used to construct crude temperature phase diagrams of these lipid systems. Based on these initial observations and supporting measurements obtained from dynamic light scattering and polarized optical microscopy, promising regions of the phase diagrams were examined in closer detail by small angle neutron scattering (SANS) at the NIST Center for Neutron Research. By this method, mesoscale morphological changes were mapped out as a function of temperature, concentration, and lipid composition. With regards to protein crystallization, one of the more important phase behavior features of these lipid systems is the temperature at which a liquid-to-gel phase transition occurs. This phase transition is significant because it underscores short-range correlations involving the temperature required for a useful protein-bicelle mixing phase and longer-range correlations relating to the formation of protein proto-crystals. We have investigated the dependence of the liquid-to-gel phase transition temperature on the T_m of the long-chain phospholipid as a means of tuning the phase behavior of these bicelles to the characteristics of specific proteins.

Loyola College in Maryland

Performance Analysis of 3D Flash LADAR
Jacqueline Kenney

Flash LADAR cameras capture real-time 3D data of a scene using active sensing and a focal plane array. Due to increasing performance and decreasing cost they have been applied to a variety of areas including manufacturing, construction, security and autonomous navigation. This study evaluates four different flash LADAR devices in order to characterize their performance. The study considers the effect of distance, target material and angle of incidence on accuracy and precision of their range data. In addition the uniformity of their light sources is examined since, unlike scanning LADARs which point a constant beam of light at each location, the distribution of LADAR light varies over the scene. The information collected identifies the limitations of each of the LADAR devices as well as the causes of the limitations.

Massachusetts Institute of Technology

Fabrication and Characterization of Polymer Microsphere Test Standards for Trace Explosive and Narcotic Detection Portal Systems

Jacqueline Brazin

In recent years, there has been a growing interest in the development and deployment of new screening technologies for trace explosive and narcotics detection to support homeland security, counter terrorism and law enforcement. One very promising technology is the trace explosive (narcotics) detection portal (TEDP) which is currently being extensively deployed by Transportation Security Administration (TSA) for the noninvasive and rapid identification of airline passengers who may be carrying or were exposed to explosives. Portal systems rely on the removal, collection and preconcentration of explosive particles that are dislodged from the passenger as they pass through the portal device. A person entering the portal is subjected to a series of pulsed air jets. Particles released by this process are collected onto a metallic grid which is subsequently heated to produce vapor which is sampled by ion mobility spectrometry (IMS). One of the key issues facing the effective utilization of this new technology is the concurrent development of standard test particles (containing explosives or narcotics) to evaluate the operational status, sensitivity and particle collection efficiency of these systems. Appropriate test materials must meet a number of criteria including uniformity of the particle size, quantitative incorporation of the analyte molecule, stability of the particles over time, safety of the materials used, and ease of production..

In this work, we demonstrate a unique method for fabrication of portal test particles using an oil/water emulsion polymerization technique. A custom inkjet printer system which we call a "sphere jet" is used to deliver monodisperse polymer microdrops containing the compounds of interest into an aqueous collection bath. The microspheres cure as the dichloroethane carrier solvent is extracted into the water phase. The spheres are filtered and dried. Using this approach, polylactide co-glycolide (PLGA) microspheres containing butylated hydroxytoluene (BHT), and the explosives HMX and TNT were prepared. Operating conditions (jetting conditions, polymer and analyte concentration, jetting frequency, curing conditions) were varied to produce spheres of various sizes and analyte concentrations. PLGA was selected as a carrier because it is biodegradable and approved for use in drug delivery systems. Similarly, BHT is a food additive that is approved for human consumption. The use of nontoxic starting materials is important to address potential health issues associated with the eventual use of aerosolized test particles in public venues such as airports. Characterization of the fabricated microspheres was carried out using optical particle counting, differential thermal analysis, fluorescence microscopy, scanning electron microscopy, focused ion beam analysis, and secondary ion mass spectrometry. Particle size analysis and fluorescence microscopy demonstrated the uniform size distribution and the monodispersity of the microspheres, which ranged from 20-40 ± 5 μm. Evaluation of the microspheres by ion mobility spectrometry (IMS) detected the presence of analyte (negative ion peak) in the microspheres and the PLGA offered no interfering peaks. The microspheres described here meet the requirements for an appropriate test material for detection of trace explosive particles in portal detectors. Ongoing studies will aim to characterize the surface and cross sectional distribution of the analyte molecules in the microspheres. Finally, the microsphere fabrication and characterization approaches developed in this work are applicable to

the development of standards for next generation polymer microsphere drug delivery systems which will be the subject of another investigation in our laboratory.

Combinatorial Designs and Their Impact on Software Testing
Michael A. Forbes

From straightforward device drivers to complex mathematical modeling programs it is clear that program correctness is needed for both security and reliability but is unclear how to face the insurmountable problem of producing bug-free code. There are many ways to approach this problem including constructing better programming languages, performing more code review and additional by-hand testing as well as automated code checking. However, none of these methods really guarantee the type of testing that identifies all logic bugs.

To combat this problem, notions from combinatorial design are being used to create sets of input to cover all possible test cases sufficiently well. To cover all possible test cases would require an exponential amount of work, but a "good" coverage has been shown to have roughly logarithmic growth with the number of parameters. Full coverage would require all possible cases for all possible parameters to be present. "Good" coverage can be defined as requiring all possible values to be tested for any subset of size t of the k parameters available, for some value of t. Empirical testing has shown that if t=6 this is sufficient to expose most bugs. While this gives hope to creating test sets for programs that can quickly and efficiently expose bugs, it does not answer some of the vital questions such as what the minimal size of such test sets can be as well as how to construct such sets. Current research is aimed at proving bounds on the size of minimal test sets and improving existing algorithms for constructing such test sets.

A collaboration of researchers at NIST, the University of Texas at Arlington and George Mason University have developed a program called FireEye that generate test sets by incrementally covering parameters. This strategy is called In-Parameter-Order (IPO). Currently, IPO is a deterministic algorithm that includes two phases, horizontal growth and vertical growth. It has been shown that the vertical growth algorithm has optimal efficiency but optimal algorithms for horizontal growth take exponential amounts of time. The existing algorithm takes a greedy approach that leads to good results. However, by making the algorithm "more greedy" by expanding its search space and randomizing the greedy selection noticeable decreases in the size of the resulting test set have been achieved.

High Resolution X-Ray Diffraction: Characterizing Aspects of a NIST SRM
Phyllis Xu

This presentation focuses on the High Resolution X-Ray Diffraction (HRXRD) Standard Reference Material (SRM) development project at NIST. The HRXRD structure consists of two thin, single crystal layers (Si, SiGe) grown on a Si substrate wafer. We focused on two research topics, artifact uniformity and modeling interpretation. First we examined the uniformity of the calibration artifact's structural parameters. The HRXRD method allows us to determine the thickness and composition of the thin Si and SiGe layers and in turn provides us with information on the overall wafer deposition quality. We measured structural parameters at the small-scale (1 mm) and the wafer-scale (75 mm), which showed measurements ranging between

a 1% to 2% deviation in both scales. This was comparable to the standard uncertainties predicted by the commercial modeling software, which ranged from 0.4% to 2%. In the modeling interpretation study, we compared commercial and online open source HRXRD software to test the consistency between the two models' input parameters. We found that all parameters need to be input correctly in order to produce identical patterns and that several parameters between the models are not uniformly defined (strain versus lattice variation). Within the commercial modeling software, changes in two different parameters (composition and strain) generated similar changes in the pattern, making structural model refinements ambiguous. In conclusion, the deposited structure is reasonably uniform within the standard uncertainty determined by the modeling software, but we are still unsure as to which additional input structure parameters (e.g. strain) are necessary for the SRM modeling.

Miami (Ohio) University

Performance Comparisons of InGaAs, Extended InGaAs, and Short-Wave HgCdTe Detectors Between 1 µm and 2.5 µm
Matthew Dopkiss

Traditional photovoltaic detectors such as PbS and PbSe are limited in their ability to conduct low noise measurements for small very small signals. The noise permitted by the low shunt resistance of these detectors leaves them unsuitable for measurements requiring extremely low uncertainty. This study provides characterization and analysis of three different varieties of photodiodes whose band-gap wavelengths span the near-infrared spectrum. The three types of detectors examined include Indium Gallium Arsenide (InGaAs), extended InGaAs and short-wave Mercury Cadmium Telluride (MCT) detectors with active areas of either 1mm or 3mm. These photodiodes are thermoelectrically cooled over a range from room temperature to -85^{o} C in order to measure their temperature-dependent shunt resistances, spectral power responsivities and noise equivalent power characteristics. The detectors' spectral power responsivities are determined against a pyroelectric detector (standard with constant responsivity versus wavelength) to determine the absolute spectral power responsivity of each detector. Measurements reveal InGaAs shunt resistances can increase to 5 GΩ when cooled to -20^{o} C. Both extended InGaAs and MCT shunt resistances were measured to be about 11 MΩ at -70^{o} C. The importance of selecting an appropriate temperature (and therefore shunt resistance) relative to load resistance is critical to the design of high-precision photodiode measurement techniques.

Millersville University

Ph-ISFETs in Microfluidics: Qualitative Analysis of Variance and Comparison with Fluorescent pH Indicator
Amelia Fillipo

Lab-on-a-chip type devices require accurate and reproducible sensors for quantitative determination of analyte concentration in small volumes of flowing solution. Previous studies have used fluorescent dyes for pH measurement in microfluidic systems, however, ion-sensitive field-effect transistors (ISFETs) may be more appropriate for some applications because of their small size and planarity. The purpose of this study is to qualitatively determine how flow-rate

and ionic strength of buffered aqueous solutions affect the output voltage of a pH-ISFET embedded in a planar microfluidic system. The prototype microfluidic ISFET system also allows for optical pH measurements in the same device thus facilitating comparison of the two orthogonal measurement techniques.

The prototype pH-ISFET system comprised a molded elastomer microfluidic channel (cross sectional area of about 250 μm wide by 50 μm high) positioned on top of the silicon nitride gate insulator of a FET (gate length = 20 μm, gate width = 500 μm). A planar Ag/AgCl quasi-reference electrode was integrated into the same fluidic system. The microfluidic channel over the ISFET was filled with various buffer solutions and the channel over the Ag/AgCl electrode was filled with 3 mol L^{-1} KCl. Determination of pH with the ISFET was accomplished by measuring the drain to reference voltage, V_{DR}, at a constant drain to source current. Calibration of the ISFET at steady state gave a repeatable near-Nernstian response slope of 63.2 ± 6.2 mV pH^{-1}. Volumetric flow rates of a phosphate based pH 7 buffer were varied from 2 to 14 μL min^{-1} while V_{DR} was monitored. Separately, V_{DR} was measured while the ISFET was exposed to pH 7 solutions adjusted with NaCl to different ionic strengths (12 to 120 mS), all at similar flow rate. After a time dependent drift in V_{DR} was accounted for, neither flow rate nor ionic strength was observed to strongly correlate with variance in the output voltage.

Optical measurements of pH by utilizing the fluorescent dye 2,3-dicyanohydroquinone (DCHQ) in the same fluid channel system are currently underway. When exposed to a mercury arc lamp through an excitation filter centered at 365 nm, the fluorescent light from DCHQ was collected through a long pass filter (420 nm). Both the fluorescent intensity and rate of photobleaching are pH dependent and are thus used in conjunction to determine pH.

Comparing the fluorescent dye calibration to the ISFET calibration should increase confidence in the accuracy of the pH measurements for both techniques. Since pH accuracy can be independently verified and since the system variables of flow rate and ionic strength were shown to have little or no effect on the accuracy of ISFET based pH measurements in the microfluidic format, it has been shown that the ISFET has the potential to be a robust sensor for use in a wide variety of lab-on-a-chip and microfluidic applications.

Application of Parallel Tempering to Neutron Reflectometry Data

Ed Schwartz

Thin films are of immense interest from both the applied and fundamental research communities. The characterization of such films is critical to both communities. Neutron reflectivity provides a way of determining parameters such as roughness and layer thickness. It is one of the only probes capable of determining magnetization density. However, the fitting of reflectivity data suffers from the presence of many local minima in the parameter space. To address this global minimization problem, we have developed a self-optimizing parallel tempering algorithm.

One commonly used global optimization technique is known as simulated annealing. This technique is derived from ideas developed in the study of spin glasses. In the technique, a set of parameters is randomly generated. A theoretical curve is then produced from this parameter set and compared against measured data. Parameter choices which improve the fit are always

accepted. However, parameters which generate worse fits are also accepted, with a probability based on how worse the fit is, and the "temperature". Worse fits are more likely to be accepted at higher temperatures. At high temperatures a large portion of the parameter space is explored, and as the temperature lowers, less exploration occurs, however, it is still possible to escape from local minima. However, if the cooling rate is too fast and the fitting surface is too rough, it is still possible to become trapped in local minima, where the temperature is insufficient to allow the algorithm to escape from that minima to explore more of parameter space. This deficiency is addressed by parallel tempering, which runs several replicas at the same time. Each replica consists of a set of parameters. Replicas adjacent in temperature can be swapped depending on the difference between goodness of fit for the replicas, and temperature difference between them. This allows replicas to move in a random walk through temperature space and to always have the opportunity of escape from local minima.

For our test functions, we found parallel tempering to be more efficient than simulated annealing, so we proceeded to modify our algorithm to make it even more efficient. We then integrated this algorithm into a reflectometry fitting program used at NIST called KSRefl.

Dynamic Web-Based Repository for Healthcare Standards Information

Jennna Yocklovich

The health care industry has many standards and specifications that deal with a wide variety of health care services. This variety makes it quite difficult to examine and trace the entire health care industry, which hinders many development efforts. Standards users and organizations become frustrated by the difficulty involved in understanding and adopting needed standards.

The NIST Health Care Standards Landscape (HCSL or Landscape) was designed to address these issues, and allow easy use and viewing of information about health care standards using a public web-based repository. It includes information about the standards, the organizations that use, develop, or promote the standards, related health care information, and links to other resources (note, the Landscape contains no actual standards). It is intended to help the health informatics community and interested users search for health care standards' information. In addition, because of extensive and ever-changing health care standards field, the Landscape also allows organizations and users to register and add content (i.e. publish), as well as update and delete existing obsolete content on relevant health care standards' information.

The Landscape provides a rich set of features and capabilities for publishing, managing, discovering, and retrieving health care standards information. This presentation describes the work of developing test data and scenarios for testing the Landscape capabilities, and briefly summarizes some of the test procedures and results. Extensive testing was conducted, and will continue to be performed to ensure that the Landscape capabilities and software function correctly for all users. As new Landscape features are added to expand its functionality, these will also need to be tested. It is the hope of the developers that the HCSL will continue to become more useful as more users contribute healthcare standards information to the database, thus making it even more useful to the health care community.

Montgomery College

Microstructural and Thermal Conductivity

Chi T. Do

Fire resistive materials have been utilized in both industrial and residential applications, and have proved their significance, especially when fireproofing is applied in high buildings and large-scale structure. Porous fire resistive materials are used to protect steel columns and other structural components such as fire-rated walls or exhaust hoods. However, the relationship between their microstructure and performance has not been established yet. Thus, this project focuses on further developing linkage between the microstructure and thermal properties (mainly thermal conductivity) of fire resistive materials. Experimental measurements of thermal conductivity were made using a Hot Disk thermal constants analyzer. Microstructural characterization was performed using optical and scanning electron microscopy. Finally, computer microstructural models and analytical relationships were applied to examine relationships between microstructural features and measured thermal performance, for instance, how thermal conductivity changes at various temperatures due to microstructural changes. It was found that for porous fire resistive materials, pore size and porosity do take an important part in how the materials perform, especially at high temperatures.

Moorpark College

Literature Study of the Supply Change of Medical Devices

Sam Toutounchian

Communication is an intricate portion of the supply chain management of any industry, including medical devices. The shelf price of medical devices are determined by the interactions between the various vendors and buyers throughout a supply chain, which is said to be the chain of vendors and buyers that raw materials go through between the time that they are acquired, to the time that they are in a finished potentially life saving device. The prices throughout the supply chain are determined by the supply and demand for each respective product or raw material that is involved in the specific transaction between the involved members of the supply chain. The only way to optimize this complex system of various supply and demand curves is to have superior methods by which to predict the demand at the various points in the supply chain. Communication is arguably the most important task in demand forecasting. The most obvious solution would be an automated system of computers that report sales data throughout the supply chain. A literature study was conducted to investigate the implementation and utility of current standards for automated e-business communication. There are several standards in use today, none of which lend themselves to the supply chain management of medical devices. These standards include: Electronic Data Interchange, UN/EDIFACT, ebXML, and XML. Certain transactions sets using core components of the current standards were created to better serve the medical device industry. The future of this field of research holds promise to greatly improve the efficiency and dependability of the medical device industry.

