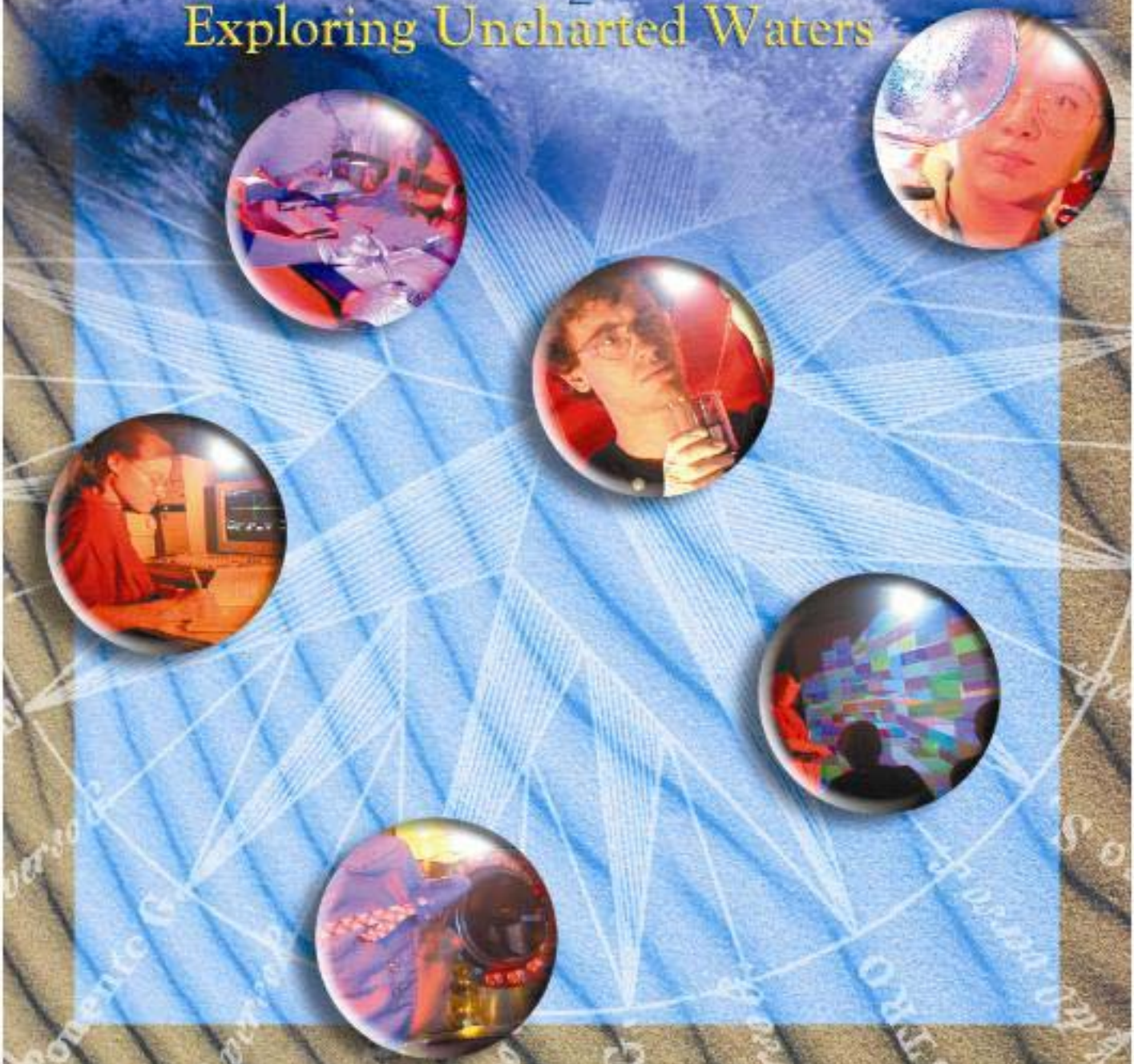
National Science Foundation

SURF Twentytwo

summer undergraduate research fellowship

Exploring Uncharted Waters



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

INTRODUCTION

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. As of 2002 all seven of NIST's measurement and standards laboratories are participating in this exciting program: Building and Fire Research, Electronics and Electrical Engineering, Information Technology, Manufacturing and Engineering, Materials Science and Engineering, Chemical Science and Technology, and Physics.

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. This program exposes students to applied research procedures in a unique environment while working one-on-one with world-class NIST scientists.

In addition to the laboratory experience, SURF seminars, extramural group activities, and an end-of-the-summer SURF Symposium enhance the students' experience. The SURF seminars feature lectures by leading industrial researchers, academic leaders, and world-class NIST scientists that expose the students to a variety of research applications. At the end of the summer, the students feel pride and a sense of accomplishment as they participate in the SURF Symposium. This symposium provides an opportunity for the students to present their summer work before their fellow SURF students and the NIST scientific community in a conference-like setting. During the following school year, students are strongly encouraged to present their research results at national meetings. This book provides you a glimpse of the 2002 SURF program at NIST from the schools and students involved, student activities, seminar speakers, and an abstract of the final student presentations. We hope that by reviewing this information you will consider joining us in this exciting program.

Intentionally Blank

Table of Contents

The Summer Undergraduate Research (SURF) Program at NIST

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 the Building and Fire Research Laboratory (BFRL), Information Technology Laboratory (ITL), Manufacturing Engineering Laboratory (MEL), the Materials Science and Engineering Laboratory (MSEL), and the Chemical Science and Technology. 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 attending a U.S. college or university.

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. 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
As of 2002, all seven of NIST's measurement and standards laboratories are participating in the SURF programs: the 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, in addition to travel and housing allowances. A limited number of 9-week fellowships are available for students that cannot attend the full 12-week program. Students attending the 9-week program will receive a $3,000 stipend, in addition to travel and housing allowances. Universities are encouraged, but not required, to share in the program in such ways as providing student credits, travel or housing allowances.

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 close of business February 15th or the first business day following that date. Visit http://www.surf.nist.gov/ surf2.htm for this years' 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). 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). To receive an application by mail, you may also contact:

Anita Sweigert
NIST
100 Bureau Dr., Stop 8400 (Building 221, Room B160)
Gaithersburg, MD 20899-8400
Telephone: 301-975-4200 Fax: 301-975-3038
E-mail: sweigert@nist.gov

2002 SURF Summer Seminars and Activities

May 28 First official "work" day and Orientation

May 29 Welcome Picnic – NIST Picnic Grove

The SURF Directors provided the burgers, salads, snacks, and sodas. The SURF students were responsible for the entertainment, Frisbees, music, etc.

May 30 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, lab safety, and radiation safety.

May 31 "How's It Going" Rap Session

This was a general session for students to discuss their expectations and those of their advisors and to air any concerns or feedback about things to date.

May 31 Dr. Marc F. Desrosiers
Physics Laboratory SURF Director and Research Chemist, NIST Physics Laboratory, Ionizing Radiation Division

Anthrax in the Mail: NIST Calibration Services to the Rescue

Scientists in the NIST ionizing radiation program played a critical role in the government's response to the recent anthrax attacks. Under the direction of the Office of Science and Technology Policy, NIST led the multi-agency technical task force (U.S. Postal Service, Department of Defense, Department of Energy, Food and Drug Administration, and the U.S. Department of Agriculture) and facilitated the adaptation of current irradiation technology to decontaminate the U.S. mail. High-energy x-ray and electron beams are proving to be effective in eradicating anthrax in contaminated mail. The talk detailed the fundamentals of this technology, as well as chronicled NIST's efforts to alleviate this problem.

June 5 NIST Virtual Library (NVL) Demos and NIST Research Library Tour

The sessions provided an overview and tour that includes demonstrations of the Library facilities, both manual and computer-based.

June 14 Dr. John T. Armstrong
NIST Chemical and Science Technology Laboratory, Surface and Microanalysis Science Division

The Disputed Discovery of Element 43 (Technetium)

In 1925, Ida Noddack, Walter Tacke and Otto Berg reported discovery of a new element having atomic number 43, which they named Masurium. Their discovery was based on line identification of x-ray emission spectra from chemically concentrated residues of various U-rich minerals. These results, however, were disputed and eventually the discovery of element 43 (Technetium) was generally credited to Perrier and Segre, based on their chemical separation of neutron-irradiated molybdenum in 1937. The scientific career of the brilliant chemist Ida Noddack was badly damaged by this controversy.

Using first principles x-ray emission spectral generation algorithms from the NIST DTSA spectral processing program, we have simulated the x-ray spectra that would be expected in the experiments of Noddack et al., using their likely analytical conditions and sample compositions (derived from their papers and contemporaneous reports). The resulting spectra are in close agreement with that reported by Noddack et al., place limits on the possible residue compositions, and are supportive of the presence of detectable amounts of element 43 in their sample. Moreover, the calculated mass of element 43 shown in their spectrum is consistent with the amount that would be now expected from the spontaneous fission of U present in the ores they studied. The history of the original Masurium/Technetium controversy and the means used to reexamine the original record were presented in this scientific detective story.

June 17 First "official" work day and Orientation for Session 2 students

June 18 NIST Safety Orientation for Summer Students – 2nd SURF Group Entrance

The session provided an overview, including how to report emergencies, use of personal protective equipment, general safety, office ergonomics, lab safety, and radiation safety.

June 19 Welcome Picnic for Session 2 Students – NIST Picnic Grove

The SURF Directors provided the burgers, salads, snacks, and sodas. The SURF students were responsible for the entertainment, Frisbees, music, etc.