Mount St. Mary's University

Surface Derivatization of Thermoplastics for Increased Hydrophilicity

Ashley Keeney

In February of 2004, The National Institute of Justice estimated the backlog of criminal cases involving DNA evidence to be 500,000. They provided several reasons for this backlog, including inadequate funding due to the high cost of DNA analysis (an average analysis costs $1,100) and the length of time required to process DNA evidence. The use of microfluidic devices can reduce the cost and time required for DNA analysis. The development of these devices is still relatively new, but their construction using economical plastics is showing great promise. One of the challenges of using plastic for DNA analysis is that the DNA non-specifically adsorbs to the plastic surface, resulting in low analysis resolution. To address this problem we investigated the ability of several oxidizing agents to alter the surface chemistry of poly(methyl methacrylate) (PMMA), a common plastic used in microfluidic devices, so that it would absorb a layer of poly-N-hydroxyethylacrylamide (polyDuramide) which has been shown to be an effective a dynamic coating on silica capillaries. The oxidizing agents we used were aqueous solutions of sodium chlorite, potassium permanganate, potassium chromate, and a 4:3:1 solution of deionized water, sulfuric acid, and hydrogen peroxide, which is also known as piranha. By coating the PMMA we can change its surface chemistry to eliminate or reduce the non-specific adsorption of DNA to its surface. The effectiveness of each oxidizing agent in altering the surface hydrophilicity was evaluated through contact angle measurements. It was concluded from these measurements that piranha was the most effective in derivatizing the PMMA surface to allow for the polyDuramide to adsorb to it, creating a surface more suited to DNA analysis. In addition, the effectiveness of piranha to alter the surface hydrophilicity of polycarbonate was evaluated through contact angle measurements. However, these measurements were inconclusive. Thus, current monitoring, a technique to measure zeta potential (surface charge density), was used to further characterize the absorption of polyDuramide to polycarbonate following a treatment with piranha. Based on these measurements we were able to calculate the average electroosmotic mobility (a measure of surface charge density) for native polycarbonate and treated polycarbonate. The native polycarbonate had an average electroosmotic mobility of 0.000435 $cm^2/(V*sec)$ and the polycarbonate treated with piranha and polyDuramide had an average electroosmotic mobility of 0.000181 $cm^2/(V*sec)$, which is approximately a 60% reduction in electroosmotic mobility. These results show that the polyDuramide effectively absorbed onto the surface of the polycarbonate.

Northwestern University

Immuno-Fluorescent Staining for Telomerase: Cell Population Expression Variability

Adrienne Smith

Modern cancer diagnostics rely heavily on histopathology. Such analyses involve subjective interpretations by a pathologist that are often times inconclusive. Consequently, there is a need for quantitative methods for objectively differentiating between stages of cancer. Telomerase is a protein that may be utilized as a biomarker in this endeavor. Responsible for immortalization

via the addition of chromosomal telomeres, telomerase is expressed in 85-90% of all human cancers, but not in normal adult, non-stem cell somatic tissues. An immuno-histochemistry (IHC) standard protein chip for telomerase expression would allow biopsy tissue to be stained with fluorescently marked antibodies and compared for objective analysis.

An IHC chip has been developed and fabricated by photolithography using a thiolene polymer. In order to create a reliable standard, the effect of the substrate on cell proliferation and telomerase expression was studied. Cells from the IMR90 (normal fibroblast) and VA13 (representative stage two cancer cells) lines were seeded on glass slides and thiolene chips. Fluorescently labeled telomerase antibodies, nuclei stains and cell membrane stains were used in conjunction with fluorescence microscopy to evaluate the effect of the substrate surface.

We have developed a data analysis macro to examine the distributions of cell area, telomerase expression and fluorescence intensity on each of the respective substrates.

Pennsylvania State University

Electrical Measurements of Self Assembled Monolayers
Chad Althouse

A Self Assembled Monolayer (SAM) is a material that is created by molecules that "self assemble" themselves into a plane that is a single molecule thick. SAMs have prospects to be used as conductors or dielectrics in electronic devices. In addition, theorists have published hypotheses that some SAMs have switching properties and therefore might serve as a replacement for silicon transistors in the future. However, until recently, few electrical measurements have been made of SAMs because of complications in forming an electrode on top of the SAM. One solution to this problem is the use of PEDOT:pss, an electrically conducive polymer. This talk will cover the use of PEDOT:pss in creating a top electrode for a SAM and the results of electrical measurements of SAMs.

Evaluation of the Stability of NIST Natural-Matrix Radionuclide SRM
Kevin Cheng

Humans are exposed to radiation in various ways. Most radiation exposure from sources in the environment results in small doses which are not particularly harmful. For pathway assessment, samples are gathered from various locations but are not always immediately analyzed. Some samples may take several years before the full analysis is complete. But how can you be sure that the stability of the sample has not affected the accuracy of the measured activity? Similarly, when environmental radionuclide quality control test samples are made up but stored for a number of years, could the stability of the sample over time affect the results of the test? This poses a concern to whether natural-matrix radionuclide samples are stable under stored conditions. In this work, NIST Radiochemistry Intercomparison Program water and synthetic urine samples that have been stored for a number of years were analyzed radiochemically for alpha, beta and gamma-ray emitting nuclides such as Mn-54, Co-57, Sr-90, U-234, Pu-238, and other isotopes as well. Older samples along with more recent ones were examined to determine any change in activity level. One might expect that when the results are compared with previously confirmed massic activities (Bq/g), the radionuclides will show various degrees of

stability in their respective matrices. Early results show a reasonable recovery percentage when analyzing for alpha-emitting nuclides. However when analyzing for gamma-ray emitting nuclides, it appears that older samples showed a lower activity. The issue of instability may apply to Standard Reference Materials (SRM); some radionuclides may indeed not be stable over extended periods of time. The results of this work provide important new information that would be very useful to: a) prioritize the analysis of future environmental samples, and b) determine the useful storage time of archived environmental samples, quality control test samples and reference materials.

Towards the Redefinitiion of the Kilogram: Magnetic Levitation of Mass Standards

Carolyn Denomme

As the only SI unit still based on an artifact rather than a fundamental physical property, the kilogram faces many problems. The international prototype kilogram may be damaged or destroyed and it seems the mass is even drifting with time. Scientists are working toward a redefinition that would be based on fundamental physical constants. NIST's watt balance is a foremost player in this redefinition process. The watt balance's accuracy will be improved with a better connection between the kilogram in the watt balance, which is held in vacuum, and NIST's kilogram standard, which must be kept in air. A magnetic levitation system is being designed for this purpose. Currently, the first phase of this magnetic system is being designed and tested to help determine parameters for the final levitation system.

Measurements and Modeling of Contact Potential Difference with Scanning Kelvin Force Microscopy

Thomas Walker

The contact potential difference (CPD) between a surface and the probe of a scanning Kelvin probe microscope (SKPM) was measured at different probe heights above the surface. The results matched the findings of Park et al.; both the present study and Park's study found that CPD vs. lift height either increases or decreases rapidly (the trend depends on phase angle), and in a nonlinear fashion. Both studies also found that CPD at different lift heights is shifted uniformly when phase angle changes.

The CPD of interest is a DC voltage between surface and probe, at each position of the probe as it moves along the surface. Koley et al. provide expressions for the differential capacitance of the tip and cantilever on a probe. From this model a computer program, FAST Scanning Kelvin Simulator (FASTSKS), was adapted. The model was used to find the CPD caused by different commercially-available probes. The Koley model was modified per the model by Saint Jean et al., however, to consider the tip as two separate components – a hemispherical point, and a conical shank. This change allowed the investigation of differential capacitance for each component of the probe, between minimum and maximum heights.

It was found from this altered model that a long blunt tip's differential capacitance will dominate the overall differential capacitance, more than that of a short sharp tip. This finding, along with the comparison of short sharp tip CPD model to long blunt tip CPD model, suggests that the

latter tip yields results closer to the empirical results. Eventually the electrostatic analysis used in the Koley model will be extended, to see if shielding the shank will let the tip dominate further from the surface. It is expected that this adjusted model's results will be closer to the real CPD.

Polytechnic University of Puerto Rico

File Change Analysis OS Startup (System Boot)
Billy Medina Torres

High profile investigations, criminal activities and civil litigations create a challenging scenario for computer forensics examiners. The analytical and investigative techniques to identify, collect, and examine evidence should be performed in a manner where the data should be kept as unaltered as possible during the forensic process.

As a first guideline procedure, preservation of evidence in the acquisition phase must be a top priority.Nevertheless an accidental system boot can occur, which in turn can modify the forensic evidence collected (the hard drive's file system information) and potentially jeopardize the investigative process.

My project consisted of identifying the changes that may have occurred during a system boot sequence and consists of two primary phases. First I developed a means to image the target data and created some scripts to automate this process. This acquisition was done without the assistance of the subject operating system and can be referred to as a "*dead analysis"* (i.e. we are not looking at a live system). Then I used a variety of forensic analysis tools to assist with identifying changed content and present test results in an easily understandable format.

Overall, my project provides a means to identify potentially the quantity and types of files that may be modified during the boot process. The impact of my research will assist investigators and forensic examiners in determining how to proceed if original evidence (hard drives) has been incorrectly examined and subjected to being booted directly.

Princeton University

Towards a Simple, Effective Database of Medical Codes
Siddharth Bhaskar

In the healthcare industry, diagnoses and procedures are associated with various schemas of numbers, which are referred to as "codes" in this context. These codes facilitate record keeping, and give physicians, laboratories, and insurance companies a common standard by which they can coordinate tests, prescriptions, billing, and the like. Two of the main coding schema are the International Classification of Diseases, version 9 (ICD-9) and Current Procedural Terminology, version 4 (CPT-4). In the United States, these two are the de facto standard for diagnoses and procedures respectively.

As the number of codes and the information contained wherein is extensive and growing, computer-based databases are the obvious solution for storing the codes. The American

Association of Clinical Endocrinologists (AACE) has requested a low-cost, user-friendly database of ICD and CPT codes. Similar databases intended specifically for coding exist, but are plagued by superfluous graphics, confusing interfaces, and exorbitant costs. We intend our product to be a simple and minimal solution, which also provides further functionality by letting users add links between ICD and CPT codes, for example.

We chose to build our product on the Veterans Health Information Systems and Technology Architecture (VistA), created by the Veterans Administration (now the Department of Veterans Affairs). It is a comprehensive database intended for hospital administration. VistA has ICD-9 codes already built in to the database, and CPT-4 codes may be integrated with a download from the American Medical Association (which copyrights CPT codes). Therefore, all that needed to be written were scripts which allowed a user to query and modify the database from a browser, made possible by VistA's Application Programming Interface. Like VistA itself, these scripts were written in MUMPS, or M, a language mostly used in database-heavy applications, such as in healthcare or banking.

Furthermore, VistA is completely open-source. One may download VistA, and an implementation of MUMPS to run it on, for free. The AMA's copyright on CPT-4 codes prevents us from merely putting our product on the internet for the general public; however, we feel that choosing to build our code on open-source databases makes our product more sound in the long run, because of a large network of free support and the growing potential for additional functionality.

Rensselaer Polytechnic Institute

Behavior of Single Walled Carbon Nanotubes in Aqueous Suspension

Bryant Walker

Single walled carbon nanotubes (SWNTs) are molecules of intense interest due to their outstanding theoretical mechanical and electrical properties. One promising method of testing SWNT mechanical properties is by analyzing their Brownian motion in water. This test method eliminates concentration gradients that can be caused by physical implementation instruments, and should give a more accurate measurement of SWNT bending modulus. Our experiment focused on measuring the deformation of 10-50μm SWNTs in aqueous solution. In addition, we sought to define a reproducible method to transfer SWNTs grown on TEM grids into aqueous suspension. Such a procedure could have future use in the field of wet-phase nanofabrication.

SWNTs were grown on TEM grids using the chemical vapor deposition (CVD) growth technique. The grids were then analyzed in a low voltage electron microscope (LVEM) using transmission electron microscopy to determine the SWNT yield of different methods of CVD. The grids were then placed in a flask with 1wt% aqueous sodium dodecyl sulphate (SDS) and sonicated in the presence of fluorescent dye (PKH26 or PKH67). The solution near the grid was then extracted and sealed between a slide and cover slip. Fluorescence microscopy yielded video recordings of SWNTs 10-20 μm long in solution. After a few seconds, the tubes collapsed on themselves by either folding or breaking. This process happened repeatedly, both within each

sample and in samples with varied sonication times. This unusual behavior might indicate defects in the nanotubes or could be the effect of fluorescent dye photo bleaching.

Rice University

Ontolex: Extending the Computational "Basic Reference Model" for Second Language Learning
Emily Fortuna

Around the same time Herbert Simon and Allen Newell developed their computer Information Processing Language for problem solving, Noam Chomsky produced his book *Syntactic Structures*, then *Aspects of the The Theory of Syntax* and other works that changed Linguistics. As Computer Science and Linguistics progressed, the idea of creating cognitive computer models emerged as a method to study the mysterious black box of the human mind. In fact, Chomsky believed that humans had evolved a specialized "Language Acquisition Device (LAD)", but could not yield a feasible model. Newer theories which work at the syntax *plus* semantics level may lead to better models in both Computer Science and Linguistics.

The goal of this project is to aid future second language learning studies by providing an easily extensible, web-accessible computer model framework for researchers to expand and use for comparison with other models. While learning his or her first language, a child also forms an ontology as he or she gains an understanding of the underlying concepts behind words. The framework, called *Ontolex*, focuses primarily on second language learning through the written word and assumes that the individual has already developed a simple hierarchal ontology of concepts. This intelligent learning system expands upon the "Basic Reference Model" developed last summer and models three general phases in the human second language learning process: vocabulary building, formulaic speech and translation, and unique utterance generation with user feedback. This adaptable framework is partly inspired by Construction Grammar and Lexical-Functional Grammar theories from Charles Fillmore, James Pustejovsky, Raymond Jackendoff, George Lakoff, Yehuda N. Falk, Mirjam Fried, and Jan-Ola Östman.

Saint Joseph's University

A Study of New Colorimetric Radiation Dosimeter
Nora Graneto

Ionizing radiation is used in various areas of industry for product sterilization, pasteurization, and material modification (*e.g*., polymer crosslinking). The radiation treatments are carried out in large-scale irradiation facilities by the manufacturer. For most processes a range of absorbed dose is sufficient, and the delivery of this dose should be accurate and reproducible. The role of dosimetry is to assist in the process design and for quality control of the process. Electron-Beam (EB) Fast Check Strips are new radiation dosimeters introduced by the Spectra Group Ltd. Spectra Group claims these dosimeters can be used to obtain dose profiles, monitor dose, and determine the power of EB energy sources. They are composed of three dye-coated squares on a rectangular adhesive-backed strip. Ideally these color strips can be used in industry as a quick visual indicator. They can be fixed onto selected boxes in the assembly line of product boxes

and, upon exit from the irradiation area they can be examined to verify that the box was processed. Since Spectra Group claims that the dosimeters can be used to quantify dose, a series of tests were designed to evaluate the quality of this assertion. Because the color change is not easily quantified visually, techniques that would quantify the subtle changes were examined. After some initial tests, it was decided to use *Lab* color space and the Minolta Chroma Meter CR-300. In Lab color space the *L*-value measures lightness, the *a*-value measures green (negative *a*) and red (positive *a*), and the *b*-value measures blue (negative *b*) and yellow (positive *b*). The instrument detects subtle changes in color that the eye cannot see. The goal of this experiment is to assess some of the company claims on the usefulness of these colorimetric radiation dosimeters. Dosimeters are typically sensitive to light, temperature and humidity. Also, the response of some dye dosimeter systems are known to be time dependent. The dosimeter response did change with exposure to room light, so precautions were taken to prevent light exposure. The time dependence of the dosimeter's radiation response was halted by annealing the dosimeters at 87 °C. The talk will focus on studies of the dosimeter system's radiation dose response, relative humidity effects and accuracy as a visual indicator. To evaluate the accuracy of the visual recognition of absorbed dose for these dosimeters a visual test was developed and tested with volunteers.

Saint Mary's College of Maryland

Quantification of Capsaicinoids in Hot Peppers Using Liquid Chromatography / Mass Spectrometry

Nathaniel Doane

The "hotness," or pungency, of chili peppers is due to the family of compounds known as capsaicinoids. Medicines for nerve pain, spicing for food, and pepper sprays for law enforcement use these compounds as active ingredients. Pungency has traditionally been measured in Scoville Heat Units (SHU) and measurement based on a taste test accounting for only the cumulative capsaicinoid concentration. Other methods have derived ways to measure capsaicinoid levels in peppers including capillary gas chromatography and liquid chromatography. Different types of peppers have specific ratios of each capsaicinoid (i.e. capsaicin, dihydrocapsaicin, etc.). The ratio of these capsaicinoid concentrations makes each type of pepper unique. Therefore, it is optimal to separate each capsaicinoid from each other in order to quantify the concentration of each specific capsaicinoid. To achieve complete separation and identification, the method of using liquid chromatography/ mass spectrometry (LC/MS) was employed to identify eight capsaicinoids. A phenyl stationary phase was used to achieve complete separation of the capsaicinoids and norcapsaicin was used as an internal standard. Different types of peppers in both the fresh and dried state were analyzed for consistency and to compare the different capsaicinoid profiles of the different peppers. Of the eight capsaicinoids analyzed, capsaicin and dihydrocapsaicin were the two compounds prominent in the hot pepper profile. The water content of these peppers was found to be about 90% resulting in higher concentrations of capsaicinoids in dry peppers. The method of separation proved to be applicable to a wide assortment of peppers.

Development of a Computer Based Fire Fighter Training Tool

Tabitha Huntemann

The best way to learn how to fight fire is to fight fire. However, this is expensive and particularly dangerous for the trainee. Many fire situations that must be trained for are too large and hazardous to re-create in a training setting involving real fires. In addition, environmental concerns limit the amount and kind of live fire training available in many areas of the country. Methods are needed to allow fire fighters to gain valuable experience by using virtual reality techniques applied in other fields so that they may learn about fire behavior and the impact of fire fighting tactics on the fire without the possibility of harming themselves or others. A computer-based fire fighting training tool will improve training opportunities while lowering costs and the risk of death and injury. This research contributes to the development of this training tool by developing comparisons between real and modeled training scenarios.

Fire experiments representative of fire fighting training exercises were conducted at the Maryland Fire and Rescue Institute and in the NIST Large Fire Facility. In order to demonstrate extreme temperatures encountered by fire fighters, an arrangement of wooden pallets was ignited in the corner of a burn room. The experiment was instrumented to record changes in fire conditions. The data output was used with NIST Fire Dynamics Simulator (FDS) to model the training facility and fire. Smokeview visualized FDS results by drawing shaded temperature contours. Initial models accurately predicted the location of the hot gas layer. However, temperatures in the modeled burn room were approximately one-third lower than real burn room temperatures. Dimensions of a burn room doorway were refined to keep heat and flames in the burn room. In addition, the wooden pallet arrangement was altered to more accurately reflect the real fire geometry. This alteration resulted in partial blockage of the burner, in effect halving the heat release rate and further depressing temperatures. The wooden pallet arrangement was again refined to unblock the burner. This change resulted in modeled temperatures very similar to the temperatures measured in the real burn room. Additional work is needed to create a more accurate depiction of the pallet arrangement without blocking the burner.

Realistic scenarios are also being developed for the trainer. For example, FDS and Smokeview were used to simulate kitchen training fires. Stovetop fires show the effects of vented stove hoods on fire spread as well as the fire suppression provided by sprinkler systems. Real kitchen experiments will be conducted to compare the model's ability to accurately predict the effects of fire suppression tactics.

This research shows that fire models can be used to create fairly accurate reproductions of live fire experiments. However, real confidence in model predictions can only be gained if the modeler checks that the model is working properly for the given scenario.

Quantitative and Qualitative Analysis of the Uptake of Polystyrene Microspheres by Human B-Lymphocytes

Fred Nawabi-Ghasimi

Increased application of nanomaterials throughout various industries demands an examination of their degree of toxicity and risks associated with the environment. As a model study, we have

recently utilized 1.0-μm polystyrene microspheres (beads) coated with amino (-NH3) and carboxylate (-COOH) chemistries to study their rates of uptake and direction by human B-lymphocytes. More specifically, these beads were determined to be attached to or internalized by 10-15-μm wide Epstein Barr Virus (EBV) transformed cell line, PB-6, acquired from a peripheral vein of a *Homo sapien* Caucasian male. Additionally, these cells were diluted 1: 20mL at log phase of growth ranging from 2.0-3.0*10^6 cells/ mL and incubated with beads diluted to 1μl: 10mL. Using counts from five trials, a t-Test: Paired Two Sample for Means revealed two-tail P-value of 0.043224547 for attached and 0.061587832 for internalized 1.0-μm polystyrene microspheres coated with amino (-NH3) versus carboxylate (-COOH) surface chemistries. Furthermore, y-axis error bars acquired from standard deviations displayed an overlap for both beads attached and a very slight difference between beads internalized. Thus, we can conclude that the difference between 1.0-μm polystyrene microspheres coated with amino (-NH3) and carboxylate (-COOH) chemistries attached to cells was not due to chance and is statistically significant. Conversely, the difference between internalized beads by the cells is due to chance and is not statistically significant.

Salisbury University

A Fourier Transform Analysis of Human Images for Evaluation of Thermal Imaging Cameras

Matthew Strawbridge

Thermal imaging cameras (TIC) have become a very useful tool for first responders by enhancing visibility in hazardous environments such as inside dark or smoky structures. Current research focuses on the daunting task of recreating first responder scenarios in order to develop appropriate performance test methods.

The goal of this project was to define a relationship between an image of a human body and the frequency of a square wave bar target. With this correlation, repeatable laboratory experiments can be performed using well defined bar targets while retaining a relationship to the human target that a first responder might seek. In support of this goal, infrared and visible images were collected of pairs of human targets (male and female) at four different distances (2m, 3m, 5m, 10m) using eight thermal imaging cameras and a visible camera. These distances where chosen because it is reasonable to expect that first responders might need to recognize human forms at these distances. The two human targets were dressed in either street clothes or fire fighter turnout gear based upon the fact that search and rescue victims could be fire civilians or other first responders. The correlation will be found by performing a Fourier Transform on the human images. The Fourier transform is a method used to transform objects in space or time into a "frequency space" by breaking an image down into its sine and cosine components. This method generates a complex valued vector for each image pixel, where the magnitude of the complex vector tells us how much of a certain frequency is present and the phase tells us where in the image this frequency is located.

Santa Monica College

Determination of Caffeine and Caffeine-Related Analogs in Candidate NIST Green Tea SRMs

Kristin Wong

There is an escalating need to develop analytical methods and reference materials that can be used to verify label claims and to assess product authenticity in the dietary supplement industry. In general dietary supplements have been mislabeled, adulterated and/or contaminated by other substances such as pesticides or toxic botanicals. With an increasing concern for public health, the Analytical Chemistry Division of the National Institute of Standards and Technology (NIST) collaborated with the National Institutes of Health's Office of Dietary Supplements, along with a few other research agencies, to establish a suite of SRMs that consists of authentic, well-characterized reference materials to help support the needs of the dietary supplement community.

One suite of SRMs that is currently being produced at NIST to support these needs is the Green Tea Dietary Supplement Suite. Green tea (*Camellia sinensis)* contains alkaloids (caffeine, theophylline and theobromine) and other compounds such as catechins (polyphenolic antioxidants), amino acid, minerals and trace elements. Green tea is used as a stimulant and is being used as a replacement for ephedra, which was recently pronounced an adulterant by the Food and Drug Administration. The aim of this project is to establish an analytical method to measure the concentration of alkaloids, specifically caffeine, in candidate green tea SRM samples.

Reversed-phase high performance liquid chromatography-ultraviolet absorbance detection (RP-HPLC-UV) is the method used for the analysis of the SRMs in this study. Caffeine and its derivatives are eluted using isocratic chromatographic conditions employing acetonitrile and 0.5% aqueous acetic acid. The UV absorbance wavelength of 274 nm is used to maximize the detection of caffeine. Chromatographic conditions are optimized using a standard mixture that contains theobromine, theophylline and caffeine in water. Samples are infused and sonicated for about 15 minutes prior to injection onto a C_{18} column. We are able to consistently separate caffeine, theobromine, and theophylline in the candidate materials by using 8 % acetonitrile: 92% aqueous acetic acid at a flow rate of 0.8 mL/min. The total run time is 30 minutes for each analysis.

The external standard method is currently being used to quantify the amount of caffeine in the samples. Initially β-hydroxyethyltheophylline was the proposed internal standard. However, this analyte co-eluted with a constituent in the candidate green tea SRM sample and hence did not serve as a sufficient internal standard. Other potential internal standards will be evaluated in the future. The measurement of caffeine in the candidate green tea SRMs using the external standard method will be discussed.

Smith College

Development of 3-D Geometries for Respirator Flow Field Modeling

Hillary Sackett

The flow of gases and particulates inside a respirator mask is not well understood, especially in the presence of a leak. A firefighter wears a respirator mask to protect his/her lungs from hazardous atmospheric agents associated with their line of work. Respirators are used where there is an insufficient oxygen supply or in atmospheres with smoke, dust, fumes, or gases. The National Institute for Occupational Safety and Health (NIOSH) approves all respirators, filters, and cartridges for firefighter use. Air purifying respirators (APR) employ filters. APRs cannot be used in oxygen deficient conditions or in an atmosphere immediately dangerous to life or health (IDLH). Atmosphere supplying respirators, such as self-contained breathing apparatus (SCBA) units, provide breathable air from a clean air source. In smoke and fire related contaminated atmospheres a positive pressure SCBA provides the most effective respiratory protection. Several variables interfere with the fit of the mask, including facial hair, dentures, jewelry and eyeglasses. A poorly fit mask may result in a leak. Computational fluid dynamics (CFD) utilizes specialized software that can be used to analyze the flow fields inside the respirator. CFD helps researchers predict and identify exposure levels and determine the most effective place to put a sensor inside the mask.

In our research, a three-dimensional scan of an experimental head form was converted from a point cloud into a set of surfaces using Raindrop Geomagic three-dimensional modeling software. Raindrop Geomagic generates accurate digital models of physical objects into files that can be exported in IGES format for industrial applications including CFD. Using this software the 3D scans of APR and SCBA masks were also converted into surfaces and merged with the head form separately to create an IGES file of the head "wearing" each mask. The surfaces were trimmed and smoothed to define a discrete spatial domain between the head and mask. A mesh was then applied to the spatial domain in CFD-GEOM, dividing the volume between the surfaces into discrete cells. CFD-GEOM is a pre-processor for a commercial mathematical modeling software package, equipped with an extensive set of geometry manipulation and mesh generation capabilities. The physical modeling was performed using CFD-ACE+, multi-physics software that enables simulation of fluid behavior given fluid properties and boundary conditions. CFD-ACE+ applied a suitable algorithm to solve simultaneous differential conservation equations, such as the Navier-Stokes equation of motion. We were most interested in the pressure and velocity inside the mask. After CFD-ACE+ simulated the flow problem through the domain, the results were examined and interpreted utilizing the tools in CFD-VIEW. This software allowed us to visualize pressure and velocity through color mapping, track the flow of a specific particle from inlet to outlet, and create flow vector animation through an entire breath cycle. This research project will continue to explore the fluid dynamics of respirator and head geometries for better understanding of respirator fit and best placement of a sensor inside respirator masks.

Auto-Generation of C-Code to Improve Efficiency of a PDE Solver Written in Python
Katherine Travis

FiPy is an object-oriented partial differential equation solver written in the Center For Theoretical and Computational Materials Science by James Warren, Jon Guyer, and Daniel Wheeler. Written in Python, this powerful and versatile tool is aimed at scientists who would otherwise spend valuable time developing their own case-specific solvers. Much of FiPy code is used to perform large array operations, which are very slow written in pure Python code. C, a lower-level programming language, can perform these operations much faster, depending on the context, possibly up to 16 times as fast. This could allow a user to obtain a result in days rather than weeks, or months rather than years. Using existing tools such as Weave, which allow us to write C code in Python modules, we can step out of Python at the moment when we actually perform these operations. The challenge is converting high-level variables with different dimensions and other specific attributes into simple arrays that C can recognize. In addition, we can now write C code that can be auto-generated for most situations, rather than hand-writing code for each operation and type of array. Preliminary tests of the new inlined code show a great deal of improvement over the old version of FiPy.

State University of New York, Binghamton

Adhesion and Release in Nanoimprint Lithography
Andrew Gardner

The goal of the project this summer was to design and conduct a test for the rapid quantitative analysis of adhesion and release of nanopatterned molds in imprint lithography. The devised test is based on the asymmetric double cantilever beam (ADCB) test, which is used to measure the adhesion between two materials. Additionally, the feasibility of incorporating combinatorial methods into such a test was investigated. The model system utilized was a dimethacrylate resin between two beams, consisting of a glass substrate and silicon mold. After the resin was cured using ultraviolet light a thin wire was inserted between the beams to slowly pry them apart and the resulting crack length was recorded. This information along with the material properties of the silicon and glass allowed for the adhesion energy of the system to be calculated.

Mechanisms of Water-Induced Adhesion Loss
Joshua Goldman

In recent years, the use of polymeric adhesives has increased in structural, technically demanding applications. The driving force for this development is the many advantages that they offer over the more traditional methods of joining such as welding, riveting, mechanical fasteners, etc. However, there are some issues that have limited the wider application of adhesives. The most important of these issues is the lack of knowledge concerning the durability of adhesive joints upon exposure to an adverse environment. The most destructive and most commonly encountered environment for adhesive joints is water. The presence of water in adhesive joints not only affects both the physical and mechanical properties of the bulk adhesive itself, but also the nature of the interface between the adhesive and substrate.

Indeed, it has been widely observed that the loci of failure of un-aged adhesive joints are cohesive in the adhesive layer, but apparent interfacial failures between the adhesive-substrate interfaces are often observed after water attack. It is widely speculated that subsequent accumulation of water at the interface is assumed to be the primary reason for failure of adhesive joints. The objective of this study is, therefore, to establish direct experimental evidence of the fundamental mechanism for water-induced adhesion loss of adhesive joints exposed to humidities. Many adhesive joints undergo a dramatic loss of adhesion once the relative humidity of the environment has exceeded a critical value. Thus, it is aimed to elucidate the mechanism of adhesion loss at the critical relative humidity. This study employs the shaft-loaded blister testing method to ascertain the adhesive fracture energy of the joints as well as attenuated total reflectance Fourier transform infrared spectroscopy to characterize the mechanism of failure of the joints.

How to Pull a Nanowire: Developing Nanomechanical Testing Configurations

David Henann

As modern components and devices scale down to micron and sub-micron sizes, accurate mechanical property measurements of the materials and interfaces in these devices are crucial for their design and for an assessment of their mechanical reliability. Accordingly, we are developing standardized testing configurations and methodologies with wide applicability that can be used for localized mechanical measurements of micro- and nanoscale structures, such as nanowires. A particularly promising test configuration is that of a theta-like geometry loaded vertically in compression in a nanoindenter, thereby subjecting the horizontal ligament, the gauge section, to uniaxial tension. However, the data obtained from such a test characterizes the load-displacement behavior of the entire specimen, including the frame. Therefore, a linear superposition model is developed relating external load with gauge section stress and load-point displacement with gauge section strain. Three-dimensional finite element analysis is used to verify the validity of this model by examining linear elastic gauge sections of varying geometries.

Computer-Controlled Instrumentation for a Silicon Carbide Power Device Long-Term Reliability Test Circuit

Jay Huang

Recently a new semiconductor material, Silicon Carbide (SiC), is used to implement power devices for high voltage high frequency power conversion applications. SiC is a wide bandgap semiconductor material, and power devices that utilize SiC could be used in many applications such as power converters, power distribution/transmission systems, energy storage systems, and ship propulsion systems. SiC based power devices have the promise of much higher efficiency for high voltage combined with high frequency operation. Current research SiC devices are demonstrating higher than 10kV switching operations with 50ns voltage transitions. By comparison, the currently preferred silicon device for high power applications, the IGBT, is capable of only 6.5kV with switching speeds more than an order of magnitude slower.

Although SiC based power devices can provide higher performance, the device stability under long-term application condition is still unclear. In order to facilitate the commercialization of SiC power devices, it's important to test the long-term reliability of the devices. Reliability considerations include single event failure due to exceeding static or dynamic safe operation limits, and long term degradation due to cumulative conduction time and switching events. To establish the long term reliability of high-voltage, high-frequency SiC power devices, a specially designed power converter has been developed to apply long-term switch-mode operation while also recovering the power that is processed by the devices.

The objective of this SURF research project is to develop software tools to control and monitor the long-term reliability power converter test system. The software tools consist of routines that control instruments to implement burst mode operation of the power converter, monitor parameters from the power device under test, and perform data logging. The tools contain routines that monitor the system temperatures, including heat sink temperature and junction temperature of the power devices. In the event that any temperature exceeds a safe value, or any monitored parameter changes, the software tool initiates a system shutdown to prevent damage to the devices. The software tools are also responsible for periodically recording stress time and monitored device characteristics to maintain a history of each device.

A Study of Electrochemical Joining for Micro-Wires
Jordan Peck

An experiment was designed and carried out to test the strength of electrochemically formed joints between micro-scale wires and flat substrates. The final experimental protocol requires an SI traceable calibration of a pre-market Asylum Research NanoIndenter; the spring constant of this indenter is measured with low uncertainty. This indenter was then used as a tensile tester to apply small forces and test the joint strength for homogeneous and non homogenous electrochemical joints formed in-situ between Ni and Pt micro-wires and flat Ni substrates.

State University of New York, Geneseo

Investigation of Source Detection Algorithms for Radiation Portal Monitors
Christopher Wahl

In recent years, heightened security concerns have prompted increased interest in radiation portal monitors, instruments capable of detecting, and in some cases identifying, gamma-ray and neutron emitting radioactive material passing through them. These monitors are currently deployed at important sites around the nation to monitor traffic for radioactive sources. Along with efficient and reliable physical detectors, such monitors need software capable of analyzing the resulting signals in order to effectively catch weak radioactive sources. The software should be able to distinguish between the sometimes subtle signals due to weak sources and the varying background. After investigating several possible source-detection algorithms, a program has been developed to locate signals from weakly radioactive sources in real time. By including corrections for background suppression due to trucks shielding the detector and changing background levels, this program is capable of detecting significantly weaker sources than current software. The limitations of this method will also be discussed.

State University of New York, Stony Brook

An Optical Vortex-Based Azimuthal Lattice for a Bose-Einstein Condensate

Azure Hansen

Many properties of Bose-Einstein condensates, including band structure, momentum distribution, and atomic interactions, have been studied in linear optical lattices produced by the interference of two counter-propagating laser beams. We propose to instead use an azimuthal lattice created by the interference of off-resonance co-propagating Laguerre-Gaussian laser beams of opposite helicity. This new ring-shaped lattice provides a uniform atom density and periodic boundary conditions that approximate an infinite lattice. Varying the rotation rate of the lattice imparts angular momentum to its trapped atoms, the same way that accelerating a linear lattice by chirping one beam's frequency accelerates those atoms.