June 19 Professor David Goodman
Electrical and Computer Engineering Department, Polytechnic University

Wireless Internet

The big 1980s development in information technology was the personal computer. In the 90s it was the Internet and cellular telephones, which until now have followed separate paths. The revolution anticipated in the present decade is the convergence of wireless communications and the Internet, but wireless LAN and cellular technology have not fulfilled the expectations. This talk examined the ability of emerging technologies to realize the potential of a Wireless Internet and the value of a top-down approach to technology that first examines the information needs of a mobile population, and then confronts technical constraints to obtain the benefits of the "wireless revolution".

June 21 Dr. John L. Gross
NIST Building and Fire Research Laboratory, Materials and Construction Research Division

NIST Response to the World Trade Center Disaster

June 25 NIST Virtual Library (NVL) Demos and NIST Research Library Tour

The sessions provided an overview and tour that includes demonstrations of the Library facilities, both manual and computer-based.

June 27 Dr. Thomas A. DeFanti
Distinguished Professor, Computer Science Department, Director, Electronic Visualization Laboratory, University of Illinois at Chicago

StarLight: a Facility for Experimental Networks and e-Science Applications

The availability of wavelengths is accelerating the bandwidth capacity of all networks at an incredible rate. In the City of Chicago, a number of metro, national and international advanced optical networking infrastructure initiatives are converging. In particular, the Electronic Visualization Laboratory (EVL) at the University of Illinois at Chicago (UIC), the International Center for Advanced Internet Research (iCAIR) at Northwestern University (NU) and the Mathematics and Computer Science Division at Argonne National Laboratory (ANL) are partners in creating a carrier-neutral co-location facility at Northwestern University's campus in downtown Chicago. This facility, called *StarLight*, anchors over $40 million of new government and university investments in optical networking infrastructure. StarLight is a research support facility built ***by*** researchers ***for*** researchers. These researchers are networking engineers and electrical/computer engineers, computer scientists and e-Scientists and their applications programmers. StarLight is designed to support a network-rich future, operating switching/routing at the highest experimental levels, but also laying the foundation for future experimental and production fully optical (O-O-O) switching. Indeed, StarLight researchers are already experimenting with an optical networking testbed based on O-O-O switching, using MEMS devices.

June 28 Dr. Timothy J. Foecke
Materials Scientist, NIST Materials Science and Engineering Laboratory, Metallurgy Division

The Metallurgy of Shipwrecks: Titanic, Arizona and Hunley

With proper care, an iron ship can last for hundreds of years on the surface on the water. Sink it, and all bets are off. Corrosion, biocorrosion, biofouling, wave action, collisions and nettings all take a toll on a ship's structure and cause it to decay and collapse. Many historical wrecks around the world are rapidly falling apart, and several are being actively investigated to determine if their structures, and their historical legacies, can be preserved. In this talk, past projects and work in progress on ships like the Titanic, Lusitania, USS Arizona, USS Monitor, CSS Hunley and the Andrea Doria were discussed. Corrosion is the main enemy of a wreck – after all, rust is what most metals want to be!

July 8 Dr. Nicholas Carino
NIST Building and Research Laboratory, Materials and Construction Research Division

Seeing with Sound: The Impact-Echo Method for NDE of Concrete

July 8 2002 SURF T-Shirt Design

It has become a "tradition" each year for the group to design a T-shirt during the summer. This is the front and back design that was chosen. There were over 160 students, advisors, and other NIST staff sporting this year's design around the campus.

July 9 Dr. Manuela M. Veloso
Professor, Carnegie Mellon University

Autonomous Muti-Robot Teams

My long-term research passion is the study of complete autonomous intelligent agents that can continuously perceive the world, act, achieve goals in dynamic and uncertain environments, and learn to improve their performance. Creating such effective agents, in particular as members of a team in the presence of opponents, is a challenging problem. Robotic soccer has offered an interesting concrete environment for research in multiagent planning, execution, and learning. With my students, I have been pursuing research in robotic soccer in three different technical setups: fully distributed multiagent simulation, small-wheeled robots with centralized perception, and fully autonomous Sony legged robots. We have participated in the RoboCup international competitions since 1997 and have been champions several times. In this talk, Dr. Veloso reviewed their work in the different leagues and some of their main underlying research contributions, including a robust perception-biased probabilistic localization algorithm, a real-time path planning and replanning algorithm, and a variable learning rate multiagent learning algorithm. Dr. Veloso set his research goals in perspective and discussed some of the fascinating open questions to be addressed towards truly creating teams of autonomous robots.

July 12 Ms. Elena Messina and Mr. Adam Jacoff
NIST Manufacturing Engineering Laboratory, Intelligent Systems Division

Robots to the Rescue

NIST researchers developed a test bed to evaluate autonomous mobile robots that aid in Urban Search and Rescue (USAR) operations. This work is part of their efforts to develop measures for robots and other intelligent systems. When a building collapses (due to earthquakes or other disasters) the first thing that rescuers do is try to locate victims and potential hazards in the buildings and then they work on finding a way to remove the victims. In a USAR scenario, robots can be used in collapsed buildings to locate victims and hazards, map

the environment, and communicate the locations of those victims and hazards back to the human rescuers. The USAR domain is just one example of several domains in which robots may be well suited to perform dangerous and difficult activities. The challenge is to quantify how well the robots work. NIST test arenas are being adopted worldwide as *de facto* reference tests for mobile robots. They are being used by the American Association for Artificial Intelligence and RoboCup Rescue competitions. The talk described the design considerations in creating reproducible and transportable arenas, what the challenges are for autonomous mobile robots, and videos of robots in arenas from recent competitions were shown.

July 18 Arlene Modeste Knowles and Suzanne Otwell
Education and Outreach Department, American Physical Society

July 19 Mr. Kirk Rice
Program Manager, NIST Electronics and Electrical Engineering Laboratory, Office of Law Enforcement Standards

A Modern Knight's Tale – Weapons and Protective Systems for 21st Century Law Enforcement

Law enforcement officers rely on a variety of protective equipment so that they can perform their duties more safely and effectively. In some sense, they are like modern knights, sworn to protect and serve those in their communities. Like their medieval counterparts, their specialized equipment (weapons and armor) is designed to meet the types of threats they expect to encounter. The Office of Law Enforcement Standards (OLES), within the Electronics and Electrical Engineering Laboratory at NIST, develops performance standards for many types of equipment used by law enforcement. These standards are published by the National Institute of Justice, and they are often cited in procurement specifications so that law enforcement agencies can purchase equipment that performs satisfactorily. This presentation highlighted some of the important equipment performance standards that have been developed, some that are underway, and provided an overview of the standards development process.

July 25 Dr. Norman P. Neureiter
Science and Technology Adviser, Office of the Secretary of State, Department of State

International Science

July 26 Dr. Bert Rust
Research Mathematician, NIST Information Technology Laboratory, Computational Sciences Division
Fitting Nature's Basic Functions

This was a tutorial lecture on the art of least squares modeling of measured time series data using combinations of the most basic functions governing the dynamics of natural processes, with a particular emphasis on cyclical and exponential behavior. The techniques described were applied to the historical records of global total fossil fuel production, atmospheric carbon dioxide abundance, and global average temperatures of the lower troposphere. Standard statistical diagnostics were used to assess the models that were developed and the connections between them. Short-term extrapolations into the future were considered.

July 29 Dr. Cynthia Howard Reed
Environmental Engineer, NIST Building and Fire Research Laboratory, Building Environment Division

Investigating Indoor Air Quality and Ventilation: A Tour of the NIST Test House

July 31 Dr. Michael Gaitan
Semiconductor Electronics Division, NIST Electronics and Electrical Engineering Laboratory

Dr. Gaitan talked about the manufacture of MEMS using CMOS compatible designs and processing. This concept, which today is widely used throughout the industry, was pioneered by Dr. Gaitan nearly a decade ago. Some past and current metrology applications of MEMS, including thermally activated devices, RF power sensors, and thin film stress sensors will be described. Finally, the use of MEMS for single molecule manipulation and measurement (SM3) was discussed.

August 2 Mr. Donald Swenholt
Donald Swenholt Associates, Inc.

Giving Successful Presentations

Mr. Swenholt presented a few techniques and up-to-date procedures to assist the students in presenting their talks for the end-of-the-program SURF student symposium.

August 8 Dr. Ana Ivelisse Aviles
Mathematical Statistician, NIST Information Technology Laboratory, Statistical Engineering Division (and former SURF student)

From SURF to Stats: Mixed Effects Models

The speaker was a NIST SURF student several years ago, and she told about some of her experiences and how the opportunity affected her acquisition of the Ph.D., which later led her back to NIST. The main objective of the talk, however, was to discuss experimental designs for the estimation of fixed effects and two variance components, in the presence of nested random effects.

August 12 Final Presentations by SURF Students moderated by invited guests

August 12 Lunch with special invited guests

August 13 Final Presentations by SURF students moderated by invited guests

August 14 Final Presentations by SURF students moderated by invited guests

August 15 Final Presentations by SURF students moderated by invited guests

August 16 Last Day for SURF students - Farewell Party!

Student Abstracts from the 2002 Program at NIST

American University

Realization of the ITS-90 Below 84K
John Patrick Casey

Our work is concerned with maintaining the International Temperature Scale of 1990 in the cryogenic range below 84K. The ITS-90 is defined by fixed points of a number of elements. By utilizing resistance thermometry, temperature data can be obtained on fixed-point cells, such as the triple points of e-H_2, Ne and Ar at cryogenic temperatures. These points are realized by freezing and melting the cell and observing the temperature plateaus during these processes. Two methods can be used to obtain the extremely low temperatures needed. The first involves the use of a bath cryostat. The cell is enclosed in multiple layers, which are pumped to vacuum and filled with cryogenic liquids to cool the cell down to the appropriate temperature. This method is very slow and expensive due to the use of the liquid cryogens although it produces stable conditions for data acquisition.