Laguerre-Gaussian (LG) beams, the optical vortex mode, have a spiral phase distribution and therefore a characteristic region of undefined phase on the axis of the beam where the amplitude is necessarily zero. The interference pattern between two vortex beams of equal and opposite helicity resembles dark and bright beads regularly spaced on a ring. The trapping potential of the lattice comes from the optical dipole force, which depends on the intensity of the light and its detuning from the atomic resonance. We create LG beams using a computer-generated hologram (CGH) implemented in either a static phase grating or a spatial light modulator (SLM). A CGH is the calculated interference pattern between a plane wave and an LG mode. This has a "fork" discontinuity that introduces the vortex singularity when used as a diffraction grating.

The azimuthal lattice is rotated by introducing a phase shift in one of the co-propagating LG beams that create the interferogram. If the LG beams are produced using the SLM, this phase change can easily be programmed into the CGH code. However, in testing this method we found that the maximum rotation rate that could be achieved is too slow for our application. Therefore, we have developed and tested another system that has the desired time response, spatial resolution and stability. Vortices produced by a "fork" phase grating are interfered in a modified Mach-Zehnder interferometer in which a computer-controlled screw tilts a flat glass plate in one arm. Varying the tilt changes the optical path length and rotates the interferogram. This interferometer will soon be incorporated in our sodium BEC apparatus using a 532 nm laser.

Swarthmore College

Monte Carlo Modeling of Magnetic Cobalt Nanoparticles

Michael Gorbach

Ongoing research at NIST involves self-assembly of magnetic, cobalt nanoparticles. These particles form complex structures under the influence of their own magnetic dipole-dipole interactions and any external magnetic field. Properties of the structures formed depend on the size distribution, temperature, magnetic moment and protective surfactant layer. A Monte Carlo model was created for this system to provide theoretical insight underlying current and future experimental work.

University of California, Irvine

Redefining the SI Kilogram and Implementing a Magnetic Levitation Balance

Catherine Phan

The kilogram is the last remaining SI base unit still defined as a material artifact, the International Prototype Kilogram which resides at the International Bureau of Weights and Measures in Paris. The artifact changes at an unpredictable rate which has a consequent effect on other related base units, fundamental constants, and derived units. The artifact kilogram can be replaced with one based on a time invariant of nature by using a mechanical electrical measurement method. In this method, the "moving-coil" Watt Balance compares the mechanical power measured from weighing a kilogram in vacuum to an equivalent electrical power measured using the Josephson and quantum Hall effects. The ratio of mechanical to electrical power equal to unity will be able to link the kilogram to Planck's constant. The redefinition of the kilogram aims to achieve a level of precision on the order of 2×10^{-8} and will allow an exact value of Planck's constant to be used, eliminating or appreciably reducing the uncertainty of many other fundamental constants of physics. For improving the accuracy of the one kilogram mass a high precision balance must calibrate the kilogram in vacuum to the National Standard Kilogram in air with no mechanical link existing between them. A magnetic levitation balance will levitate one of the masses by using magnetic field inducing coils and permanent magnets while an interferometer and position feedback controller will be used to stabilize the levitation.

University of Connecticut

Collagen Matrix Micropatterning Using Localized Heat

Megan Ellis

Adherent cells have been cultured throughout the years on two-dimensional rigid surfaces such as glass and plastics. However, these materials do not resemble the in vivo environment and consequently extrapolation from in vitro to in vivo cell behavior has been constrained in many cases. There has been a growing interest in developing 3D cell cultures in recent years and efforts are underway to characterize and compare cell behavior on extracellular matrix components (in vitro), such as collagen and fibronectin, with cell behavior in vivo. Our research efforts have focused on the development of a device to generate a 3-D collagen pattern using localized heat, to further study cell morphologhy differences and cell motility. A device comprised of indium tin oxide (ITO) on glass was patterned using photolithography. A microfluidic channel composed of polydimethylsiloxane (PDMS) was placed on top of the ITO/glass wafer and collagen solution was flowed through the channel using vacuum. A calculated current was applied to raise the temperature of the device from room temperature (22ºC) to 55 ºC, a determined temperature that collagen undergoes polymerization. Results show the formation of a layer of collagen fibrils on the patterned ITO, in the order of tens of nanometers. Currently, work is in progress to improve the device heating conditions in order to obtain thicker layers of collagen, useful in cell motility assays.

Characterization of Synephrine in Dietary Supplements Containing Bitter Orange
Jose Santana

Dietary supplements containing bitter orange (*Citrus* x *aurantium*, L.) as an integrated component have rapidly replaced Ephedra-based supplements for use as weight-loss products. However, the safety of bitter orange-containing supplements has been questioned because synephrine, a key component of bitter orange, has been associated with adverse cardiovascular events. Synephrine is an adrenergic alkaloid that has thermogenic properties which promote energy enhancement and weight-loss. Synephrine can exist in any one of three different isomeric forms (para-, meta- and ortho-synephrine) depending on the position of the hydroxyl moiety on the benzene ring (Figure 1A, 1B and 1C, respectively). Many reports have been published stating that the only synephrine isoform in bitter orange-containing supplements is the para isoform; however, a recent report claimed the detection of the meta-synephrine isoform (phenylephrine). Phenylephrine is marketed as the popular decongestant "Neosynephrine". There have been no reports documenting the detection of the ortho- synephrine isoform. The para- and meta-synephrine isoforms have distinctly different toxicological, bioavailability and metabolic properties, thus reliable analytical methods are needed to detect and quantify the isoforms. Analytical methods based on the use of liquid chromatography coupled with ultraviolet detection (LC/UV) and liquid chromatography coupled with tandem mass spectrometry (LC/MS/MS) have been developed to determine para- and meta-synephrine in bitter orange-containing dietary supplements. The development and quantitative performance (limit of detection, limit of quantification, etc.) of the methods is compared and described. The utility of the methods is evaluated through the determination of the synephrine level in a suite of commercial dietary supplements. The current research supports NIST's on-going efforts to provide standard reference materials and reference methods in the areas of health and nutrition.

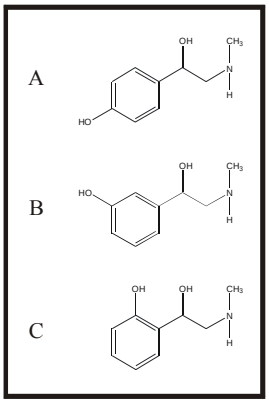


Figure 1.

<u>University of Delaware</u>

Calibration of Radioactive Seeds Used in Brachytherapy
Steven Anton

Brachytherapy is currently a widely used alternative to beam radiation therapy for certain types of cancer, including prostate. Because of the implantation of low-energy x-ray-emitting radioactive "seeds," brachytherapy offers a much more localized dose to cancerous regions, reducing damage to healthy surrounding tissue. NIST maintains and disseminates the standard

for each type of seed approved by the FDA for clinical use. Air kerma strength, the primary calibration quantity, was measured for each seed using the Wide-Angle Free-Air Chamber (WAFAC). X-ray spectrometry was used to characterize the emergent energy spectrum and to quantify angular anisotropy of seed emissions. Radiochromic film was used to show radionuclide placement and internal seed geometry. In many cases data obtained from two different methods were cross-checked to insure validity. In addition, characterization of a novel plastic scintillator dosimeter, which was specifically designed for measurement of dose distributions around low energy photon-emitting brachytherapy sources, was done using the computational Monte Carlo package EGSnrc. X-ray pulse height distributions were calculated for a variety of scintillator configurations and depths in water. The results of simulations using experimentally measured input spectra were compared to consensus dosimetry data sets recommended by the American Association of Physicists in Medicine (AAPM). Preliminary results showed a nearly flat energy response curve for incident photon energies between 15keV and 40keV, the area of interest in low-energy photon brachytherapy.

Contrast Enhancement and Applications of Graphite Superlattice Modeling
Reza Rock

Superlattices are observed occasionally on graphite surfaces when imaged using scanning tunneling microscopy. There is, however, currently no reproducible laboratory method to create these superlattices in a controlled fashion for study. Computer models have been used to simulate these structures using the Moiré interference pattern assumption as the cause for the superlattice, modeling several layers and combining them with the equation $\phi = \sum (-1)^{n-1} W_n \phi_n$, where n is the layer number, W is the layer coefficient and ϕ is the atomic density of each layer. It is difficult to perform quantitative analyses on the output data from these simulations because the corrugation amplitude of the atomic lattice is comparable to that of the superlattice. The goal in this project was to extract useful information from the cross sections of the superlattice model by filtering and averaging. The data is smoothed by averaging within an optimum radius around each data point, and it is then possible to perform analyses on several aspects of the simulated superlattice. The effects of the W coefficients on image contrast and simulated attenuation factor between layers were studied, as well as the impact of changing rotation angle of the topmost layer of graphite on the corrugation of the superlattice. Coexisting superlattices were also simulated using six graphite layers and studied.

University of Florida

Bi_2O_3, Al_2O_3, Nb_2O_5 Equilibrium Phase Diagram
Julian Guzman

Ceramic materials are essential for electronic devices because they exhibit properties such as semiconductivity, superconductivity, high permittivity, ferroelectricity, and piezoelectricity. The Bi-Al-Nb-O study was conducted because of its potential use as a dielectric to fabricate embedded capacitors for improved electrical performance of printed circuit boards.

An equilibrium phase diagram conveys the phases and phase assemblages which are thermodynamically stable at various temperatures, pressures and compositions within a given system. To determine the subsolidus phase relations for the Bi-Al-Nb-O system, various ratios of the components (Bi_2O_3, Al_2O_3, Nb_2O_5) were mixed, pelletized, calcined overnight (700-800°C), and then heated several times in microprocessor-controlled high temperature furnaces at higher temperatures (700-1350°C) to reach equilibrium. Between heatings, samples were ground with an agate mortar and pestle to accelerate the equilibration process by increasing surface area and hence reaction rates. The attainment of equilibrium was presumed when no changes were observed on the weakest peaks of the X-ray powder diffraction pattern. The phase(s) present at each composition and their approximate ratios were determined using the disappearing phase method and X-ray powder diffraction data obtained with a Philips diffractometer equipped with incident Soller slits, a theta-compensating slit and graphite monochromator, and a scintillation detector. Compound formation and the subsolidus phase diagram showing thermodynamic stability relationships will be described.

Characterization and Optimization of Tethered Bilayer Lipid Membranes

Michelle Kinahan

An individual cell communicates with its environment primarily via its plasma membrane. Specifically, protein-membrane interactions govern many aspects of cell behavior. Synthetic membranes are useful for studying such interactions, but due to the highly disordered nature of the lipid membrane it is difficult to create a biomimetic environment that is suitable for a variety of experiments.

Solid supported tethered bilayer lipid membranes (tBLMs) present a solution to this problem. Two such systems utilizing 20-tetradecyloxy-3,6,9,12,15,18,22-heptaoxahexatricontane-1-thiol and silanized tethers were investigated with ellipsometry, electrochemical impedance spectrometry, and fluorescence microscopy. Both were found to support lipid bilayer formation.

Impedance spectrometry and fluorescence microscopy of synthetic phospholipid membranes were conducted to characterize and optimize these tethered systems, with the goal of bringing them closer to their natural counterparts. The structure and stability of membranes composed of 1-palmitoyl-2-oleoyl phosphatidylcholine (POPC), dioleoyl phosphatidylcholine (DOPC) and diphytanoyl phosphatidylcholine (DPhyPC) were considered.

Finally, the effects of cholesterol incorporation in these bilayer systems were examined. Cholesterol presence in natural cell membranes has been shown to induce the formation of lipid "rafts" which are integral in protein sorting. Both impedance and fluorescence results illustrate that cholesterol incorporation does not detrimentally affect synthetic tBLM bilayer formation.

Once optimized, these tBLM systems will offer a synthetic manner to investigate membrane-environment interactions by a much larger range of experimental methods than previously possible. They will be used to test numerous protein associations via neutron reflectometry. One area of research in which they will be utilized involves the role of β-amyloid peptide in the progress of Alzheimer's disease.

University of Maryland, Baltimore

Making Your Life Easier: Advancing Smart and Wireless Transducer Interface Standards
William Miller

Transducer technology has become extremely popular in the last few decades because their usage can improve safety, precision and efficiency in systems, such as manufacturing and automation systems. The usefulness of sensors and actuators in a wide range of technical applications has created a great commercial demand for a solution that is both easy to use and simple to apply. Traditional applications were often technically complex and costly both in terms of time and money. While advances in manufacturing and computer technology have reduced the costs involved in these applications, a better solution is still preferable. The suite of IEEE 1451 transducer interface standards address these issues and provide an efficient solution for virtually any kind of network. The most notable feature of the suite of standards is the inclusion of a Transducer Electronic Data Sheet, which is a memory device included in each transducer. The storage of specifications and functions in this memory allows for a transducer to function as a Plug-and-Play device with self-contained knowledge on what that specific transducer can do and how to do it. Another important aspect of the standard is the idea that any transducer adhering to the 1451 standards can be accessed using a common command interface regardless of its type or how it is physically connected to the network – via a wired or wireless network connection. Some parts of the IEEE 1451 standard are still being developed, however. Our present project involves implementing the 1451.2 and 1451.4 standards in Java and exploring their implementation. Platforms explored include Sun Microsystems' new Sun Spot device and implementation as a web application. The project also explores the creation of a 1451.0 HTTP API to allow for communication over a TCP/IP connection. Once completed, this API will be used to assist in the development of the 1451.5 standard, which implements wireless communication protocols.

The Hall Effect
Scott Shackelford

The Hall effect has become an increasingly important tool in materials science. Its history and significance will be discussed along with an explanation of the Lorentz force which is directly responsible for the Hall effect. The Van der Pauw method for measuring Hall voltage and resistivity of a sample has gained wide acceptance. In addition to its importance characterizing materials, there are potentially an unlimited number of Hall effect device applications, a few of which will be mentioned. The current highly cited NIST website on the Hall effect will be expanded with some of this new information.

University of Maryland, College Park

Implementation of Additional Capabilities of e-Fits Using Java Applet
Guy Cao

e-Fits is an online statistical program used to generate graphs, tables, and random numbers for univariate probability distributions. In addition, it fits user-supplied data to these distributions. e-

Fits is implemented with Perl/CGI scripts and uses DATAPLOT as its computational engine. e-Fits performs distributional modeling without user's having to install or learn a statistical program. The primary feature of the CGI model is that the computations are performed on the server rather than the user's local machine.

The CGI model is useful for the internal website. However, it is not a good model for the external server. We are developing a subset of e-Fits using Java that is intended to be used on the external NIST server. The primary advantage of this approach is the java computations are performed on the user's machine. The disadvantage is that only a limited subset of the full capabilities of e-Fits will be available.

Svetlana Rabinovich, a SURF summer student from 2005, began the implementation of the java program. She implemented the probability plot method of fitting for the location / scale distributions. My part in the project has been to extend the fitting to the case where there is a shape parameter, to add a bootstrap capability for confidence intervals, and to begin implementing maximum likelihood estimation.

Three-Dimensional Imaging of Polymer Scaffold Gradients

Shauna Dorsey

Tissue scaffold research is a multidisciplinary field for bioengineering that involves designing, fabricating, and implanting artificial tissue scaffolds to repair damaged or diseased tissues and organs. A common example is bone tissue engineering. As a result of trauma or disease where extensive amounts of bone tissue are damaged, polymer scaffolds can be used as templates to facilitate bone regeneration. Scaffolds provide the initial support necessary for bone formation as new bone cells adhere to their surface and proliferate. The scaffolds are biodegradable, leaving behind new bone tissue to heal the damaged area.

Since scaffolds made of amorphous polymers such as DTE [poly(desaminotyrosyl-tyrosine ethyl ester carbonate)] or PDLLA [poly(D,L-lactic acid)] are essentially translucent to X-rays, it is not possible to image these materials *in vivo* with X-ray radiography or *in vitro* with X-ray microcomputed tomography. In order to improve the radiopacity of scaffolds made from DTE, we have blended DTE with DTE-I_2, an iodinated analog of DTE which is radiopaque due to covalently linked iodine atoms. The presence of iodine should not interfere with cell growth ensuring that an iodinated scaffold implanted into the body is non-toxic. The iodine allows the polymer scaffold's progress *in vivo* to be conveniently tracked by X-ray radiography as it degrades or develops during bone formation. The iodine also allows *in vitro* analysis of scaffold microstructure by X-ray microcomputed tomography.

Combinatorial methods are valuable for characterizing biomaterials for tissue engineering applications by accelerating research through the efficient collection of large data sets. Thus, we have used a combinatorial method for screening polymeric tissue scaffolds to determine the amount of X-ray contrast agent required to enable imaging of tissue scaffolds by X-ray radiography and X-ray micro-computed tomography. We fabricated salt-leached polymer scaffold gradients with DTE -I_2 at one end and DTE at the other. The DTE/DTE-I_2 gradients

were imaged using X-ray microcomputed tomography and X-ray radiography to determine the percentage of iodine required to enable imaging using X-ray technology. The results demonstrate the feasibility of a novel, combinatorial approach for determining the optimum tissue scaffold composition for imaging by X-ray radiography and X-ray microcomputed tomography.

Light Polarization and Spatial Light Modulation
Dylan Erwin

We show that through the combination of a few simple polarization elements, and two 127 pixel hexagonal array spatial light modulators (SLM's), spatial control over amplitude and linear polarization angle of light transmitted through the system can be achieved. In bright field microscopy, we can use such a device for amplitude and polarization control of the microscope illumination, or as a spatial filter on the collected image, by placing the device at the appropriate conjugate plane. In particular, the use of the device at a conjugate back focal plane in the illumination path grants the experimenter control over the amplitude and polarization of each illumination angle at the sample. We will discuss how different back focal plane configurations can be created from simple polarization matrix computations, the realization of these configurations using a LabView program, and the application of the device to scatterfield microscopy for semiconductor metrology.