Another method more suited to this application uses a multi-stage Gifford-McMahon (G-M) cryocooler. This does not require the use of liquid cryogens. Helium gas is pressurized and expanded in a cycle, which produces a cooling effect. This system is desirable where temperatures below 10K are not needed. It is faster, cheaper and will hopefully produce results comparable to that of the cryostat method. Preliminary realizations of the e-H_2 triple point with a G-M cryocooler have been completed and results are now being compared with previous realizations performed in other systems.

Appalachian State University

QCSim: A Quantum Computer Simulation
Matthew Cass

Designing a quantum computer simulator is essential to testing and exploring the power behind these theoretical super computers. The need for this simulator grows from the need to be able to evaluate different error correcting codes, quantum circuit layouts, and variable assignments.

I set out to write a quantum computer simulator in the C++ programming language. This model would implement basic, common quantum computing gates and eventually quantum circuits. The first complete simulator, QOne, was a simple one qubit or quantum bit simulator that performed a limited basic set of operations. Borrowing ideas from this simplified model the more complete QCSim simulator is being written. This simulator is able

to handle any number of qubits and will ultimately be able to perform any operation. Both simulators use a density matrix model for representing qubits and for performing operations.

Using the QCSim simulator, several quantum error correcting codes and quantum error correcting circuits will be tested in hopes of discovering a preferred method of error correction in quantum computers. The simulator is also designed to assist in the testing of real quantum circuits designed by physicists as a means of "answer checking" the results generated by the first lab prototypes of quantum computers.

Stability Under Shear Flow of Strings in Model Emulsions
Erin Robertson

Our group has recently reported* the occurrence of a droplet-string transition in model emulsions composed of polyisobutylene (PIB) and poly(dimethylsiloxane) (PDMS), sheared in the regime where the gap width (d) between the confining parallel plates approaches the diameter ($2r$) of the dispersed droplets. In this work we consider the stability of a long cylindrical domain of a fluid in a phase-separated mixture in a simple shear flow field. We perform steady shear experiments on a dilute PIB/PDMS emulsion, containing 4.6% mass fraction PDMS. These experiments are performed in a commercial shear cell, which consists of two optically clear quartz parallel plates (of which one plate remains stationary and the other is driven by a motor). After forming strings and letting them reach their steady state size, we decrease the shear rate. Upon reduction of shear rate, we find that the strings break up by two mechanisms: first the ends of the strings pinch off to form resultant droplets, and after end pinching occurs, the remnant string breaks up by the classical Rayleigh-Taylor-Tomotika instability. Since the strings are formed in a regime that is closer to the bulk case ($d/2r$ = 0.16), we are also able to compare our results with predictions of a hydrodynamic model by Khakhar and Ottino** for stability of strings in simple shear flow. These results will be discussed in detail in this presentation.

---

* Migler, K. B. *Phys. Rev. Lett*. **86**, 1023 (2001)
** Khakhar, D.V. and Ottino, J.M. *Int. J. Multiphase Flow* **13**, 71 (1987)

Verifying SURF III as a Standard for Source-Based Radiometry -or- Was $1.97 Million Really Worth It?
Rebecca Stamilio

At NIST's Synchrotron Ultraviolet Radiation Facility (SURF III) a new beamline was recently constructed to be a national standard of light from UV to IR. This beamline, Beamline 3, is a source-based radiometry beamline. Namely, it uses the synchrotron radiation as a standard source of light for comparison and calibration of other sources. During the summer of 2001, we designed and constructed the front end of the beamline where the current monitor device is mounted. Now in 2002, the beamline is in vacuum and it was possible to take

measurements of the synchrotron radiation at the end station and compare with theoretical calculation. A variety of filter radiometers were used with a range of electron energies to measure the angular distribution of the synchrotron radiation above and below the electron orbital plane. Theoretical values were calculated using Schwinger's equation and a synchrotron simulation program. We have compared our experimental measurements with the theoretical and the results will be presented here. Also some design on a trap detector for another beamline will be discussed.

Fire Pattern Re-Creation

Sarah E. Thompson

Arson is one of the top causes of fires and fire deaths in the United States. The annual direct dollar losses from arson are approximately $3.6 billion dollars. Recent changes in court rulings require expert testimony that is technically defensible. In other words if something cannot be proven based on scientific principles or recreated in an experiment, then it may not be admissible as evidence in court.

As part of a larger effort to develop scientific tools for fire investigation, a series of experiments were conducted to investigate the feasibility of using computer simulations to re-create quantitatively real fire burn patterns. NIST's Fire Dynamic Simulator (Version 2.2), a computer model which includes the chemistry and physics of fire phenomena, and its associated visualization program, Smokeview, were used to simulate the exposure of gypsum wall board panels to the thermal radiation of a fire. Samples of gypsum board were placed at different distances from a natural gas fired radiant panel and thus exposed to a range of heat flux values. Three separate thermocouple sensors were used to monitor the temperature at the front, middle, and back of each board. These temperatures were used in conjunction with the char depth and calcination through the board to examine the impact of a predetermined heat flux on the sample. The char area and overall burn pattern were also considered when comparing the experimental burn patterns to the burn patterns predicted by the model. A radiometric thermal imager camera was used to collect qualitative thermographs of different sample specimens. The Fire Dynamic Simulator was used to generate a heat flux map for the different distances from the panel to allow comparison to the thermographs. Preliminary results suggest NIST's Fire Dynamics Simulator can be an extremely effective method of modeling burn patterns.

Bates College

Crystallographic Orientation of Surface Facets

Amanda Slocum

The surface energy (γ) of a crystallographic solid is a function of the surface orientation. When (γ) is a constant then the equilibrium shape of the crystal is a sphere. However when (γ) varies with orientation and is anisotropic enough, then the equilibrium shape will consist of flat facets.

The atomic force microscope (AFM) has been used to image a polycrystalline alumina (Al_2O_3) sample after the sample was heated in a furnace. During heating the initial flat surface becomes faceted, a process in which the original surface breaks up and surfaces of different orientation are exposed. In the AFM, a probe in contact with the sample is scanned across the surface. The height is recorded at fixed intervals along the surface. This height data is used to create a topographical map of the surface. From this data it is possible to see a variety of different facet orientations, and the pattern of the facets vary from grain to grain. The facets, approximately 20-40 nm in height, appear predominantly as triangular, or as hill and valley, however some grains do not appear to have faceting at all. Using visualization software AVS, the normals to the facet surfaces are calculated and displayed using the stereographic projection. The angles between adjacent facets can then be determined. Next, the sample will be loaded into the scanning electron microscope (SEM) and Electron Backscatter Diffraction (EBSD) will be performed to determine the crystallographic orientation of specific grains on which facet orientation data has been recorded. Comparing the crystallographic orientation with the orientation of the faceted planes we expect to find that facets will occur on the low index planes of low energy.

Brigham Young University

Qubit-Radiation Field Entanglement

Jacob Anderson

Moore's Law and novel algorithms have fueled research into quantum computing. Theories of quantum computation and information call for precise manipulation of quantum systems to perform calculations. This talk will provide a brief overview of quantum computation, including how practical implementations of one- and two-qubit gates often use laser fields to perform quantum operations. In many cases the qubits can become entangled with the radiation field creating a loss in gate fidelity. Using different theoretical pulses, I explored the degree of entanglement between the laser field and the qubit system as it underwent a p/2 pulse operation.

Towards Controlled Interactions Between Qubits
Yenny Martinez

Classically, information (bits) is stored in memory devices, and with logic gates makes computation possible. As the physical devices get smaller, and approach the size of a few atoms, quantum effects become important. Furthermore, it has been shown theoretically that it may be possible to use quantum bits (qubits) to solve certain problems (i.e., factorization of large numbers) much faster than with classical computers. Quantum computation relies on the special properties of quantum systems, superposition and entanglement.

Various physical implementations have been proposed to experimentally achieve quantum computation. Among them, we chose to use Bose-Einstein condensates (BECs) and optical lattices to investigate how neutral atoms could be used for quantum computation. The internal state of individual atoms would be the qubit and interactions between qubits will allow computation.

Starting with a BEC, we plan to prepare two different qubits with a Raman transition and then achieve controlled collisions between qubits by using state selective lattices. By rotating the polarization of one of the beams used to create these lattices, the qubits move according to their internal states. In this presentation, I will first focus on the optical system designed to produce the two well-defined laser frequencies f_1 and f_2 for the Raman transition to occur. Next, I will explain the optical system used to create the state selective lattice.

Bryn Mawr College

Fourier Transform Terahertz Spectroscopy of Amino Acids, Peptide Chains and Frozen Solvents
Mary Kutteruf

Proteins are long chains of amino acids, but they do not function as stretched out long strands. Instead proteins fold into specific shapes to fulfill their biological function. The rules governing protein folding are not well understood, and are a major area of research in biochemistry. Terahertz spectroscopy (at wavelengths ~1 mm), can reveal information about molecular bending, flexing and stretching. Hence, one might expect that such spectroscopy would be helpful in analyzing the folding of proteins. Unfortunately, since proteins are extremely large molecules, they tend to not give sharp spectra. Single amino acids and small peptide chains, however, give sharp, distinct spectra at terahertz frequencies but little if any research has been in this region. My research involved taking terahertz spectra of numerous amino acids and peptide chains (ca. 35 solid state species) in order to begin understanding the interactions and structures of these molecules. The amino acids were also modeled using the computer program Gaussian 98. Computer generated spectra differed greatly from experimental spectra, probably due to hydrogen bonding, presence of water and solid state effects. Two amino acids, serine and cysteine, were modeled extensively, due to their similar

structure. Hydrogen bonding was accounted for by adding water molecules to the calculation and by using the solution function of the Gaussian program. It was hoped that any solid-state spectral artifacts could be removed by dissolving the amino acids in solvents and then freezing the solution. To this end spectra of frozen water, ethanol, methanol and acetone were taken. While spectra of frozen alcohols and acetone are also revealing, unfortunately, spectra of amino acid solutions did not show significant differences from the solvent spectra, proving this approach ineffective.

Preparation and Characterization of Nanostructures for Surface Enhanced Raman Spectroscopy (SERS)

Jessie Rosenberg

As part of a large, multi-laboratory NIST program called Single Molecule Manipulation and Measurement (SM^3), this research effort focuses on the optical characterization of single biological molecules using vibrational spectroscopy. To obtain the sensitivity necessary for single molecule spectroscopy, signal enhancement via metallic nanoparticles is employed. The goal of this summer project is to synthesize and characterize cobalt nanoparticles, a previously unexplored metal substrate for Surface Enhanced Raman Spectroscopy (SERS).

As Raman cross sections are inherently low ($\sim 10^{-30}$), enhancement of the scattering is necessary to observe vibrational bands originating from low concentrations of analyte. Enhancement factors for inelastic scattering of $\sim 10^{15}$ have been achieved with nanoscale metallic (gold and silver) colloids, either in solution or on a surface. A detailed understanding of the relationship between the characteristics (ex. size, shape, density, etc.) of the metallic nanoparticles and the enhancement factors is as yet unavailable. However, the enhancement originates from both a chemical or molecular effect and an electromagnetic or field effect.

The goal of this summer project is to explore the synthesis of cobalt nanoparticles by various chemical methods and to characterize the resulting nanostructures by multiple, complementary methods. Also sought is a comparison of the Raman enhancement from the cobalt nanoparticles with that from known nanoparticle systems such as silver. Ultimately, the surface enhancement capabilities of cobalt nanoparticles will be combined with magnetic manipulation. Production and characterization of specialized magnetonanoparticles, such as gold or silver coated cobalt, is of particularly high interest. A magnet (up to 8 Tesla) coupled to a Raman microscope will permit studies of both the enhancement of the Raman scattering and the alignment capabilities of the particles.

Bucknell University

Characterization of Derived Porous Silicates and Bioencapsulated Catalytic Proteins

Matthew S. Paoletti

Characterization of sol-gels is increasing due to their possible applications as novel pharmaceutical and catalytic biomaterials. Consequently, the desired applications of these silica gels and bioencapsulated catalytic proteins will be discussed. Small-Angle Neutron Scattering (SANS) was employed to determine the mean-pore distribution of silica hydrogels. Experimental results permit a characteristic length scale of the pores to be determined, allowing us to infer which proteins, based on molecular size consideration, may be encapsulated in these gels. In order to tailor the pore size and distribution of the gels, the composition was varied by employing silica solutions at several concentrations and through the addition of polymers of different molecular weight and volume fraction. Results from the SANS experiment are compared with images obtained with an Atomic Force Microscope (AFM).

In addition to the aforementioned experiments, dynamics of proteins encapsulated within the silica gel pores have been examined by incoherent quasi-elastic neutron scattering using The Disk Chopper Spectrometer at the NIST NCNR. Two proteins were examined and are compared with the corresponding data for these proteins in solution. By utilizing different silica solutions of varying concentrations and an array of polymers, it should be possible to either inhibit or maintain the dynamics of these proteins to suit a particular, desired application.

Calvin College

Two-Beam-Excited Conical Emission

Michael C. Scholten

By intersecting two beams of same-frequency near-resonant light in a rubidium vapor cell, a circular cone is emitted between the two beams. Degenerate four-wave mixing in the alkali vapor, which is a result of the non-linearity of the medium, causes this effect. Due to energy and momentum conservation, we expect both spatial and temporal correlation of the photons in the emitted cone. In order to determine if correlation exists, we use heterodyne spectroscopy to compare the energy spectra of the cone and the input beam, and use a pair of avalanche photodiodes to detect time-correlated photon pairs.

Potential future applications of this experiment include correlated photon pair production for quantum communications and quantum cryptography, as well as creating a convenient source for atom optics experiments.

Carnegie Mellon University

Displaying Fourier Maps in FOX Using the Marching Cubes Algorithm
Michael Polyakov

FOX (Free Objects for Xtallography) written by Vincent Favre-Nicolin is a program for *ab-initio* structure determination from powder diffraction data. As well, FOX can display a crystal structure in 3D using OpenGL. This is valuable because it allows the structure to be manipulated in three dimensions allowing the geometry to be understood, as opposed to most crystallographic visualization software, where rotation must be done one view at a time. This visualization would be even more powerful, if one could also visualize the electron or nuclear charge density around atoms that is derived crystallographically from Fourier maps. Our goal is to import and display Fourier intensities derived using the GSAS package. GSAS (General Structure Analysis System), is a comprehensive system for the refinement of structural models from both x-ray and neutron diffraction data. It can generate these Fourier maps, but it does not offer graphics as highly advanced as FOX. In this project we are adding a new feature to FOX that will allow it to display a Fourier density in a region of space defined by the user using the Marching Cubes visualization algorithm. Marching Cubes is optimized to be most effective for rendering charge distributions, with a recursive approach when the number of 'objects' to be graphed is known, alternately a brute-force algorithm must be used. A second aspect of this project has been to add the capability of export of structural information into the XML format used by FOX into the EXPGUI program. Finally, a novel idea for a 3D cursor that could be used to select boundary volumes in the Fourier map is being explored.

Characterization of MEMS Microheating Elements
Michael Vahey

Understanding the conditions in which a microelectronic device operates and the subsequent response of the device to these controlled stimuli is an integral part of research in micro electromechanical systems, or MEMS. The objective of this project is to characterize the various behaviors of a microheating element, a MEMS device comprised essentially of a resistive bridge (encapsulated in silicon dioxide and suspended over an etched pit) across which a voltage is applied, leading to joule heating. By measuring the device's behavior in both the steady state and transient cases through electronic, optical, and mechanical techniques, a more robust characterization of the device can be obtained. Towards this end, the following approach has been adhered to. First, an IV characteristic for the device is obtained, from which temperature information can be extrapolated. Optical measurements of temperature can also be acquired through the use of a scanning infrared microscope. Computer modeling is then employed as a means to connect these two sets of data and to reconcile any disparities between them. In so doing, information about the convective, conductive, and radiative properties of the device is obtained. The subsequent knowledge of the device's parameters, in conjunction with measurements from a Doppler vibrometer in

which the device is excited both mechanically (through a piezoelectric transducer – a miniature shaking table) and electronically (through various direct input signals), allows one to form a more fully standardized picture of the device's operation and aids in the interpretation of future measurements.

Case Western Reserve University

Reference Value Estimators in Key Comparisons

Margaret Polinkovsky

Key comparisons are international interlaboratory comparisons for weights and measures that combine information from National Metrology Laboratories (NMIs) around the world. The purpose of Key Comparisons is to establish the equivalence on different NMIs in measuring a key reference value. The participating laboratories conduct parallel experiments using agreed-upon procedures and common artifacts or common definitions of the event. Each laboratory calculates its best measurement (estimate) and gives an associated experimental variance (Type A) and a "Type B" uncertainty. "Type B" uncertainty arises from fluctuation in the experimental equipment and other outside sources that affect the entire experimental procedure at each participating laboratory. The problem is how to combine the estimates from the various participating laboratories. Since each laboratory has its own "Type B" uncertainty (as well as its experimental variance), several different overall estimates have been suggested.

The performance of six competing estimates is examined by simulation and study of several data sets from actual Key Comparisons. The competing estimators are mean weighted by experimental variance, mean weighted by combined Type A and B uncertainties, unweighted mean, median, Graybill-Deal estimator, DerSimonian-Laird estimator, and modified Mandel-Paule estimator.

Empirical probability density function were generated for the six estimators and compared. Also, the comparative offer of "Type B" uncertainty was evaluated in relation to the Type B/Type A ratios. Simulations were based on assumption of symmetric and distributions of measurements and later will be extended to the asymmetric case. Also, the simulated model "Type B" uncertainty both as a bias and as a random effect from either a symmetric or an asymmetric distribution.

College of William and Mary

Ballistic Magnetoresistance in Nanocontacts

Andrew Busch

While the amount of information that can be stored on a hard disk is growing by leaps and bounds, there is a need to create new storage technologies if this growth is to continue. Ballistic magnetoresistance (BMR) is considered a promising way of solving this problem.

Throughout this summer, we have tried to create nanocontacts displaying this BMR effect. My talk will discuss BMR, and may illustrate several experiments performed to this end. The success and failure of several of these experiments may also be discussed.
In general, we have employed three methods to create contacts. One method uses CrO_2 to make contact between nickel wires, one uses photolithography to create CrO_2 contacts, and one uses electrodeposition to create a nickel contact between nickel wires. Both strategies were employed to varying degrees of success. In the past, electrodeposition has been used to create nanocontacts with very high magnetoresistance. On the other hand, CrO_2 has never been used to create nanocontacts, but because of its special properties, many hope that it will display a large effect. If photolithography could be used to create devices of this kind, it would be very important, because the semiconductor industry already uses this technique, and less new equipment would be needed. Once these contacts are made, we determine the magnetoresistance by measuring the resistance under different magnetic fields.