Measuring Cognitive Abilities of Artificial Systems
Shima Eshraghi

Products of informatics and Artificial Intelligent (AI) research are ubiquitous in modern life. Research in AI is concerned with producing technologies and machineries to automate tasks requiring intellectual performances.

The Defense Advanced Research Projects Agency (DARPA) is investing in funding research and development of systems that are cognitive. National Institute Standards and Technology (NIST) scientists have been investigating methods of measuring the ability and performance of intelligent systems. In particular, NIST has been developing test metrics and methods that evaluate the performance of embodied intelligent systems, such as mobile robots applied to urban search and rescue tasks. Since the cognitive capabilities of most such systems are still typically limited, we have decided to turn out attention to evaluating the overall system's performance, which takes into account physical features, such as mobility, sensing, and communications, as well as those that may be considered related to cognition, such as mapping the environment and navigating.

Our objective in this research is to investigate whether methods used to obtain "g" or General Intelligence measures for humans could be adapted and applied for artificial systems. To accomplish this subject matter, we are analyzing data from attributes of robots that participate in the RoboCup Rescue competitions. Moreover, factor analysis, which is taken to drive "g" in humans, is used to identify which attributes of a robot could predict its success in robot competitions. Information from the 2005 and 2006 RoboCup Rescue competitions is analyzed to the following categories:

(a) Derive and encode the different attributes that robots may have

(b) Determine if certain attributes were more likely to result in better performance than others.

Measuring DNA Microarray Performance
Jennifer Gehret

DNA microarrays are a tool used to study gene expression levels on thousands of genes simultaneously. Spots of short DNA segments from target genes, known as probes, are immobilized to a substrate which forms the array. Fluorescently tagged mRNA from cells under study, called targets, is then hybridized to the array. Fluorescent signals detected from these hybridized probes are proportional to the amount of regulation of the gene. Currently, there are problems interpreting the microarray results because of difficulty in quantitatively understanding the performance of the measurements in these experiments. Because of differences in designs, there is also difficulty in comparing microarray results from different manufacturers.

An experiment has been designed to validate microarray results by establishing quantitative performance "figures of merit" such as sensitivity, linearity, dynamic range, background levels, repeatability, and noise model for array data. The planned experiment involves a Latin Square design using three groups of control spikes that are added in at various concentrations and a fourth group of spikes that are added in constant concentrations throughout the experiment. The figures of merit obtained by adding spikes to the array in the fashion describe can be tracked across studies to establish confidence in the measurement performance.

A simulation was developed in Excel that generated expected data from the Latin Square experiment. This model was used to develop a useful data analysis strategy which validates the experimental design which is especially important because the experiment will be very costly to run in actuality. The data analyzed verified that the input parameters of noise, background, and probe affinity are detectable in the analysis.

Preliminary work was done to establish the concentration of spikes and validate the place in the target preparation protocol where the DNA spikes will be added. The reaction efficiencies were measured and the expected range of gene concentration was determined at the spike in point. This allows the concentration range of the spikes to be determined to accurately simulate a range of actual gene concentrations.

Validation of Stereoscopic PIV for Large-Scale Fire Induced Flow Measurements
Jeff Keslin

Experimental methods to measure the ventilation or exchange of air induced by a fire within a room have relied on physical probes such as thermocouples and modified pitot pressure probes. These measurements have served as a benchmark for validation of computational fire models. Current advances in flow measurement technology allow us to improve computational fire models. Particle Image Velocimetry (PIV) is an advanced flow measurement technique that is

non-intrusive and capable of measuring large planar fields. Stereoscopic PIV can be applied to measure all three components of the velocity vector. With seeded particles in a flow illuminated by a double-pulsed laser, CCD cameras capture the displacement of the particles and velocity measurements can be made through a planar cross-section of a doorway or vent. Here we have looked to validate the use of Stereoscopic PIV as a means of accurately measuring fire induced flows on a large scale. The effects of seed particle size and density have been examined using stereoscopic PIV experiments. Using a simulated particle map it was determined that for displacements on the order of 1 mm, measured results agreed to within 3 %. It was also confirmed that very high and very low density particle images have a compromising effect on the accuracy of the data.

Trace Detection of Illicit Narcotics Utilizing Ion Mobility Spectrometry

Rhyan Maditz

Current national priorities in homeland security have led to a unique level of utilization of trace explosive detection systems for counter terrorism and law enforcement. Ion Mobility Spectrometry (IMS) is a trace explosives detection method that has become increasingly popular after the 9/11 tragedy. People who handle explosives are likely to leave residues on surfaces that they touch or have residues on their clothes, and these residues contain trace particles of explosive that can be sampled by the IMS system. An IMS detector measures the mobility of charged molecules and compares this to a reference library of known explosives. Until recently, airports and law enforcement were able to focus on detection of negatively changed ions specifically related to most explosives. Now, the recent London train bombings suggest a growing threat from peroxide based explosives. In contrast to most explosives, peroxides are most sensitively detected as positive ions. Therefore, there is currently a high demand for a new generation of IMS instruments that operate in dual-mode to detect trace amount of both positively and negatively charged molecules. Interestingly enough, narcotics are also positively charged and are detectable in dual-mode IMS instruments. While detection of illicit narcotics have not been a top priority for the Department of Homeland Security in the past, this capability may be of particular interest to U.S. Customs and Boarder Patrol, the Drug Enforcement Agency, FBI, US Coast Guard and State and Local Law Enforcement.

This presentation will highlight the ways in which NIST is striving to optimize different types of IMS instruments by testing background levels of contamination, determining the cause of false positives and negatives, and establishing the detection limits for narcotics such as cocaine, heroin, THC, methamphetamine and flunitrazepam. We have studied sampling issues including optimal swiping methods that increase sensitivity and reducing environmental background signatures. Potential false positives are a considerable concern and we have developed a database of false alarms and interferences resulting from a wide variety of over-the-counter medications such as Claritin, Advil, and Tylenol. From these experiments, we hope to determine the metrology issues that are associated with trace narcotics screening while also helping manufacturers of future IMS instruments to optimize and calibrate their systems to provide the highest sensitivity with the lowest false alarm rate.

A User Interface to a Distributed Computing Environment

Christine McKay

Distributed computing is a very general term which refers to the use of a set of networked computers to solve a problem. Our specific focus is on a Distributed Computing Environment (DCE) which supports compute intensive scientific applications. To be appropriate for our DCE, an application must be implemented such that it can be split up into many smaller independent tasks so that they can be distributed over the computers in the network. The results of the individual tasks are then combined to form the complete solution. The runtime of such applications can be greatly reduced in this way.

Screen Saver Science (SSS) is a DCE developed by Dr. William George at NIST. It is designed to run tasks on the machines in a network when they go idle. Java, Jini, and JavaSpaces technology was used to create SSS, which facilitates interaction between clients, workers, and the JavaSpace. A central server hosts the JavaSpace, which acts as shared memory for coordinating the components of the DCE. Clients submit tasks to SSS, writing them to the SSS JavaSpace, then worker computers take and execute these tasks, sending back the results. All applications are written in Java so that any machine that can run a Java program can participate in the SSS DCE.

This summer, several important supporting features have been added to the SSS system. A method of assigning a unique set of parameters to each individual task, before submitting it to SSS, was implemented. Another feature dynamically regulates the number of tasks present in the SSS JavaSpace at any one time, with high- and low-water marks. Also, in order to run SSS on the ITL/PL cluster "raritan", it was necessary to develop a practical way for clients to submit applications to SSS. The talk will discuss SSS and the implementation of these features.

Software Assurance Metrics and Tool Evaluation to Enhance Software Security

Jeffrey Meister

In the pursuit of software security, organizations such as the Department of Homeland Security often employ automated assurance tools developed by industry. The goal of NIST's Software Assurance Metrics and Tool Evaluation (SAMATE) project is to develop specifications for these tools, test them and measure their conformance, and use this information to identify gaps in their performance and advance the state of the art in software quality assurance. The SAMATE Reference Dataset (SRD) is a growing database of test cases with known vulnerabilities designed to facilitate this tool evaluation.

The current main focus of the SAMATE team is on static code analyzers—tools which examine software at compile-time. Work is in progress on a standard for static analyzers that will reference a subset of test cases from the SRD. I populated the SRD with over 130 new candidate test cases and assisted in testing a new, more functional SRD interface. I also attended and helped organize the NIST Static Analysis Summit and heard presentations from tool developers and other interested parties in government and academia. Additionally, I worked on the development of scripts to automate the process of using SRD test cases to evaluate popular tools.

These scripts should make it easy for end-users to check the effectiveness of their software assurance tools even if they are not familiar with the tools' intricacies.

On the frontier of the SAMATE project is preliminary work on Web application vulnerability scanners. These tools perform penetration testing on Web applications to identify the unique flaws associated with this type of software, including cross-site scripting and SQL injection. As Web applications become more ubiquitous, especially in secure situations such as online banking and credit card payment processing, it is vital that vulnerability scanners perform as advertised. I researched the current status of these tools in order to clearly define their scope and develop a list of critical security flaws that they should identify, contributing toward an eventual specification.

Solution Processed Small Molecule Thin Film Transistors
James Royer

The demand for the development of low cost electronics has provided significant motivation for research in organic semiconductors. In this study we report on the electrical characteristics of organic thin film transistors (OTFTs) fabricated using halogen substituted Triethylsilylethynyl Anthradithiophene (TES-ADT) and Triisopropylsilylethynyl Anthradithiophene (TIPS-ADT) as the semiconductor layers. Thin organic films are formed from solution by spin casting or drop casting, and annealed in solvent vapor to improve molecular order and charge transport. The extrinsic field-effect mobility for solvent cast thin films of fluorinated TES- and TIPS-ADT and brominated TES-ADT are compared for devices fabricated on heavily doped oxidized silicon substrates with pre-patterned gold source and drain contacts and substrates where the silicon dioxide gate dielectric surface is functionalized with the self assembled monolayer hexamethyldisilizane (HMDS) in an effort to passivate chemically/electrically active traps at the oxide interface. To reduce parasitic contact effects and improve the extrinsic device performance we functionalized the gold source and drain contacts on selected substrates with pentafluorobenzenethiol (a strong electron withdrawing agent which forms a self assembled monolayer on gold). These combined surface treatments illustrate the importance of interface engineering for improving the performance of organic devices for low cost electronic applications.

Examining Sensor Location Algorithms from a Different Angle
John Shiu

With the current cost of wireless sensors dropping in recent years, wireless ad hoc sensor networks have become increasingly practical and in-demand. Several different applications for sensor networks have been envisioned over a wide range of fields, from military intelligence and surveillance abroad to traffic and transportation analyses at home.

One key element in deploying ad hoc sensor networks is the ability for each node in the network to identify its location. Previous investigations into sensor location algorithms have relied on signal strength data to approximate the ranges between different nodes in sensor networks. These range estimates, which are inherently susceptible to signal noise, are then analyzed by a linear program using triangle inequality constraints. Essentially, the triangle inequality constraints exploit the geometric property of triangles which states that the sum of the lengths of

any two sides of a triangle must be greater than the length of the remaining side. By applying these constraints to each triangle formed in the network, the linear program is able to add or subtract corrective residuals to the original range estimates. This allows for better range estimates that are less affected by noise and ultimately results in more accurate estimations for each node's location.

In a similar fashion to the range-based sensor location algorithm, our current project also depends on triangle constraints in a linear program to adjust for noise in measurements. However, instead of utilizing range estimates between nodes, we use angle estimates instead. Our method takes advantage of the geometric property specifying that the sum of the internal angles in each triangle must equal 180 degrees. As in the range-based algorithm, the use of triangle properties allows us to minimize the effect of noise on the accuracy of our location estimates. Our project focuses on the implementation of such an algorithm and investigates the benefits and drawbacks of using angle-based estimates versus range-based estimates for locating sensors in a network.

Assaying Peptide Gradients with Epifluorescence Microscopy

Joseph Sit

Biomaterials scientists can tailor the biological response and biocompatibility of materials used in many biomedical applications (implants, prosthetics, sensors, catheters, etc.) by modifying their surface chemistry. One way to introduce biological functionality into synthetic materials is to covalently bind peptides to the surface of materials. These peptides, which are short segments of proteins, bind to specific receptors on the surfaces of cells to provide cells with some biochemical signal that can control phenomena such as cell adhesion, proliferation, and migration. One powerful method for investigating the effects of these peptide modified surfaces is through the preparation of peptide gradients, which present a range of different molar concentrations across the surfaces. We can use such gradient surfaces to examine cellular responses to many different peptide concentrations in a single experiment; the cell response to the gradient itself can also be evaluated. One key challenge is assaying surface peptide gradients to obtain accurate measurements of the surface molar peptide concentration. Previous studies have been done using a single fluorophore as an analog for the peptide and relating the concentration to the fluorescence intensity obtained from epifluorescence microscopy. In the current study, this technique is being improved by using a second fluorophore with different excitation and emission spectra from the first. The addition of the second fluorphore as a uniform background on same surfaces that contain a gradient in the first fluorophore, provides an internal correction for optical imperfections that otherwise add noise to the intensity data. This two-fluorophore extension of the epifluorescence technique will improve the accuracy of our measurements of surface peptide concentrations. Details of the preparation of the gradient surfaces and the epifluorescence microscopy will be discussed. Results from the single-fluorophore and two-fluorophore techniques will be compared.

Positive Pressure Ventilation
Ryan Travers

Positive pressure ventilation by wikipedia encyclopedia is defined as a method that consists in creating an air flow ("wind") by raising the pressure in a part of a device or building. This is a generalized statement of what is positive pressure ventilation. When a fire occurs in a structure smoke is generated which consists of many toxic gases. Therefore, in order to make the structure safe for firefighters and workers to enter these gases need to be removed.

One common method is based on Positive Pressure ventilation that consists of using fans to force air into a structure and pressure the building. For example with a typical one story house you will open one window in the rear of the house and set a fan at the front door and force air into the house. Doing this the fan pressurizes the house and with the one window open this allows all the gases and smoke to be forced out the one window. Having more than one window open at a time while doing this reduces the effect of the fan as the pressures are reduced throughout the house. In this study we made experiments in high-rise buildings. In Toledo, Ohio experiments were conducted on a 30-story high-rise office building. Data were collected to determine how effective the positive pressure fans really are. in this study, the positive pressure ventilation method was found to be effective even in a 30-story high-rise building. These tests are crucial to the fire service as it is not often that full-scale tests are possible in a massive building. Present at the test site were members from the New York, Chicago, and Toledo Fire Departments. Using the results from our study, these fire departments are now planning on changing standard operating procedures to implement positive pressure ventilation more often.

Large Eddy Simulation of Partially-Premixed Combustion Following Ignition of a Fuel Vapor Cloud
Jennifer Wiley

The objective of this study is to examine the feasibility of a Large Eddy Simulation (LES) approach combined with a partially-premixed combustion (PPC) model for simulations of transient combustion events in fuel vapor clouds. The PPC formulation uses: a premixed combustion sub-model based on the filtered reaction progress variable approach; a non-premixed combustion sub-model based on an equilibrium-chemistry, mixture-fraction-based approach; and a premixed/non-premixed combustion coupling interface based on the concept of a LES-resolved flame index. The PPC model is implemented into the Fire Dynamics Simulator developed by the National Institute of Standards and Technology, USA. A series of benchmark simulations were performed to characterize known difficulties in the PPC model, and modifications to the algorithm were undertaken to address these difficulties.

Converting Young's Modulus MATLAB Programs to Web-Based Data Analysis Sheets
Victoria Yan

Young's modulus is a material parameter that has been eluding the MEMS community for many years. Standardization of this parameter is necessary to bring the community into consensus as to how it should be measured in order to compare results. A Young's modulus test method as

determined from the resonant frequency of cantilevers is currently being developed in SEMI's MEMS Materials Characterization Task Force. This test method is expected to attract a wide audience from NEMS/MEMS researchers interested in systematic characterization methods of resonating cantilevers for physical, chemical, and biological sensor applications to IC manufacturers interested in improving the yield in a CMOS fabrication process.

Two MATLAB programs have been written to calculate Young's modulus using resonant frequencies and layer thicknesses of cantilevers. One program obtains the Young's modulus value for a single-layered cantilever. The other program obtains the Young's modulus values of the various layers in 16 independently designed CMOS cantilevers. The cantilevers are comprised of the various combinations of interconnect and oxide layers.

This summer, these two MATLAB programs were converted into user-friendly web-based programs.

The conversion of the first MATLAB program to a Java/Html format was straight-forward and the experience was used as a stepping stone for the conversion of the second MATLAB program. The conversion of this second MATLAB program involved calling MATLAB functions from an external Java program in order to perform complex computations. The resulting data analysis sheets will be incorporated on the Semiconductor Electronics Division Web site (http://www.eeel.nist.gov/812/test-structures/MEMSCalculator.htm). They will be used as a guide, or template, for the development of any future Young's modulus data analysis sheets that will be required as the focus in the standard test method is refined.

Developing a Computer Forensics Tool to Output a Windows Registry Dataset to an XML-Based Format

Benjamin Zoller

Computer forensics investigators need the ability to analyze digital media as well as identify and gather electronic evidence. The National Software Reference Library collects commercially-available software and incorporates file profiles computed from the software into a reference dataset. It helps alleviate much of the effort involved in determining which files are important as evidence on computers or file systems that have been seized as part of criminal investigations.