20-Bit Precision Electronics for the Electrically Substituted Bolometer (ESB)

Kathryn Ellen Keister

The Electrically Substituted Bolometer (ESB) was developed for use as a direct transfer standard detector in the 200 nm – 20 μm range. Silicon-photodiode trap detectors can only be used up to about 1 μm, and room temperature pyroelectric detectors pick up too much background noise. The ESB is helium cooled to limit the noise, and the silicon bolometer can be used well into the infrared region. It will ultimately be used as a low-noise reference detector in the IR SIRCUS facility, particularly at low power levels. In initial development tests, the ESB was controlled and data was collected with an RS-5900 radiometer, which has only 15 bits of precision. The ESB has a noise floor of 10 $pW/Hz^{1/2}$; so to utilize its full range, 20 bits of precision are required. To implement this, a number of commercially available digital multimeters and function generators were combined using LabVIEW VIs and analog circuitry.

Cornell University

Quantum Computing Simulation Optimizations and Non-Gaussian Errors on a Gaussian Density Operator

Eric Hsu

The theory behind quantum computing and information has advanced well beyond any physical implementation. Many theoretical performance bounds and capabilities of complex algorithms have been established. However, leading scientists in quantum computing have developed only simple physical realizations of quantum computers. Quantum computer simulation will help bridge this disparity between high-level algorithms and quantum computer construction. Eventually we hope to optimize the layout of qubits and other physical components analogous to bits, circuits, and gates in classical computers.

Since simulating quantum information requires exponentially more processing power and resources on classical computers, we need fast algorithms and performance assessments. We developed algorithms, which create single qubit gates and controlled qubit gates, that are moderately faster than the algorithms that other quantum simulators use, and analyzed other programming practices that show noticeable improvement. Analysis was done through timing runs in Matlab and through computational complexity analysis.

In addition, we used our simulator to explore elementary quantum algorithms and their resistance to various quantum noise and errors. And we are investigating an assumption made in the design of our simulator. Specifically, we are researching the effects of non-Gaussian distributed errors on density matrices. Density matrices, which completely describe the state space of any isolated physical system, assume that all quantum noise and errors have a Gaussian distribution.

Drexel University

Translation Inference in the Process Specification Language

Joe Kopena

Development of the Process Specification Language (PSL) is an ongoing effort at NIST. PSL defines a neutral representation for business and manufacturing processes. The goal of the effort is to develop an interchange language, which can be used to exchange information between applications such as process planning, production scheduling, and manufacturing control tools.

PSL is defined using first order logic to avoid the ambiguity and informality associated with traditional standardization efforts. However, in PSL's role as an interchange format it may be seen as undesirable for applications to exchange arbitrary statements in first order logic. Such an exchange would require that both applications incorporate a first order reasoning mechanism in order to manipulate and work with exchanged information and would incur the associated computational and programmatic complexity costs. Many potential users of PSL have requested that alternative transport mechanisms be developed to avoid these issues while maintaining a grounding in PSL's formal definitions.

One technique employed in PSL to combat this issue is to restrict the form of the statements used in exchanging information. By not allowing arbitrary first order statements the computational and programmatic complexity required to process exchanged information can be constrained. This talk will explore two aspects of this technique: developing versions of PSL using less expressive languages than first order logic, such as description logics; alternately, restricting the form even more drastically and applying abstract grammars to concrete syntaxes as in traditional file formats. In particular we will discuss the development of a subset of PSL using the DARPA Agent Markup Language and using the definitions present in PSL to prove that the contents of given grammars cover intended classes of PSL entities.

Georgia Southern University

Swimming in a 3D Optical Lattice
Lisa Marie DeBeer

The goal of this project was to create a set of tools that aid both theorists and experimentalists in visualizing the optical potentials created by lasers applied to Bose-Einstein condensates and the energy spectra of these potentials. An important step along the road to the realization of a neutral-atom as quantum- computational device is the ability to manipulate atoms in an ultra-precise way. One method to accomplish this is by trapping a Bose-Einstein condensate (BEC) in a space-periodic optical potential created by counter-propagating laser beams called an "optical lattice." A Bose-Einstein condensate is a collection of atoms that all share the same quantum-mechanical wave function. Understanding the behavior of BEC's in optical lattices should be key to the design of future quantum- computing devices. Optical lattice potentials created by more than two laser beams can vary in space in a complex way so that the ability to visualize them is useful for both theorists and experimentalists. I have created two tools to perform such visualizations: (1) A stand-alone program that can execute on a windows PC, and (2) a 3-D visualization that uses the NIST Reconfigurable Automatic Virtual Environment (RAVE) facility where users can swim through the optical potentials and Band Structure landscapes interactively. I will demonstrate the stand-along program and describe the RAVE-based tool.

Grinnell College

Reference Lines in the Optogalvanic Spectra of Thorium and Uranium Over the Wavelength Range 422 – 462 nm

Sarah Campbell

The optogalvanic spectra of thorium and uranium provide reproducible, convenient, and highly accurate reference lines. These lines provide a wave number standard and aid the calibration of wavemeters for high-resolution laser spectroscopy. The optogalvanic method allows for a simple optical setup and detection. Problems associated with molecular-iodine vapor cells (Doppler broadening, hyperfine structure, complicated optical setup) and alkali two-photon transitions (high laser power, low absorption probability) are avoided.

Thorium and uranium are ideal sources due to their narrow symmetric profiles. Hollow-cathode lamps for both thorium and uranium were used, with a single-frequency ring dye laser operating in the range 422 nm to 462 nm, to observe the spectra. Eight thorium lines and nine uranium lines were measured with our Fabry-Perot wavemeter with an accuracy of a few parts in 10^8. The results improved upon earlier measurements, determined by Fourier-transform spectroscopy.

Synthesis of $HSCH_2CH_2CH_2O(CH_2CH_2O)_{3\text{-}8}CH_3$ and Characterization of Their Self-Assembled Monolayers on Gold

Thomas Parr

The synthesis and characterization of a homologous series of methyl-ω-(3-mercaptopropyl) oligo(ethylene oxides) [$HSCH_2CH_2CH_2O(CH_2CH_2O)_{3\text{-}8}CH_3$] and of their self-assembled monolayers (SAMs) on gold will be discussed. On the basis of studies of related series, such as the SAMs of $HS(CH_2CH_2O)_{3\text{-}6}CH_3$, we have found that the structure, more specifically, the conformational order of the oligo(ethylene oxide) [OEO] segments, CH_2CH_2O, is important for two very different reasons. SAMs with disordered OEO segments are, arguably, the most protein resistant surfaces known, which is important to biomedical implants/contact lenses, biosensors, and the maritime industry. On the other hand, SAMs with ordered OEO segments, which adopt a helical conformation oriented normal to the substrate, might be useful as ultrathin film thickness standards below 10 nm. This presentation will briefly describe the synthesis of the compounds, the reflection-absorption infrared spectroscopy (RAIRS) spectral characteristics of ordered and disordered OEO SAMs, our results of the RAIRS and spectroscopic ellipsometry (SE) measurements on the SAMs assembled from 95% ethanol and 100% water, and, if time permits, the results of protein adsorption experiments.

Gustavus Adolphus College

Optimization of Portland Cement Pastes Containing Fly Ash: An Empirical Approach
Chad Custer

In some instances replacing some percentage of Portland cement with fly ash results in a better product. The sample is stronger under compression tests and the permeability of the sample decreases resulting in increased durability. However, there are several different categories of fly ash and of Portland cement and these benefits only ensue when the fly ash and the cement are properly matched. If they are not, the introduction of the fly ash into the cement can result in worse performance.

In order to be able to better understand the relationship between fly ash and Portland cement, it is desirable to be able to perform many tests of the properties of the hydrating paste with varying percentages and types of fly ash and cement. Three tests, which can give a look into the properties of the cement/fly ash sample, are temperature rise, acoustic wave propagation, and conductivity changes during hydration. The purpose of this research is to develop a cell that can simultaneously measure these three properties for hydrating samples. Thus far acoustic wave propagation measurements and temperature measurements have been incorporated into a cell of size ~125 cm^3. By means of several trials, a correlation has been found between acoustic wave propagation and initial set time; however, research needs to be continued before any hard conclusions are drawn.

In the future, conductivity measurements will be incorporated into the cell and finally the cell will be miniaturized to a size of approximately 2 cm^3. Using this cell as a basis for a high volume of measurements, vast arrays of data will be able to be collected for empirical analysis thus leading to a better understanding of how fly ash and Portland cement interact leading to an optimization of fly ash/cement mixtures.

Hamilton College

Spectral Narrowing of a High-Power Diode Laser Array for Spin-Exchange Optical Pumping
James Baker

Spin-exchange optical pumping is a method to produce nuclear spin-polarized 3He gas that can be employed for neutron spin filters. In this method, the electrons in Rb atoms are polarized by a laser, and during collisions with 3He this polarization is slowly transferred to the 3He nuclei. The typical spin-exchange system uses a high-power, broadband diode laser array. The bandwidth for such diode lasers is 2 nm (1000 GHz), while the pressure-broadened absorption width of the Rb is only ~0.04 nm/bar (18 GHz/bar). We are increasing the effectiveness of the pumping system by narrowing the bandwidth of a diode

laser array from 2 nm to 0.2 nm (100 GHz). The narrowed laser is better suited for optical pumping, and can produce higher polarization values than systems with a broadband spectrum.

Harvard University

The Production of Nitrogen-13 by Neutron Capture in Boron Compounds

Monika Schleier-Smith

The $^{10}B(\alpha, n)^{13}N$ reaction was studied as a secondary activation process in which the source of α-particles is the neutron capture reaction $^{10}B(n, \alpha)^{7}Li$. This secondary activation, while relatively improbable, is of concern to an experiment for obtaining a precise measurement of the neutron lifetime by magnetically trapping ultra-cold neutrons and detecting their decay; in that experiment, boron compounds are used as neutron shielding materials, and any background radiation resulting from activation in the shielding must be taken into account. The production of the positron emitter ^{13}N, in particular, is potentially problematic because the 863 s lifetime of ^{13}N is almost the same as the neutron lifetime. To investigate the ^{13}N production in the shielding materials, samples of boron carbide, boron oxide, and boron nitride were irradiated with a high flux of thermal neutrons. For each compound, the rate of ^{13}N production was determined by subsequently counting with a high-purity germanium detector the number of 511 keV annihilation photons produced as a function of time. The results may help to reduce the uncertainty in the neutron lifetime measurement.

Jackson State University

Chemical and Electrochemical Synthesis of Gold-Polymer-Gold Nanowires for Multifunctional Sensor Investigation

Angela Denise Fortner

Nanometer scale wires composed of gold and conducting polypyrrole (Ppy) segments were successfully synthesized. First, a synthetic protocol used to prepare striped metal nanorods was modified to create these new Au-Ppy-Au nanowires. These nanowires were produced by a combination chemical and electrochemical synthesis of gold and polypyrrole inside pre-formed nanoscale templates of anodic alumina membranes. The conducting polymer was chosen due to its electrical properties and the ability to induce free volume (pores) in its matrix. This offers a unique opportunity for incorporating sensing elements into the system. Moreover, the properties were further tested, as a function of concentration, to analyze their resistance. Proteins were added to the analyzed polymer matrix. As a result of this development, it is foreseeable that these nanostructures can be used as multifunctional nanosensors able to accommodate infinite chemical and biochemical substances.

James Madison University

X-Ray Microscopy with Multilayer Mirrors in K-B Configuration
Evan Schwartz

The design, alignment and applications of x-ray microscopy are discussed using a standard sealed x-ray tube source. Two spherically curved multilayer mirrors were placed orthogonal to each other at a fixed distance apart (Kirkpatrick-Baez). The position of these mirrors was controlled by a *xyz* translation stage with pitch and yaw maneuverability. A translation stage was also used for a commercial x-ray CCD camera, which integrated several hundred frames into one composite image in less than 30 seconds. After optimizing the equipment and geometry of the system, prefabricated copper transmission electron microscope grids absorbed CuKα radiation (8 KeV) to produce a field of 100 μm and a resolution of 4 μm. Although spherical aberration limited the quality of our images, we have shown that this systems' fast imaging capabilities proves to be a valuable tool in the field of microanalysis. With the addition of a rotational sample stage, future applications of this technology could be used to do tomography or microscopy on the internal cavities of micromachined electro-mechanical devices (MEM's).

Kent State University

Calibration and Evaluation of Prostate Brachytherapy Seeds at NIST
Violeta Beleva

Brachytherapy is a form of radiation therapy in which small sealed radioactive sources, or "seeds" are injected in or near the tumor or lesion, and thus deliver radiation dose to the cancer while minimizing exposure to surrounding tissues and organs. At NIST, characterization of the strength of brachytherapy sources used in the treatment of prostate cancer involves the comparison of several measurement techniques. The relative responses of the primary standard instrument for measuring air-kerma strength, the WAFAC (Wide-angle Free-air Chamber), and three different well-ionization chambers (secondary standard instruments) are compared. The results are related to the emergent x-ray spectra of the seeds, and the effects of emission anisotropy of different seed designs are examined. To characterize the energy spectrum and the composition of the seeds, a High Purity Germanium (HPGe) detector is used. To observe emissions over an even wider x-ray and gamma-ray energy range, a new Broad Energy Germanium (BEGe) detector was implemented. The air kerma strength calculated from spectra can be compared with the results obtained by the WAFAC. The BEGe detector was also used to measure spectra at different distances from the source and investigate the effect of seed emission anisotropy on the inverse square law dependence of the air kerma rate. Additionally, by exposing the seeds to radiochromic film, the internal distribution of the radioactive material could be observed. To verify constancy of internal seed composition

and geometry with the manufacturers' specifications, x-ray transmission radiographs using Fuji plate detection were taken.

Loyola College

DNA Sequence Detection Through the Use of Peptide Nucleic Acids

Heather Begley

Peptide Nucleic Acid (PNA), a recently created nucleic acid analog, is formed by replacing the sugar-phosphate backbone of DNA with repeating N-(2-aminoethyl)-glycine units, thereby creating a neutral backbone. Despite these changes, PNA still contains the same nitrogenous bases as DNA and is thus capable of sequence-specific binding to DNA. The novel utility of PNA lies in its overall neutral charge, as this property allows PNA to form bonds with DNA that are stronger than DNA/DNA bonds. In contrast to DNA/DNA bonds in which each molecule has a negative charge, PNA/DNA bonds have no repulsive forces to overcome and thus the bonds acquire additional strength.

In our experiment, we hoped to combine the important properties of PNA/DNA interaction with the interesting research being done in the field of microfluidics. In a microfluidic channel with a temperature gradient, it is possible to balance the bulk velocity of solution against the electrophoretic velocity of a charged analyte, thereby focusing a charged species to one distinct site in the channel. Since PNA lacks a charge and is therefore unaffected by the electric fields used in electrophoresis, PNA will not focus if it is placed in the channel alone under these conditions. However, if the complementary strand of DNA is also introduced into the channel, the two species will hybridize and the PNA/DNA complex will focus to a distinct point. By tagging the PNA with a fluorophore, this focusing phenomenon can be observed spectroscopically, providing a new detection scheme for DNA in microfluidic systems.

Analysis of Ephedra Alkaloids in Dietary Supplements

Kerry Begley

Capillary electrophoresis was utilized to study the ephedra alkaloids most commonly found in certain dietary supplements. The plant genus *Ephedra*, which is also referred to by its Chinese name, Ma Huang, naturally contains the alkaloids (-)-ephedrine, (+)-pseudoephedrine, (-)-methylephedrine, (+)-norpseudoephedrine, and (-)-norephedrine (also known as phenylpropanolamine). Extracts from these plants are often found in dietary supplements, however, variations from plant to plant can lead to inconsistencies within these products, including lot-to-lot variations and deviations between the product label and actual content. In addition, because only one isomer of each compound occurs naturally, the detection of the other isomer within a dietary supplement suggests that the compound did not come from the plant. As a result, monitoring the content of these ephedra alkaloids in

dietary supplements becomes extremely important for safety reasons, as consumers are often unaware of the amount and strength of the alkaloids ingested. Therefore, ephedra alkaloids, including ephedrine, pseudoephedrine, phenylpropanolamine, and methylephedrine, were separated into their two ((+) and (-)) isomers using capillary electrophoresis. In order to optimize the separation of these compounds, the experimental parameters, specifically the pH of the buffer solution, the voltage, the temperature of the system, and the composition of the buffer, were systematically varied. Eventually, a buffer consisting of 25 mM NaH_2PO_4 and 2.5% sulfated cyclodextrin, a voltage of –12 kV, and a temperature of 20 C were decided upon and comparisons between the electropherograms of the dietary supplements and those of the ephedra alkaloid standards provided a means to analyze the actual content of the supplements being examined.

Massachusetts Institute of Technology

Structure and Magnetic Properties of Electrodeposited Co and Co-Fe Thin Films on GaAs (001)

Alexandra Ford

Co and Co-Fe thin films have been electrodeposited onto n-type (001) GaAs. The structure and texture of the Co films were investigated using x-ray diffraction and transmission electron microscopy (TEM) while the magnetic properties were examined using a vibrating sample magnetometer (VSM). For films with a thickness greater than 32 nm, a hcp-Co (1120)[001] || GaAs (001)[110] orientational relationship was observed. For films less than 32 nm thick the in-plane magnetic response was isotropic, while for thicker films (133 nm to 800 nm) four-fold anisotropy was observed congruent with the structural texture. For the thickest films (1200 nm) a significant (1010) texture developed which yielded uniaxial magnetic anisotropy. In several films (8.5 nm to 15 nm) a thin bcc-Co layer was observed between the GaAs (001) and the hcp-Co (1120) overlayer. The bcc layer formed with a cube-on-cube relationship to the GaAs (001) substrate. The structural evolution is similar to that reported for films grown by other methods, such as molecular beam epitaxy (MBE), although the thickness at which the various magnetic transitions occur differ significantly due to the different growth rates employed.

McDaniel College (formerly Western Maryland College)

Characterizing the Response of Thermoluminescent Dosimeters to Beta, Gamma, and Broad-spectrum X-Ray Radiation

Christopher Martin Drupieski

Thermoluminescence is the thermally stimulated emission of light from an insulator or semiconductor following the previous absorption of energy from radiation. Materials exhibiting thermoluminescent properties may be used as radiation dosimeters, for the

amount of light emitted by a thermoluminescent material is proportional to the dose of radiation it has received. The purpose of this research has been to examine the properties of several varieties of commercially available LiF thermoluminescent dosimeters. The dosimeters' responses to various doses of radiation from the isotopes Sr-90 and Co-60 have been measured. X-ray irradiations of the dosimeters were conducted on a low-energy x-ray calibration range, and with a 50kV handheld x-ray probe source designed for cranial brachytherapy and intraoperative applications with applicators. This research has investigated the dependence of the dosimeters' response as a function of irradiating photon energy, and has sought to determine how accurately one can predict the response of the dosimeters for broad-spectrum x-ray irradiations.

Miami (Ohio) University

Uranium and Thorium : Radioactive Refugees or Simply Irresistible?