In pursuit of the same goal, additional information could be gathered by constructing a reference dataset from the Windows registry. The Windows registry is a database that stores settings and options for Windows operating systems. It contains information about the software/hardware configuration, user preferences, and user activity that is of interest to forensic investigators. By capturing a snapshot of the registry and checking it against known registry entries, investigators would easily be able to identify and gather evidence from the registry left by malicious applications and by suspicious user activities. They would also be able to identify and ignore known benign registry entries.

This project focused on developing a program in C++ to access the registry directly using the Windows API. The program can traverse the entire registry and then output it in an XML-based format. This information could be combined with metadata about forensically interesting registry

entries. With this data, computer forensics investigators would be able to use publicly available tools to process and view the XML to find critical evidence more quickly and efficiently.

University of Minnesota

The Fate of Nanomaterials in Water Treatment
Cresten Mansfeldt

The popularity of nanomaterials such as carbon nanotubes and quantum dots spreads through a wide range of industries and usages. The applicability and complexity of nanotechnology, the construction of particles and systems on the nano scale, grows with greater demands in the electronic, cosmetic, and other industries. However, certain nanomaterials raise concerns about the possible carcinogenic threat to humans and the endangerment of wildlife health. Currently, limited research exists documenting the behavior of nanomaterials in the environment. Therefore, nanomaterial pollution may affect the natural reservoirs from which local municipalities withdraw drinking water. In response, the current water treatment methods must adequately remove nanomaterials to ensure the safe distribution of drinking water.

The size of the nanoparticles limits the effectiveness of filtration, therefore the current investigation centers around an important unit process used in drinking water treatment facilities: coagulation and flocculation. Coagulation/flocculation refers to the process of adding a coagulant to the untreated water in order to change the chemical and physical properties of the stable suspended particles. The chemicals selected promote the formation of large aggregates by neutralizing the surface charge of the particle, creating an enmeshment, developing inter-particle bridging, or compressing the electrostatic double layer surrounding the particle. These large aggregates thus are able to obey Stokes Law and settle out of the treated water.

To examine the current treatment process, experimental jar tests simulate the coagulation/flocculation unit operations present in a full scale water treatment facility. The two most popular forms of coagulant, aluminum sulfate (alum) and ferric chloride, are utilized in this investigation. The untreated, synthetic water composed of kaolin, natural organic matter, and alkalinity is dosed with carbon nanotube concentrations in order to display the nanomaterial removal efficiency. The removal efficiency of the current treatment process is quantified using UV/VIS Absorbance measurements and qualified by microscopic imaging using an Optical Light Microscope and an Environmental Scanning Electron Microscope (ESEM).

The existing treatment methods appear to be highly efficient. Carbon nanotubes associate with the dissolved clay in the untreated water creating visible particles. This association allows the carbon nanotubes to settle out of the water when treated with alum or ferric chloride.

Testing Long Term Calibration Stability of Flow Meters
James Tabat

NIST is pursuing development of a high rate hydrocarbon liquid primary flow standard by piping an array of flow meters in parallel. In order for the standard to be a practical calibration tool, the component flow meters must be able to demonstrate long term reproducibility. The objective of

my research is to compare several types of flow meters to determine which would be the best option to construct the new standard. The two types that I studied were dual turbine volumetric flow meters and Coriolis mass flow meters. Both of these flow meters operate using an oscillatory mechanism and emit square wave pulses that increase in frequency as liquid passes through at higher rates. The meter factor, or number of pulses per mass or volume of liquid passed can then be calculated. In order to evaluate reproducibility, meter factors are determined across a range of flows. To take into account slight variations in testing conditions, calculated meter factors are adjusted to specific Reynolds number values. These adjusted meter factors are then compared on a day-to-day basis to determine vertical shifts in calibration curves. Analysis of the data shows around a 0.34% and 0.38% maximum change in meter factor for any specific flow for the dual turbine and Coriolis mass flow meters, respectively. Some data suggests a relationship between liquid temperature and variation in meter output.

University of Mississippi

Electrostatic Sensing of DNA Using Field Effect Transistors
Tatsiana Aranchuk

DNA, a nucleic acid, usually in the form of a double helix, is known for separating ("melting") into two single strands with the increase of temperature. Since most biological processes involve charge transfer, electrostatic sensing of DNA melting is possible with FETs, ubiquitous switches of microelectronics industry, which can serve as excellent primary transducers.

My project involves building a measurement system to integrate the FET, fluid cell, electrical shielding with low noise and leakage, with temperatures ranging from 10°C to 50°C. The project's ultimate goal is electrostatic sensing of the DNA melting point. The talk will give an overview of the project, as well as discuss the specifics of the built enclosure, including noise and leakage current characteristics, electrostatic shielding and temperature controlling schemes.

University of Nebraska, Lincoln

High Contrast Images Made Possible by Adjustment of Illumination In the Visible and Near-Infrared Light Regions
Daniel Williams

Normally, in order to see an object, light from an outside source must be reflecting off of the object's surface into the observer's eye. Its appearance depends on the spectral distribution, or color, of the incident light and on the reflective, scattering, and absorptive properties of the object. For example, a piece of paper that appears white under a normal fluorescent ceiling light will look red if illuminated by a red light source such as that found in a photographer's dark room. Sometimes, two unique materials that look very similar under one illumination may look very different under another illumination. This increase in contrast is helpful in discriminating among different materials, which can be valuable information to have in many fields. For instance, medicine could greatly benefit from research in the area of illumination. Appropriate lighting and detection devices can aid medical personnel in many tasks from the simple administration of an IV to the determination of tissue health in a transplant organ.

This talk will focus on the science behind illumination and color, modeling what objects will look like under different light sources, and some possible applications of this science.

University of Nevada, Reno

Comparison of Density Instruments for Use in Commodity Package Testing
Danielle Ramos

For commodity packaging enforcement, the Weights and Measures Division currently require the density of products to be tested using gravimetric methods and calculating the volume contained using the acquired results. Density is the measure of mass per unit volume of a material. Research is focused on finding an alternative method for field workers to measure product density by comparing current gravimetric methods to electronic densitometers. A sample of various liquid compositions and densities from the same products that the Weights and Measures officials use were tested for repeatability assessment. Various restrictive factors that affect the quality of the density measurement will be described as part of this research. An assessment of the measurement results, proposed changes to NIST Handbook 133, identification of limiting factors, measurement issues, and general instructions to minimize potential damage to field devices will be incorporated.

University of North Carolina, Charlotte

Determining the Location of the Hip Joint Center:
Investigation of Algorithms and Factors for Location
Jereme Gilbert

Computer Assisted Orthopedic Surgery (CAOS) technologies have improved the overall postoperative results for total hip arthroplasty (THA). CAOS systems allow for greater precision and accuracy over manual techniques, by increasing the amount and quality of the information available to the surgical team. Accurate and precise location of the hip joint center (HJC) is a significant step in achieving improved postoperative results. Prior to CAOS systems, the HJC was located using anatomical landmarks. With CAOS systems, the HJC is found using optical and electromagnetic tracking systems. The quality of the model provided by the CAOS system is dependent upon the calibration of the system, therefore a calibration artifact, for preoperative calibration, is being designed. Evaluating the ability of the CAOS system to determine the hip joint center (HJC) is a vital task of the artifact. The purpose of this investigation is to assess the performance of various sphere-fitting algorithms, to be used with the artifact, for locating the HJC. Data was taken using a laser tracker interferometer and a magnetic ball bar test apparatus with a know center of rotation. This setup emulates the function of the artifact. Data was collected within a range of motion appropriate for THA candidates. Analysis will determine the factors, amount of data points and movement pattern, for optimal HJC location using the artifact.

Micromanipulation Technology

Lauren Maldonado

Manipulation and assembly of micro-scale components is necessary for the development of future technologies, including, but not limited to, microelectromechanical systems (MEMS), and the integration of nano-scale components into larger systems. Micromanipulation involves repeatable manipulation of micro-scale particles using a precision tool or mechanism, enabling the fabrication of hybrid micro-scale structures and devices. The technique used here utilizes a single sharp probe made of tungsten for the manipulation tool, combined with a high-precision XYZ positioning system. The probe and positioning system are used to push individual microspheres into specific locations and form multi-sphere configurations within two-dimensional space. The microsphere sample sits on top of a manual XYZ positioning stage. Two zoom microscopes along with digital cameras provide a top view and side view. Cameras are fed into a computer to receive video rate visual feedback. The precise motion of the probe is controlled with a joystick, which provides telemanipulation capabilities. Two different manipulation techniques are currently being implemented, pushing the microsphere using the side of the probe, and pushing the microsphere using the tip of the probe. Both of these methods have distinct advantages and disadvantages that are being weighed. The long term objective for this project is the establishment of a robust micromanufacturing process for hybrid microstructures composed of polymer microspheres that have been bonded using thermal processing. If successful, this method could be extended to stacking components in three dimensions, which would be particularly useful for the fabrication of micro-optical systems.

Physics Based Modeling of Machining

David Willoughby

During machining operations, the physical properties of both the tool and workpiece change due to thermal and mechanical effects. The affect that these changing properties have on the machining operation must be accounted for to optimize machining through accurate simulations. The Kolsky bar apparatus was utilized to measure flow stress versus strain for steel 1045 samples at strain rates, heating rates, and temperatures comparable to the conditions encounter during machining. High-speed infrared video of the sample, together with knowledge of the sample emissivity, can be used to measure the sample temperature. The same infrared video can also be used to measure temperatures during orthogonal cutting, which can then be compared to finite element modeling predictions based on the material data gathered from the Kolsky apparatus.

Several tests were performed on the Kolsky bar, both at room temperature and with heating. Three-dimensional CAD models and drawings of the Kolsky bar components were developed, so that replacement and scaled components may be produced. A sapphire-window lens protector was designed and constructed to mount and focus a series of infrared LEDs onto the thermal camera to determine the reflectivity of test samples in order to derive the necessary emissivity. Test discs and a mounting piece for orthogonal cutting operations were designed and implemented, which will allow direct comparisons between finite element models and real world machining operations.

University of Oregon

Self-Assembly of Fluorinated Surfactants in Ionic Liquids

Yevgeniya Turov

Volatile organic compounds have long been used as solvents for chemical reactions, but they pose an environmental hazard as they contribute greatly to air pollution. Recently, room temperature ionic liquids (organic salts that are liquids under ambient conditions) have been investigated as "green" alternatives because they typically have incredibly low vapor pressures. Due to the ease with which the cation and anion pairs can be changed, ionic liquids have a wide range of chemical properties that allow them to be useful in myriad reactions, even exhibiting selectivity and catalytic ability in certain instances. The solvent abilities of these room temperature ionic liquids have not yet been extensively investigated, so several important characteristics such as whether they exhibit hydrogen bonding and how they interact with solutes compared to water or other organic solvents is not known. Surfactants are an interesting solute used to study the solvent abilities of ionic liquids because they behave differently depending on concentration and form a range of structures that can be examined using microscopy or neutron scattering.

Surfactants consist of a hydrophilic head portion and a hydrophobic tail portion, so they typically form micelles in polar solvents so that the hydrophobic tails aggregate away from the bulk solvent. There is a variety of self-assembly structures, including spherical micelles, cylindrical micelles, and surfactant bilayers. Oftentimes, surfactants also exhibit phase behavior and form liquid crystal phases with long-range order; the most common of these phases are the lamellar, hexagonal, and cubic phases. These phases can then be examined using polarizing microscopy and show a range of fan- and finger-like structures, ladder structures, and even Maltese crosses.

A novel ionic liquid, n-ethylmethylammonium trifluoroacetate (EMATF), was synthesized by a proton transfer reaction between a strong organic acid and strong base. The ionic liquid was characterized using Fourier transform infrared spectroscopy and also proton nuclear magnetic resonance spectroscopy. The self-assembly structures of several fluorinated surfactants (Zonyl FSN-100, Zonyl FSO-100, and Zonyl FSP) and one hydrogenated surfactant (didoceyldimethylammonium bromide) were investigated using polarizing microscopy and small angle neutron scattering (SANS), which is useful for examining microstructures in the nanometer size scale. A range of concentrations of all of these surfactants was utilized to see at what point the surfactants began to self-assemble. Promising SANS data seems to indicate that aggregates form at high concentrations (greater than 20%) of the surfactants in EMATF. In addition, it has been found that the hydrogenated surfactants behave differently from the fluorinated surfactants, indicating that the composition of the ionic liquid affects how it interacts with a solute.

University of Pennsylvania

Application of Thin-Film NiSi Kinetics to Nanocalorimetry of NiSi

Edward Nie

Semiconductor devices continue to become smaller and smaller, including computers, PDA's and cell phones. As they shrink, the chips that run these devices have to become more complex, and hence Moore's Law. The law predicts that the transistor density of semiconductor chips would double every 18 months, and so far it has held true. This means the transistors have had to have become smaller and smaller. However, as they have become smaller, the thinning silica (SiO_2) dielectric used in the gate stack begins to leak current, which compromises the effectiveness of the transistor. Therefore, new materials are being developed to replace the silica, such as Hafnium Oxide (HfO_2). The application of nanodifferential scanning calorimetry will be to use combinatorial studies to examine the interfacial reactions of these new dielectrics with Si. However, before that can happen, the nanocalorimetry process is very new, so it must be developed and refined because there is no experimental database on the subject. NiSi has been chosen to be the test material to be experimented with in the nanocalorimeter. The kinetics of NiSi must first be studied in order to create a model to extrapolate from when interpreting the nanocalorimetric data. For this project, NiSi films of 100nm thickness are deposited by E-beam deposition onto Si (100) wafers, which are then cleaved into 15mm squares. Using rapid thermal annealing and x-ray diffraction, the phase compositions of these squares are examined at various temperatures. The integrals of the x-ray peaks are plotted and used to create a basic model of the kinetics of reaction between Ni and Si. Of course, the kinetics is important in understanding the reaction rates as the samples undergo processing. As the nanocalorimetric process is being refined through testing, the hope is to use it in the near future to examine the interfacial relationships of other compounds with silicon on a nanoscale.

University of Puerto Rico, Mayaguez

The Effectiveness of Combinatorial Methodology on the Exploration of TaAlN Metal Gate Electrodes on HfO_2

Coral Cruz

The use of polycrystalline silicon (poly-Si) for the metal gate of traditional CMOS (Complement Metal Oxide Semiconductor) devices has encountered some severe limits (poly-Si depletion and Boron dopants diffusion) with the continuously aggressive scaling driven by the Moore's law. Metal gates offer an advantage over poly-Si due to their intrinsically higher conductivity. However, elemental metal gates, even with appropriate band structure, may suffer adhesion and thermal stability problems. Alloy metal gates might be a better solution, since one can tailor the desirable properties. However, exploring metal gate electrode alloys is not trivial, since fabrication based on a one-composition-at-a-time approach is too time consuming to investigate even one of the many possible alloy systems. Combinatorial methodology offers a viable approach, since it incorporates high throughput and rapid characterization in parallel, and a large number of samples may be characterized. The goal of this research is to demonstrate the efficiency of combinatorial techniques to enable rapid exploration of the electrical and physical properties of the combinatorial metal gate electrode system on HfO_2, through the deposition of a

combinatorial TaAlN composition spread "library". Wavelength Dispersive Spectroscopy (WDS) characterization showed a wide composition range, and scanning x-ray micro diffraction showed polycrystalline of TaN and amorphous or nanocrystalline structure of AlN. Flat band voltage shifts (ΔV_{fb}) and leakage current density (J_L) were measured to offer a basis for understanding the gate stack properties on the TaAlN/HfO_2 capacitors.

Electrical and Chemical Characterization of Multi-Walled Carbon Nanotubes Coated in Streptavidin

Jose Garcia

Carbon nanotubes (CNT's) have sparked much excitement in recent years ever since their discovery in 1991 by Sumio Iijima; with much research being dedicated to their understanding. These macro-molecules of carbon are not only light and flexible, but are also extremely strong with some CNT's having to been found to be up to one hundred times as strong as steel. As part of this investigation multi-walled carbon nanotubes were grown using a method known as chemical vapor deposition (CVD). CVD is a process in which a substrate prepared with a layer of metal catalyst particles is heated to temperatures well above 700º C in a tube furnace while a blend of a gases, a process gas and a carbon containing gas, are passed over it. These MWNT's were then coated in Steptavidin, a tetrameric protein in order to be able to study differences between coated and bare MWNT's in electrical resistance and heat transfer to surrounding liquids. Currently, our laboratory is in the process of conducting these experiments as well as characterizing these MWNT's coated in Streptavidin through the use of SEM, TEM, and XPS imagery.

Radiolabeling of p-SCN-Bn-DOTA with Po-210 for Applications in Angiogenesis-Targeted Radioimmunotherapy: HPLC Method Development

Michael Santiago

Research in the development of new radiopharmaceuticals for use in the treatment of certain types of cancer continues to increase. Most of the effort has focused on techniques that employ beta-emitting radionuclides (e.g., ^{90}Y) for delivery of cytotoxic dose. However, recent investigations into the use of alpha emitters for targeted radioimmunotherapy indicate that alpha-emitters may be advantageous in localizing therapeutic dose, while minimizing damage to healthy tissue. The higher degree of specific localization is a result of the high linear energy transfer, which is characteristic of the massive, high energy alpha particle emissions (when compared to beta particle emission). This characteristic minimizes the destruction of healthy cells while maximizing the cytotoxic dose to the pathogenic tissue. One promising candidate for targeted therapy using alpha radiation is ^{210}Po. Properties of ^{210}Po that are considered advantageous include: (1) a relatively long half-life (138 days, which allows more time for delivery to patient); (2) a simple decay scheme (it virtually decays 100% through alpha decay to a stable daughter nucleus); (3) promising metallic characteristics that should allow for stable in-vivo complexes for target delivery; and (4) it is available in a highly pure form at a reasonable cost.