Kathryn A. Lee

A resistate is a mineral that resists weathering and chemical treatment. Some resistates contain isotopes of uranium and thorium. This can produce inaccurate data when scientists analyze samples of soil if not all of the sample is dissolved. Seven common resistates (allanite, apatite, monazite, pyrochlore, titanite, xenotime, and zircon) were chosen and heated in solutions of hydrofluoric and nitric acids for up to 14 days in order to test how much of each resistate dissolved. These samples were also tested to see how much uranium and thorium were released by the acid treatment. The results indicated that allanite and zircon contained considerable quantities of U and Th but very little was released during strong acid treatment. On the other hand, a considerable amount of titanite dissolved. Although we found that some resistates are more readily dissolved by strong acids, these data can be used to help evaluate the efficacy of radioanalytical methods and improve the certification of standards.

New Mexico State University

Scalability and Performance Limits of Planar and 6D Parallel Cantilever Bi-Axial Micro-Positioner (PCBMP)

Derek Powell

The talk will contain a brief description of the project that I have worked on over the summer of 2002. The aim of this project was to create scale models of preexisting two and six degree of freedom PCBMPs designed here at NIST. Using the parametric modeling capabilities of Pro/Engineer, CAD models of the planar and the six-degree of freedom (6DOF) positioners were made so that they could be scaled to any size needed. A brief description of the design of the current XY micro-positioner and the results of a finite element analysis on this model will be presented. The results will include the maximum displacement and stress behavior

for three different sizes of the planar micro positioner. Based on the result from the analysis a 1/4 sized model of the current micro-positioner is going to be constructed. Problems encountered as well as the method for analysis will be worked in with the discussion. The pros and cons of the finite element program Pro/ Mechanica, which is integrated into Pro/E will be presented. The design for the 6DOF micro-Positioner will be looked at and I will discuss how the final design of this model will be based on the parametric model that has been created. The ability for Pro/Engineer to read data from a text file and modify the final design of the 6DOF will be necessary. A mathematical program that is already in use can define the size and movement range needed from the linear stages used to operate the 6DOF design. A user will identify the output needed from the 6DOF stage; the program will give the required inputs from the linear stages and print a text file with the information needed by Pro/E. Pro/E can then regenerate the model and any analysis needed could be performed at that time. This whole process will be summarized as well as the process by which a basic analysis in Pro/Mechanica is run.

North Carolina State University

Synthesis and Characterization of Titanium Dioxide (TiO_2) Nanoparticles and Nanostructured Films

Robyn Bloch

Due to its photocatalytic properties, Titanium Dioxide, or TiO_2, has expanding applications that reach far beyond the common use as a pigment or filler for coatings, plastics, or paper. Some of these applications include air and water purification, self-cleaning window glass, anti-microbial surfaces, bioweapon decontamination, and even non-toxic cancer treatments. The scope of the project was to find an optimal method of preparing a continuous film of TiO_2 and then determine what physical properties optimize or minimize photoreactivity. Preparation methods included solvent casting of both pigmentary and nanoparticle size TiO_2 as well as sol-gel synthesis. Physical characteristics such as particle size, morphology, and topography were observed using a confocal microscope. Metal contacts were deposited on the surface of the films and photoconductivity was measured. With this information we will be able to relate the physical properties of TiO_2 to its photocatalytic response.

Northeastern University

Fusion of Face-Recognition Algorithms via Nonparametric Dependence Characteristics

Igor Malioutov

The statistical problem of combining classifiers has important applications in biometrics. By fusing the similarity scores from different face-recognition algorithms one can gather additional information about the identity of the probe images. The underlying theoretic methods devised for this task also have important applications in fields other than biometrics.

In our study four nonparametric fusion methods based on the weighted averaging approach were proposed. The resulting classifiers were tested on three large datasets of similarity scores for the best four preselected face-recognition algorithms. Several different criteria were used for evaluating performance. These included the Cumulative Match characteristic (CMC) and Receiver Operator Characteristic (ROC) Curves for the classifiers, the expected values of the distribution functions, i.e., the mean rank assigned to the true images, and areas under the ROC curves. In general, the outcomes of our simulations show that these criteria resulted in similar characterizations. Other factors such as computational efficiency and numerical tractability of the methods were assessed.

Simulations for the proposed methods demonstrated a superior, robust performance that matched and at times exceeded that of the best constituent face-recognition algorithms. However, numerical optimization for the methods is desirable. Further generalizations for different metrics such as Cayley's, Footrule, and Kendall's distances were considered. Other considerations such as studying the effect of varying sizes of training datasets on algorithm performance and the potential improvements when combining multiple algorithms are put forward.

Pennsylvania State University

BaO-ZnO-Ta2O5 and BaO-ZnO-Nb2O5: Phase Equilibria for Talking Ceramics

Evan Pickett

Ceramic dielectric resonators and filters are essential components for cellular base stations and hand-held wireless devices. The system BaO-ZnO-Ta2O5 had not been previously investigated but contains the commercially important compound Ba3ZnTa2O9, used in 2.2 GHz base stations. The system BaO-ZnO-Nb2O5 likewise had not been investigated but contains the compound Ba3ZnNb2O9, which may be commercially developed. Understanding the phase equilibria in these two systems may facilitate improvements in the processing of these ceramics, lowering costs and improving performance.

NIST research maps out the phase behavior of the system in question and provides this map to industry as a processing tool. Three new compounds were discovered in each of these two systems. The ultimate goal is to determine the precise composition, melting point, and crystal structure for each of the six compounds discovered.

This presentation details the research that was conducted, the methods that were involved, and the pertinence of the results to the ceramics industry.

Purdue University

Effects of Surfactant Polymerization on Micellar Structure
Thomas Young

The effects of counterion polymerization of a cationic surfactant didodecyldimethyl-ammonium 4-vinylbenzoate are investigated with regard to the changing stability of the micellar structure with temperature, concentration, and solvent polarity. Conclusions about the nature of polymerized micelles are drawn from small angle neutron scattering measurements. Models are fitted to the SANS data to characterize the internal structure of the micelles. Several surfactant and surfactant/salt solutions such as cetyltrimethylammoniumvinylbenzoate and dodecyltrimethylammoniumvinyl tosylate/ NaBr were made to compare similar effects in different surfactants. The overall micellar structure in the polymerized samples will be measured with light scattering, and the absence of the vinyl group after polymerization will be shown via NMR and Infrared Spectroscopy. The micelles are hypothesized to consist of a nonpolar tail region on the interior encased in an area of ionic head groups, which is further encased in a stable "jacket" of polymer chains. The effects of polymerizing with varying amounts of initiator and copolymerizing with styrene, ethyleneglycol dimethacrylate, divinyl benzene, and methylmethacrylate are also discussed.

Radford University

Multi-Component, Three Dimensional, Viscoelastic Flow
Tim Dutton

A computer simulation program to model the flow of a multi-component, three dimensional, viscoelastic flow is in the process of being written. The program implements the use of the Giesekus constitutive equation to describe the rheological behavior. Similar programs have been written for Newtonian fluids but these do not account for any amount of the viscoelasticity, which is inherent in Non-Newtonian fluids. The way in which suspended drops in a viscoelastic blend break up is greatly different from blends of Newtonian fluids, and is important for industrial purposes. This program would be the first to accurately describe these actions for a viscoelastic fluid in three dimensions.

Rensselaer Polytechnic Institute

An Adaptive Leasing Mechanism for Jini™
Kevin Bowers

Distributed computing environments require strategies by which components can detect and recover from failures in remote, collaborating components. Many protocols for distributed systems employ a strategy based on leases, which grant a leaseholder with access to data or services for a limited time (the lease period). If the leaseholder does not renew a lease before expiration of the lease period, the lease grantor assumes the leaseholder has failed, and terminates the lease (withdrawing the previously granted access). Choosing an appropriate lease period requires consideration of tradeoffs among resource utilization, responsiveness, and the number of leaseholders. We investigated these issues in the context of Jini™ Networking Technology, a service-discovery protocol created by engineers and researchers at Sun Microsystems. We began by modeling the current Jini implementation, aiming to establish an optimal lease period. We found that system responsiveness is directly proportional to the lease period. Further, because leases with shorter periods must be renewed more often, we found an inverse relationship between lease period and bandwidth utilization. Based on our results, we can now determine the optimum lease period (and therefore the best responsiveness that can be achieved) for a specified bandwidth and number of leaseholders. However, as the number of leaseholders varies, Jini cannot easily adjust lease periods to maintain the best responsiveness. We propose a modification of Jini leasing procedures that allows lease periods to be dynamically adjusted to maintain optimum responsiveness for fixed bandwidth utilization as the number of leaseholders varies. We anticipate that similar procedures could add adaptive capability to other systems that rely on leases as well.

Building a Multi-Biometric Authentication System
Jack Damerji

Tightened security nowadays brings the need to search for more secure systems. Multi-biometric authentication systems using different types of biometrics - iris recognition, face recognition, hand geometry, and fingerprint scan - are being implemented to accomplish security objective. Examples from each of these systems were installed and studied.
A number of problems and challenges were inherent in each biometric system.

For example, Iris Recognition exposed problems during the enrollment process; users wearing eyeglasses had difficulties at enrollment and verification due to the reflective light from their lenses. Face Recognition showed a definite dependency on lightning backgrounds and on the number of pictures stored for each user. Also, recognizing faces that had changed, like growing a beard or having a different haircut, produced longer identification delay times or even non-recognition of some users. Hand Geometry reader could be tampered with easily since the reader includes the door controllers making it a security vulnerability. Also, the way the hand is placed on the Reader's scanner is essential for proper enrollment and verification. Finally, fingerprint depends on the quality of the user fingerprints. Dry or cracked hands may cause some irregularities.