The focus of this project is the development of a high performance liquid chromatography approach for assessment of radiolabeling yields of 210Po with chelator 1,4,7,10-tetraaza-4,7,10-

tris(carboxymethyl)-1-cyclododecylacetyl (DOTA). My experiments were designed to investigate the elution behavior of p-SCN-Bn-DOTA that results from systematic changes to the isocratic mixture of two solutions (.1%TFA diluted in deionized water and .1% TFA diluted in acetonitrile). Once the elution time is well understood, a solution of p-SCN-Bn-DOTA mixed with Po-210 under variable conditions is injected into the column under identical conditions. If the Po-DOTA complex has not been achieved, ^{210}Po elutes rapidly, not being retained by the column. If the DOTA complex is labeled with Po-210, it is expected the elution time of the DOTA will be the same as the elution time of the polonium, as detected by their respective detectors. Most of our parameters in the HPLC tests were taken from our collaborators in the University of Maryland.

This investigation lays the groundwork for the future stability and kinetic studies of the radiolabeled Po-DOTA complexes with a targeting mechanism specifically designed for combating angiogenesis of cancerous tumors. By targeting and minimizing angiogenesis in tumors their development can be halted noticeably, since tumors need new blood vessels to grow and metastasize.

University of Couthern California, Los Angeles

Rubidium Tools: Atomic Beam Production and Quantum State Manipulation

Alexandra Schnieders

Laser cooling is a technique that uses light to change the kinetic properties of atoms and to cool atoms to temperatures on the order of ten μK. These laser-cooled atoms are then magnetically trapped and further evaporatively cooled. At about 100 nK, the ultra-cold atoms undergo Bose-Einstein condensation; such Bose-Einstein condensates (BECs) are intriguing because quantum properties can be observed on a macroscopic scale.

To study these properties, we are interested in developing an improved rubidium oven that will produce a collimated atomic beam to facilitate efficient cooling and trapping. In the new design, the atoms pass through a 1 mm thick glass capillary array (GCA) with an aspect ratio of 40:1; rubidium atoms then exit as a collimated beam. In previous designs, the GCA decomposed into a black tacky substance as temperatures neared the expected operating values (140°C for ^{87}Rb and 200°C for the GCA). We suspect that the highly reactive rubidium atoms are chemically reacting with the volatile compounds that permeate the glass. Further testing will establish functional operating temperatures to produce a collimated atomic beam and avoid the decomposition of the GCA.

After atoms in the beam have been cooled, we can begin the study of quantum properties. The hyperfine spin state is an important parameter to control in our ultra-cold atoms. The hyperfine ground states are separated by $\Delta E \sim h * 6.8$ GHz, and can be manipulated with microwave radiation. We designed and constructed a device to manipulate the hyperfine states of rubidium atoms in the BEC without further obscuring optical access to the experiment. Our device is a carefully-tailored open copper tube that selectively delivers a microwave signal to the atoms. This "directional horn waveguide" sends the majority of a 6.8 GHz signal toward the atoms and minimizes the amount of the signal that exits the other end. We first generated the 6.8 GHz

radiation and launched it into the copper waveguide. We then optimized the geometry of the device to maximize the signal sent to the atoms. Once installed, the waveguide will allow us to "spin flip" atoms in the $5^2S_{1/2}$ ground state between the F=1 and F=2 states.

University of Southern Mississippi

Photobleaching of Cy3 in Single-Molecule Fluorescence Studies
Carrie Walker

In single-molecule studies of DNA, short strands are commonly tagged with a fluorescent dye (such as Cy3) and excited by laser light while being observed under a microscope. With careful signal collection and optical filtering, the fluorescent signal from the dye can be detected with high resolution. The feasibility of such single-molecule fluorescence experiments is limited greatly by the length of time the fluorescent dye can be observed before photobleaching occurs. Previous studies have found that the simultaneous exposure of Cy3 to an excitation laser and near infrared light (as with the use of optical tweezers) greatly increases this photobleaching rate. In the proposed mechanism for this process, a fluorophore already in the first excited state absorbs a near infrared photon and then enters a pathway that leads to accelerated photodestruction. Previous studies using surface tethered molecules suggest that modulating exposure of the fluorophores to the trapping and fluorescent lasers prevents premature photobleaching by this two-photon process. We would like to confirm and quantify this effect for Cy3 contained in hydrosomes by identifying an optimal modulation frequency and duty cycles for the fluorescent and trap lasers. In combination with the optical tweezers and single-molecule fluorescence microscopy setup, we employ acousto-optic modulators to alternate hydrosome exposure to the trapping and fluorescent lasers. Preliminary results indicate that modulation of the fluorescent and trap lasers does in fact significantly lengthen the photobleaching time for Cy3 dye while still allowing for stable trapping and manipulation of the hydrosomes.

University of Toledo

Improving Voting Standards
Jameela C. Hudson

In collusion with the Help America Vote Act (HAVA), NIST is assisting the Election Assistance Committee (EAC) with improving national voting standards. This work shows that there are other venues available to improve the standards in voting systems such as security, privacy and usability by those who are disabled. While doing internet research on operating systems used in the top voting machines in the nation, it was discovered that not every machine within one company is using the same operating system. Trusted computing platforms would sanction for better protected and secured voting operating systems. Furthermore, through the testing and analyzing of these voting machines, it was discovered that options available to those voters who are disabled were not offered to those voters assumed not to be disabled. HAVA (Section 301) requires that voting systems "shall be accessible for individuals with disabilities, including non visual accessibility for the blind and visually impaired, in a manner that provides the same

opportunity for access and participation (including privacy and independence) as for other voters.

University of Tulsa

Microhotplate Characterization and SoC Development

Joshua Buck

Chemical microsensors using microhotplates represent one important application for Micro-Electro-Mechanical Systems (MEMS) technology. The CMOS microhotplate is the foundation on which thin film conductance-based gas sensors are fabricated. A System-on-Chip (SoC) implementation gas sensor implementation integrates an array of microhotplates with on-chip digital circuitry to facilitate programmable control and data gathering. This SoC incorporates a wide range of components: a MEMS microhotplate-based gas sensor array, an 8051 microcontroller, and on-chip interconnect and peripherals. The SoC approach exploits increases in transistor count to deliver simultaneous benefits in performance, power dissipation, reliability, footprint and cost. For efficient implementation, the operational parameters of the microhotplate devices need to be known. Electrothermal characterization of microhotplate includes the measuring of the temperature coefficient of resistance of the polysilicon heater, the thermal efficiency, and thermal time constant of the microhotplate structure. We developed new power control algorithms for the microhotplate heating element that are tested on General Purpose Interface Bus (GPIB) controlled source meters configured for four-wire Kelvin measurement to control the microhotplate power consumption and assist in microhotplate characterization. The new algorithms developed and measurement results will eventually be used by the 8051 microcontroller software for control of the microhotplate.

Optimizing and Characterizing Systems for Microchip-Based Microwave-Heated PCR

Shannon M. Burke

DNA analysis routinely requires amplification of a specific sequence of a gene by the polymerase chain reaction (PCR), generating *in vitro* millions of copies of the sequence. Although conventional PCR is widely used for its sensitivity and accuracy, it requires large sample volumes and it is labor-intensive, time-consuming and prone to contamination. Alternatively microfluidic-based PCR offers automation capabilities, faster reaction rates and an enclosed environment (thus minimizing risks of contamination). In addition on-chip PCR enables point-of-care analysis in situations when immediate results are required (e.g. organ transplants, bioterrorist threats). One foreseeable requirement is a fast and sturdy PCR system. A multi-disciplinary group at NIST is developing a chip-based microwave-heated PCR set-up to this end. With microwave heating the delivery of the energy is targeted to the sample; further enhancing heat transfer and reducing reaction times. The development of a sturdy PCR system (sample composition and protocol) is paramount for testing and characterizing this set-up.

Our experiments focused on establishing a robust system to amplify DNA. A standard 25µL PCR sample is composed of DNA (1µL, 50ng/µL), YieldAce® HotStart DNA polymerase (0.5µL, 5U/µL), PCR buffer (2.5µL , 10x), primers (2.5µL, 10mM), dNTPs (5µL, 1mM) and water (13.5uL). Experiments were performed on an i-Cycler thermocycler. A standard

thermocycling protocol is as follows: (1) 2min at 92°C, (2) 10 cycles of 30s at 95°C, 30s at T_m-5°C, 1min at 72°C, (3) 30 cycles of 30s at 95°C, 30s at T_m-8°C, 1min at 72°C, and (4) 7min at 72°C. The annealing temperatures vary with the melting temperatures(T_m) of each primer set.

Three genes were targeted: Rab1b, Vitronectin, and MAP2. Standard primers were first optimized. Additional primers tested the effect of GC-clamps on the polymerase binding to the template. These six primer systems were optimized by testing various concentrations of the polymerase (0.025U/μL-0.1U/μL) and of the primers (125μM-1000μM). Higher yields were obtained with the modified primers than with their standard counterparts. The three most efficient systems were the standard primers for Vitronectin, and the modified primers for Vitronectin and Rab1b. These systems demonstrated strong temperature stability (5°C range) for the denaturation, annealing and extension phases. Calibration curves for DNA concentration (0.001ng/μL to 100ng/μL) were developed for each system. All three systems displayed a linear response in the 0.01ng/μL - 1ng/μL range.

This project has identified and characterized three sturdy PCR systems. Optimum ranges for DNA concentrations and temperatures were successfully established. This work will enable our team to develop a microwave-heated PCR set-up with confidence.

Probing the Molecular-Level Understanding of Protein Adsorption to Surfaces

Ryan Vierling

Protein surface interactions play an important role in a variety of biomedical and maritime industry applications. Biofouling (the covering of a surface with protein material) can cause failure of prosthetic and cardiovascular devices doctors use to cure disease and help return mobility to the physically impaired. Surfaces that prevent non-specific protein adsorption are essential for making these devices last as long as possible. In addition, the specific adsorption of protein, with out the lost of its native 3D conformation would help advance the field of "protein chips," a diagnostic tool that doctors/researchers/clinicians could use to better diagnose certain conditions based on the adsorption of proteins from the blood to specific antigens on the chip.

The current model system for studying protein adsorption at surfaces on the molecular scale is oligo(ethylene oxide) [OEO] monolayers on Au. Prior research shows that molecules of this type arrange on the Au to form highly ordered self-assembled monolayers (SAMs). The molecules adopt a 7/2 helical conformation when the surface coverage approaches 100%. The molecules previously under investigation had a $–OCH_3$ terminus, and protein adsorbed at low and high surface coverages due to bare Au patches and highly entropic (ordered), conformationally confined chemisorbed molecules, respectively. However, high resistance to protein adsorption occurs at intermediate surface coverages in which the underlying Au is screened by uniformly distributed, conformationally mobile compounds. In these earlier studies surface hydrophobicity and SAM order increased simultaneously. Thus it was unclear whether the protein adsorption at the near 100% coverages was due to the increasing hydrophobicity of the surface, or the order of the individual molecules presenting a smooth surface for the protein to interact with.

Studies this summer were focused on new OEO compounds and SAMs derived from them that should decouple surface order and hydrophobicity. To this end $HSCH_2CH_2CH_2O(CH_2CH_2O)_xH$, where x = 5 and 6, were synthesized and/or purified. These OEO SAMs have a hydrophilic -OH terminus and hydrophobicity is expected to remain constant or decrease as the SAM order increases. Our data on the SAMs prepared this summer will be presented. SAM thickness and, indirectly, surface coverage was determined using spectroscopic ellipsometric data. The degree of order for the individual molecules was studied using reflection-absorption infrared spectroscopy and hyrophobicity of the surface was determined using contact angle measurements.

University of Wisconsin, Platteville

Exploring Millennial's Information Habits and Expectations of Library Resources
Andrew Schaumberg

In the next few years, the NIST employee base will begin to include an influx of the "millennial" generation. Multiple studies have indicated that this millennial generation functions very differently than previous generations, "generation X" and the "baby boomers". To better understand these issues, a study was designed to answer the question, "How should NIST's Information Services Division position itself to best serve the millennial generation's information needs?" This study was to have a two pronged approach: study of the SURF population to learn their information seeking habits and preferences, and if time permitted, a proof of concept design in response to SURF students' survey responses. Participants in NIST's Summer Undergraduate Research Fellowship program served as model millennials and participants in this study. Informal discussions among groups of three to seven participants led to the creation of a moderated online forum available for all participants to share their thoughts and experiences, including their perception of research, their use of electronic devices, their preferred sources for gathering information, and challenges they have encountered during the research process. Upon review of the discussion responses, the project team developed a survey to better quantify the responses of the participants. This survey was designed and will be administered next year. In the survey design process it was decided that creating a user satisfaction survey for NIST staff seeking similar trends would be useful for ISD planning to respond to all the populations it serves. After review of other library products, responses on the forum, and software libraries, a prototype software solution based on the Ruby on Rails framework was presupposed. This software was designed and implemented as a proof of concept search and index service for millennial researchers. It was intended to reduce the amount of time spent gathering information by harvesting metadata from external databases having an Open Archives Initiative Protocol for Metadata Harvesting (OAI-PMH) interface and creating *one* local searchable archive for NIST researchers to use rather than leaving these researchers to navigate many sites on their own.

Villanova University

Modeling of Aluminum and Copper Interconnect Features with Dee-Sub-Micrometer CDs at GHz Frequencies

Robert Sorbello

In high speed VLSI integrated circuits, copper has been replacing aluminum as the material of use for interconnects. The reason for this is because copper has lower resistance than aluminum for all geometries. Using a program called HFSS (High Frequency Structure Simulator), I was able to create a model of the interconnect wire, and then calculate how the resistance of the wire changed with frequency increasing. HFSS is a very complex program because of the many factors you have to consider when making the model, such as the ground plane, radiation, wave ports, excitation boundaries and much more. So my advisor and I were questioning whether we were setting up the interconnect model exactly the right way. Even after running numerous tests with HFSS we were not really sure if we can trust the results we were getting. My next task was to analyze the interconnect structure so that it will successfully replicate the results that were outputted by another program called Maple. After analyzing our model we need to validate the results we needed to compare solutions with the function outputted by Maple, which used Maxwell based differential equations having Bessel Function solutions. The only advantage HFSS has over Maple is that it solves actual IC conductors while Maple only solves the Bessel Functions. In order to replicate the Maple function, I would shift the copper wire to different distances from the ground plane on the IC, and from there, see which height came closest to the Maple graph. The simulations that were run were with the copper wire having a radius of 5 microns and .5 microns.

Virginia Military Institute

Spin Diffusion Transistors

Tom Shaffner

Since the invention of the integrated circuit there has been a continual drive for smaller devices in processors. Spintronics has come to light recently as a field of study that could potentially augment this downward size trend. Application of spintronic effects may allow logic circuits to decrease in size not through reducing the physical transistor size as in the past, but through a reduction in the number of transistors required to form a single gate.

This work has investigated one type of transistor, which is a modified bipolar junction transistor with two additional layers of magnetic material/tunnel barrier. The effect of this addition should allow the base current to remain a factor in the current flowing through the transistor, while adding a second layer of control through the application of magnetic fields. These fields, when applied, can change the magnetic orientation of the magnetic material in the device junctions, which in turn will change the resulting spin injection and thus the collector current.

This new device was tested over a range of plus or minus one Volt applied from collector to emitter, and plus or minus ten nanoamps base current. Magnetic field tests were run with an initial saturation of at least 2000 Gauss, and data was taken by sweeping the field over the ±

500 G range. Initial results indicated a consistent gain value in the range of one, and magnetic field tests indicated a marked effect on current at certain field values, but further work is necessary to refine the signal.

Williams College

Obtaining Slow Light Via Electromagnetically Induced Transparency

Kristen Lemons

Electromagnetically induced transparency (EIT) is a technique used to make an opaque medium transparent. Associated with this change in absorption is a rapid change in the refractive index with respect to frequency. This results in a very low group velocity hence a pulse propagating in the material moves much slower than the usual speed of light in a vacuum. This is called slow light. Our ultimate goal is to incorporate our slow light cell into an existing correlated photons experiment by sending one of two twin photon beams through the cell so that we can observe the effects of the delays.

We were able to achieve EIT by sending two beams of light, a strong pump beam and a weak probe beam, into a cell of heated rubidium atoms (50-70^{o}C). We worked on the D1 line of ^{87}Rb and set the frequency of the pump beam to that of the F=2-F'=2 transition line. We then used two acousto-optic modulators to scan the probe frequency a few MHz on either side of the pump frequency in order to be able to observe the full transparency window. The two beams were circularly polarized in opposite directions. We studied the effects of the power in the pump beam on the width and height of the EIT spike. Both properties decreased as the pump power decreased, but the width of the peak seemed to be limited by the magnetic field in the cell at about 125 kHz, for which we needed to lower the pump power to about 150 μW with 10-20 μW in the probe beam. In the correlated photons experiment we expect to need a width of a couple MHz, which means we will need 10-25 mW in the pump beam.

In order to measure the slow light, we sent pulses of light as the probe beam and measured the delay due to traversing the cell. Although the cell was only 5 cm long, we observed delays close to 2 μs. While studying these slow light delays, we have discovered that their behavior is much more complicated than what is expected from the simple EIT model.

Yale University

Developing a Rapid LSC Screening Method for ^{90}Sr Contamination in Urine

Evan B. Crawford

Strontium-90 is one of the most insidious fallout products of nuclear fission. Radioactive but difficult to detect due to its characteristics as a pure beta emitter, it is relatively long-lived with a ~29-year half-life. Its daughter yttrium-90 is another pure beta emitter, further complicating the detection of ^{90}Sr. Strontium is chemically analogous Ca; thus, in the body ^{90}Sr is deposited in bones and teeth, its radioactive isotopes causing long-term complications such as leukemia in humans. Current ^{90}Sr bioassay methods require a few days to several weeks per sample and involve time- and labor-intensive chemical separations. This time frame is unacceptable for

mass human screening in the event of the release and environmental dispersion of considerable quantities of ^{90}Sr.

A rapid (~1 hour or less) method was developed over the past two years to screen human urine samples for ^{90}Sr contamination via parallel Cerenkov and cocktail liquid scintillation counting. Determination is complicated by chemical and color quenching varying with different urine samples. Mathematical corrective quench curves can be quickly and simply generated on a sample-by-sample basis by splitting the sample and spiking one fraction with a radioactive isotope for comparison against an unquenched sample, reducing or eliminating the necessity of chemical separation processes. Alternatively, a ~10 min. activated charcoal chemical process can be used to decolorize the sample in order to reduce quenching effects. Due to its relatively low maximum beta energy, only ~0.5% of ^{90}Sr activity will be counted via Cerenkov LSC, while >90% is counted via cocktail LSC. A calibration constant is calculated to allow for the comparison of these two measurements and thus the ^{90}Sr fraction in the urine is resolved. The method also allows for the resolution of ^{89}Sr and ^{90}Y from the energy spectra. This method is robust and flexible, allowing for rapid mass screening of the population affected by the dispersion of radiostrontium.

Further research has been done to streamline the method and determine its accuracy, using a spectrophotometer to determine a correlation between color quenching and Cerenkov LSC efficiency. Somewhat by accident, it was discovered that generic store-bought Pekoe tea is a good spectral match for urobilin, the compound which gives urine its color, and thus different dilutions of brewed tea can be used to simulate color quenched urine samples. The efficiency and effectiveness of tea bags filled with activated charcoal at removing color quench from samples has also been examined. Thus, alternative options exist for the use and deployment of the method, allowing for users of the method to tailor it as needed given differing instrumentation and resource availability at potential measurement sites.

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APPENDIX A. QUICK CROSS-REFERENCE – SURF 2006

STUDENT	UNIVERSITY	TALK TITLE	OU
Althouse, Chad	Pennsylvania State University	Electrical Measurements of Self Assembled Monolayers	EEEL
Ames, William	College of William and Mary	Measurements of Radon Diffusion Coefficient with NIST Radon Standard as a Source	PL
Anton, Steven	University of Delaware	Calibration of Radioactive Seeds Used in Brachytherapy	PL
Aranchuk, Tatsiana	University of Mississippi	Electrostatic Sensing of DNA Using Field Effect Transistors	EEEL
Baler, Kevin	Cornell University	In Search of Anisotropy in Cobalt Nanoparticles	MSEL
Bhaskar, Siddharth	Princeton University	Towards a Simple, Effective Database of Medical Codes	MEL
Brazin, Jacqueline	Massachusetts Institute of Technology	Fabrication and Characterization of Polymer Microsphere Test Standards for Trace Explosive and Narcotic Detection Portal Systems	CSTL
Brown, Roger	Colorado School of Mines	Quantum Phase Transitions in the Hubbard Model	PL
Buck, Joshua	University of Tulsa	Microhotplate Characterization and SoC Development	EEEL
Burke, Shannon M.	University of Tulsa	Optimizing and Characterizing Systems for Microchip-Based Microwave-Heated PCR	EEEL
Campbell, Daniel	Hamilton College	Neutron Beam Collimation Using Monte Carlo Simulation Techniques	PL
Cao, Guy	University of Maryland, College Park	Implementation of Additional Capabilities of e-Fits using Java Applet	ITL
Cheng, Kevin	Pennsylvania State University	Evaluation of the Stability of NST Natural-Matrix Radionuclide SRM	PL
Christopher, L. Bailee	Appalachian State University	Modeling a Medical Particle Accelerator Using Monte Carlo Simulation Methods	PL
Clayton, Daniel	Davidson College	Optimization, Quality Assurance, and Quality Control in Neutron Detector Development	CSTL
Cope, Stephanie	Georgetown University	Simulating Heat Transfer in a Water Calorimeter for Use in Radiation Dose Standardization	PL
Cotts, Sarah	College of William and Mary	Interfacial Molecular Charge Transport in Monolayer Films	CSTL
Crawford, Evan B.	Yale University	Developing a Rapid LSC Screening Method for ^{90}Sr Contamination in Urine	PL
Cruz, Coral	University of Puerto Rico, Mayaguez	The Effectiveness of Combinatorial Methodology on the Exploration of TaA1N Metal Gate Electrodes on HfO_2	MSEL
Denomme, Carolyn	Pennsylvania State University	Towards the Redefinition of the Kilogram: Magnetic Levitation of Mass Standards	MEL
Do, Chi T. (William)	Montgomery College	Microstructure and Thermal Conductivity	BFRL
Doane, Nathaniel	St. Mary's College of Maryland	Quantification of Capsaicinoids in Hot Peppers Using Liquid Chromatography / Mass Spectrometry	CSTL
Dopkiss, Matthew	Miami (Ohio) University	Performance Comparisons of InGaAs, Extended InGaAs, and Short-Wave HgCdTe Detectors Between 1 µm and 2.5 µm	PL
Dorsey, Shauna	University of Maryland, College Park	Three-Dimensional Imaging of Polymer Scaffold Gradients	MSEL
Dunne, Cody	Cornell College	Human Computer Interfaces of Tomorrow: How Science Fiction Has Become Reality	MEL
Dunstan, Robyn M.	Elizabethtown College	Suppression of Coherence in Electron Microscopy	PL
Ellis, Megan	University of Connecticut	Collagen Matrix Micropatterning Using Localized Heat	EEEL
Erwin, Dylan	University of Maryland, College Park	Light Polarization and Spatial Light Modulation	PL
Eshraghi, Shima	University of Maryland, College Park	Measuring Cognitive Abilities of Artificial Systems	MEL
Fillipo, Amelia	Millersville University of Pennsylvania	Ph-ISFETs in Microfluidics: Qualitative Analysis of Variance and Comparison with Fluorescent pH Indicator	EEEL
Forbes, Michael A.	Massachusetts Institute of Technology	Combinatorial Designs and Their Impact on Software Testing	ITL
Fortuna, Emily	Rice University	*Ontolex*: Extending the Computational "Basic Reference Model" for Second Language Learning	ITL
Garcia, Jose	University of Puerto Rico, Mayaguez	Electrical and Chemical Characterization of Multi-Walled Carbon Nanotubes Coated in Streptavidin	CSTL
Gardner, Andrew	State University of New York, Binghamton	Adhesion and Release in Nanoimprint Lithography	MSEL
Gehret, Jennifer	University of Maryland, College Park	Measuring DNA Microarray Performance	CSTL

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Gilbert, Jereme	University of North Carolina, Charlotte	Determining the Location of the Hip Joint Center: Investigation of Algorithms and Factors for Location	MEL
Goldman, Joshua	State University of New York, Binghamton	Mechanisms of Water-Induced Adhesion Loss	BFRL
Gorbach, Michael	Swarthmore College	Monte Carlo Modeling of Magnetic Cobalt Nanoparticles	PL
Graneto, Nora	St. Joseph's University	A Study of New Colorimetric Radiation Dosimeter	PL
Green, Nelson	Kansas State University	Thermophoretic Sampling of Soot from a Diffusion Spray Flame	CSTL
Guzman, Julian	University of Florida	Bi_2O_3, Al_2O_3, Nb_2O_5 Equilibrium Phase Diagram	MSEL
Hackenmueller, Sarah	Gustavus Adolphus College	Towards Protein Resistance of Silicon	EEEL
Hansen, Azure	State University of New York, Stony Brook	An Optical Vortex-Based Azimuthal Lattice for a Bose-Einstein Condensate	PL
Henann, David	State University of New York, Binghamton	How to Pull a Nanowire: Developing Nanomechanical Testing Configurations	MSEL
Hong, Sam	Boston University	Polyelectrolyte Deep Eutectic Solvents	MSEL
Howley, Iris	Drexel University	Developing a Robot Classification System for Urban Search and Rescue	MEL
Huang, Jay	State University of New York, Binghamton	Computer-Controlled Instrumentation for a Silicon Carbide Power Device Long-Term Reliability Test Circuit	EEEL
Hudson, Jameela C.	University of Toledo	Improving Voting Standards	ITL
Huffer, Craig	Indiana University, Bloomington	Surface Barrier Detector Properties for the Precise Neutron Flux Measurement	PL
Huntemann, Tabitha L.	St. Mary's College of Maryland	Development of a Computer Based Fire Fighter Training Tool	BFRL
Keeney, Ashley	Mount St. Mary's University	Surface Derivatization of Thermoplastics for Increased Hydrophilicity	CSTL
Kenney, Jacqueline	Loyola College in Maryland	Performance Analysis of 3D Flash LADAR	MEL
Keslin, Jeff	University of Maryland, College Park	Validation of Stereoscopic PIV for Large-Scale Fire Induced Flow Measurements	BFRL
Kinahan, Michelle	University of Florida	Characterization and Optimization of Tethered Bilayer Lipid Membranes	MSEL
Lemons, Kristen	Williams College	Obtaining Slow Light Via Electromagnetically Induced Transparency	PL
Maditz, Rhyan	University of Maryland, College Park	Trace Detection of Illicit Narcotics Utilizing Ion Mobility Spectrometry	CSTL
Maldonado, Lauren	University of North Carolina, Charlotte	Micromanipulation Technology	MEL
Mansfeldt, Cresten	University of Minnesota	The Fate of Nanomaterials in Water Treatment	CSTL
Manweiler, Justin	College of William and Mary	NIST Conformance Testing Framework Promotes HL7 Compliance	ITL
McKay, Christine	University of Maryland, College Park	A User Interface to a Distributed Computing Environment	ITL
Medina, Billy	Polytechnic University of Puerto Rico	File Change Analysis ***OS Startup*** (System Boot)	ITL
Meister, Jeffrey	University of Maryland, College Park	Software Assurance Metrics and Tool Evaluation to Enhance Software Security	ITL
Miller, William	University of Maryland, Baltimore	Making Your Life Easier: Advancing Smart and Wireless Transducer Interface Standards	MEL
Morgan, Brian	Gettysburg College	Effects of Surface Roughness on Instrumented Indentation	BFRL
Nawabi-Ghasimi, Fred	St. Mary's College of Maryland	Quantitative and Qualitative Analysis of the Uptake of Polystyrene Microspheres by Human B-Lymphocytes	CSTL
Nie, Edward	University of Pennsylvania	Application of Thin-Film NiSi Kinetics to Nanocalorimetry of NiSi	MSEL
Noonan, Kathryn	College of Holy Cross	The Development of a Raman Standard for 633 nm Excitation Source	CSTL
Ostapenko, Tanya	Gettysburg College	Temperature Corrections in Industrial Irradiation Processing	PL
Peck, Jordan	State University of New York, Binghamton	A Study of Electrochemical Joining for Micro-Wires	MEL
Peterson, Eric D.	Appalachian State University	Plasma Oxidation of Ultra-Thin Aluminum Layers for Magnetic Tunnel Junctions	PL
Phan, Catherine	University of California, Irvine	Redefining the SI Kilogram and Implementing a Magnetic Levitation Balance	MEL
Polimeni, Gina	Kennesaw State University	Using Small Angle Neutron Scattering to Investigate the Phase Behaviors of Mixed Lipid Systems	MSEL

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Ramo, Jarred	Cornell University	Spatial Statistics for Carbon Nanotubes	ITL
Ramos, Danielle	University of Nevada, Reno	Comparison of Density Instruments for Use in Commodity Package Testing	MEL
Rastogi, Ashwin	College of William and Mary	Quantum Mechanics of a Magnetic Field Generated by Non-Abelian Vector Potential	PL
Rock, Reza	University of Delaware	Contrast Enhancement and Applications of Graphite Superlattice Modeling	MSEL
Royer, James	University of Maryland, College Park	Solution Processed Small Molecule Thin Film Transistors	EEEL
Sackett, Hillary	Smith College	Development of 3-D Geometries for Respirator Flow Field Modeling	BFRL
Santana, Jose	University of Connecticut	Characterization of Synephrine in Dietary Supplements Containing Bitter Orange	CSTL
Santiago, Michael	University of Puerto Rico, Mayaguez	Radiolabeling of p-SCN-Bn-DOTA with Po-210 for Applications in Angiogenesis-Targeted Radioimmunotherapy: HPLC Method Development	PL
Schaumberg, Andrew	University of Wisconsin, Platteville	Exploring Millennial's Information Habits and Expectations of Library Resources	MEL
Schirmer, Daniel	Colorado School of Mines	Phases of Ultra Cold Gases in the Fermi-Bose Hubbard Model	PL
Schnieders, Alexandra	University of Southern California, Los Angeles	Rubidium Tools: Atomic Beam Production and Quantum State Manipulation	PL
Schwalbach, Edwin J.	Illinois Institute of Technology	Examining Lipid Bilayer Molecular Dynamics by Neutron Scattering and Molecular Dynamics Simulations	MSEL
Schwartz, Ed	Millersville University of Pennsylvania	Application of Parallel Tempering to Neutron Reflectometry Data	MSEL
Shackelford, Scott	University of Maryland, Baltimore	The Hall Effect	EEEL
Shaffner, Tom	Virginia Military Institute	Spin Diffusion Transistors	MSEL
Shen, John	California Institute of Technology	Investigation of Hot Particles in Rocky Flats Soil Material	PL
Shiu, John	University of Maryland, College Park	Examining Sensor Location Algorithms from a Different Angle	ITL
Sit, Joseph	University of Maryland, College Park	Assaying Peptide Gradients with Epifluorescence Microscopy	MSEL
Smith, Adriennne	Northwestern University	Immuno-Fluorescent Staining for Telomerase: Cell Population Expression Variability	MSEL
Sorbello, Robert	Villanova University	Modeling of Aluminum and Copper Interconnect Features with Dee-Sub-Micrometer CDs at GHz Frequencies	EEEL
Strawbridge, Matthew	Salisbury University	A Fourier Transform Analysis of Human Images for Evaluation of Thermal Imaging Cameras	BFRL
Tabat, James	University of Minnesota	Testing Long Term Calibration Stability of Flow Meters	CSTL
Toutounchian, Sam	Moorpark College	Literature Study of the Supply Change of Medical Devices	MEL
Travers, Ryan	University of Maryland, College Park	Positive Pressure Ventilation	BFRL
Travis, Katherine	Smith College	Auto-Generation of C-Code to Improve Efficiency of a PDE Solver Written in Python	MSEL
Turov, Yevgeniya	University of Oregon	Self-Assembly of Fluorinated Surfactants in Ionic Liquids	MSEL
Vierling, Ryan	University of Tulsa	Probing the Molecular-Level Understanding of Protein Adsorption to Surfaces	CSTL
Wahl, Christopher	State University of New York, Geneseo	Investigation of Source Detection Algorithms for Radiation Portal Monitors	PL
Walker, Bryant	Rensselaer Polytechnic Institute	Behavior of Single Walled Carbon Nanotubes in Aqueous Suspension	MSEL
Walker, Carrie	University of Southern Mississippi	Photobleaching of Cy3 in Single-Molecule Fluorescence Studies	PL
Walker, Thomas	Pennsylvania State University	Measurement and Modeling of Contact Potential Difference with Scanning Kelvin Force Microscopy	EEEL
Wiley, Jennnifer	University of Maryland, College Park	Large Eddy Simulation of Partially-Premixed Combustion Following Ignition of a Fuel Vapor Cloud	BFRL
Williams, Daniel	University of Nebraska, Lincoln	High Contrast Images Made Possible by Adjustment of Illumination in the Visible and Near-Infrared Light Regions	PL
Willoughby, David	University of North Carolina, Charlotte	Physics Based Modeling of Machining	MEL
Wong, Kristin	Santa Monica College	Determination of Caffeine and Caffeine-Related Analogs in Candidate NIST Green Tea SRMs	CSTL
Wright, Amelia	Johns Hopkins University	Wind Load Factors for Tall Buildings	BFRL

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Xu, Phyllis	Massachusetts Institute of Technology	High Resolution X-Ray Diffraction: Characterizing Aspects of a NIST SRM	MSEL
Yan, Victoria	University of Maryland, College Park	Converting Young's Modulus MATLAB Programs to Web-Based Data Analysis Sheets	EEEL
Yocklovich, Jenna	Millersville University of Pennsylvania	Dynamic Web-Based Repository for Healthcare Standards Information	ITL
Zoller, Benjamin	University of Maryland, College Park	Developing a Computer Forensics Tool to Output a Windows Registry Dataset to an XML-Based Format	ITL