We evaluated each system and assessed the strengths and weakness and determined their best configuration settings. We are planning to build a combination of these existing systems. By using the combinations, we will be able to solve most of these problems and minimize false rejections and acceptance rates.

Fire Pattern Re-Creation
Maureen Elizabeth Desi

Arson is one of the top causes of fires and fire deaths in the United States. The annual direct dollar losses from arson are approximately $3.6 billion dollars. Recent changes in court rulings require expert testimony that is technically defensible. In other words if something cannot be proven based on scientific principles or recreated in an experiment, then it may not be admissible as evidence in court.

As part of a larger effort to develop scientific tools for fire investigation, a series of experiments were conducted to investigate the feasibility of using computer simulations to re-create quantitatively real fire burn patterns. NIST's Fire Dynamic Simulator (Version 2.2), a computer model which includes the chemistry and physics of fire phenomena, and its associated visualization program, Smokeview, were used to simulate the exposure of gypsum wall board panels to the thermal radiation of a fire. Samples of gypsum board were placed at different distances from a natural gas fired radiant panel and thus exposed to a range of heat flux values. Three separate thermocouple sensors were used to monitor the temperature at the front, middle, and back of each board. These temperatures were used in conjunction with the char depth and calcination through the board to examine the impact of a predetermined heat flux on the sample. The char area and overall burn pattern were also considered when comparing the experimental burn patterns to the burn patterns predicted by the model. A radiometric thermal imager camera was used to collect qualitative thermographs of different sample specimens. The Fire Dynamic Simulator was used to generate a heat flux map for the different distances from the panel to allow comparison to the thermographs. Preliminary results suggest NIST's Fire Dynamics Simulator can be an extremely effective method of modeling burn patterns.

Temperature Control of the NIST Electronic Kilogram
Reza Hosseinzadeh

The ultimate goal of the NIST Electronic Kilogram project is to redefine the SI unit of mass (Kilogram) by an accurate determination of Planck's constant. This project uses a 2-story high Watt Balance that requires good temperature stability. The focus of this presentation is the implementation of a control system, which regulates the air temperature in the non-magnetic building where the NIST Watt balance resides. To accomplish this task, hardware interfacing was installed and a LabVIEW program was developed for the temperature control system. The control system is implemented for 5 different areas and controls the temperature to 0.1 Kelvin accuracy.

Design and Development of a Measurement and Control System to Calibrate Line Pitch Samples on the AMRAY Scanning Electron Microscope
Eranga Tyrrol Crossley Jayewardene

The Nanoscale Metrology Group of the Precision Engineering Division measures the pitch spacing on silicon samples to the lowest uncertainty possible. These samples are then used by the semiconductor industry to calibrate the magnification levels on their own scanning electron microscopes (SEM). The AMRAY SEM has been upgraded with a new measurement and control system and since uncertainty of instrument is pushed to the nanometer level, developing an analysis system to evaluate the pitch measurement becomes increasingly important. This talk will discuss the design and development of a new LabVIEW based measurement and control system and the analysis capability that has been completed.

Wafer Inspection at Low Dimensions: Automated Resistivity Mapping System
Mark Matarazzo

Integrated circuits (ICs) are dependent on the uniformity of the semiconductor they are composed of. Great variations or defects in the properties of the semiconductor over small distances can interfere with the operation and performance of ICs made from that material. Therefore, it is essential to ensure that current methods of growing semiconductors result in uniform properties throughout the growth.

In 1991 Joseph J. Kopanski showed that resistivity variations in a silicon wafer could be mapped with high spatial resolution. This was accomplished using an Alessi ECC-01 probe station, equipment to measure voltage and current, and a four-probe measurement technique designed to eliminate probe contact resistance. Since that time technology has evolved to the point where the program used to control the process, written in ASYST, is obsolete. With the advent of Gallium Nitride (GaN) use in the semiconductor industry and the current difficulty to grow uniform wafers of GaN, resistivity mapping is necessary once again. A program to control the process was written for use with current technology and results comparable to those found previously were obtained.

1-, 2-, and 4-probe systems of measurement were explored over the course of the project in order to test various configurations of the equipment. Similarly, three different types of measuring resistance were employed to accommodate varying requirements users might have. Equipment included a personal computer (PC), a Keithley 426 source/measure unit, and an Alessi ECC-01 probe station. A program was written to filter outliers out of the data and the data was graphed using Matlab. When compared to data taken in the original study, it was clear that the same patterns existed in both sets of data taken.

Future applications of this project include the mapping of GaN wafers grown both locally and remotely and future tests of various masking procedures. The process will show variations in resistivity as small as two percent at scales of thousandths of an ohm-centimeter. This will clearly show small differences in resistivity at chip- and wafer-scale passes.

Rice University

Speaker Verification

Eliot Flannery

Since the inception of computing, passwords have served as the best protection against unauthorized access available to the casual computer user. Unfortunately casual computer users despise passwords, seeking at all times to beat the system and use an easy to remember (and hence easy to guess) password. Worse yet, passwords can be stolen, traded among groups, given out over the phone, or even written on a sticky note and affixed to a computer monitor. Biometrics seems to defuse this problem. The user simply presents his fingerprints, voice, eye, or some other physical aspect of himself and requests that he be approved by the computer. Voice verification is an attractive form of biometric authentication as it requires no special devices or expertise. Aside from using a microphone, voice verification can be performed entirely in software. This project successfully integrated voice verification with the Linux Pluggable Authentication Module framework, effectively allowing the user to recite a series of numbers into a microphone in place of a password. The voice verification program showed improved performance over the basic program it was based upon and ran successfully on a personal digital assistant. The voice verification program calculates a pitch

contour as well as Mel-scaled cepstral coefficients for a user speech sample. It then utilizes dynamic time warping to match up the similar aspects of the submitted speech sample and the stored reference template the user had created earlier when enrolling in the voice verification system. If the speech sample matches the reference template well enough the user is authenticated successfully. The verification system's performance was improved by averaging the submitted speech sample's features with those of the reference template upon successfully authentication. This voice verification program was shown to be portable across varied systems as well as effective in correctly authenticating users, though its performance is not yet ready for more than research or hobby use.

Rochester Institute of Technology

Magneto-Optical Indicator Film Imaging of Magnetostrictive Thin Films

Matt Aggleton

Magneto-Optical Indicator Film (MOIF) Imaging is being used to examine magnetic domain motion in magnetostrictive thin films. These materials are either amorphous TbFe and TbFe/FeCo multilayers acting as actuators or amorphous FeCoBSi (Metglas) and FeCo/CoB multilayers to be used as field or stress sensors. Initial shape, orientation, and the subsequent development of domains in these materials are being observed as either a magnetic field or an external stress is applied to the nanostructured materials. A description of this apparatus, including the special jig for applying the stress, will be presented along with results of the observations.

2002: A Nanoparticle Sizing Odyssey

Brad R. Conrad

Ceramics have been made for more than twenty five thousand years and are a thirty five billion dollar annual business in the United States. The use of ceramics is vital in such diverse areas as magnetic storage media, glass fiber optics, building materials, and even human implants. An important fact to keep in mind is that the process of manufacturing most ceramics starts with powders. Primary standard reference materials are vital considering that powders are an integral part of such a big business. Unfortunately, standard reference materials (SRMs) made of ceramic materials with size distributions below one micrometer are not currently available. The reference materials that exist exhibit chemical as well as physics properties that are significantly different than those demonstrated by ceramic powders. A reference material with more representative properties including particulate shape, size distribution, and even agglomerate distribution properties is vital for quality control and process monitoring during the manufacturing process. Lacking useful reference materials deters standardization of manufactured goods, restrains compatibility, and inhibits precise industrial and commercial communication. This talk will discuss and outline information gathered this summer in the qualification studies for a sub-micron titanium

dioxide powder for development as a size standard with a particle distribution between 100 nm -500 nm. The influence of sample and sample preparation parameters (e.g. dispersant, concentration, etc.) on the size and size distribution analyses by electron microscopy, laser light scattering and X-ray disc centrifuge will be discussed.

Saint Mary's College of Maryland

Comparison of Scanning Electron Microscope Simulation Programs MONSEL and Metrologia

Kevin Beanland

Metrologia and MONSEL are programs that use Monte Carlo simulations to simulate the pathways of electrons in the SEM. Metrologia's advantages are that it has more flexibility in the kind of sample geometries that can be used in the simulations; the disadvantage is that it also contains certain free parameters such as a "secondary depth" parameter, which is used to calculate the probability of secondary electron detection, and a scale factor parameter. These parameters make it inherently less accurate than MONSEL, which follows the pathways of the secondary electrons until they are detected. MONSEL however does not allow the same kind of flexible sample geometries. Since it would be beneficial to have the geometrical flexibility of Metrologia with the accuracy of MONSEL, simulations were run to find the Metrologia depth parameters and scale factors that produced secondary electron yields best matching the corresponding secondary electron yields of MONSEL. Sample geometries, involving varying tilt angles of the sides of the lines, were used to find the parameters for three materials; silicon, silicon dioxide, and PAR 810 resist, having two to three different incident electron energies per material. The results matched most accurately at 600 eV beam energy for silicon dioxide and PAR 810 and at 1 keV beam energy for silicon. The worst matches were for the 5 keV silicon and silicon dioxide simulations and the 1 keV PAR 810 simulation. We will test these parameters using more complex geometries to ensure they remain accurate.

Micro-Force Measurement with Piezo-Resistive Cantilevers

Jonathan Mulholland

Force is realized through the base SI units the kilogram, the meter, and the second. For the realization of very weak forces, the meter and the second can both be accurately measured on a small scale. Deadweights, the realization of mass, are only accurately manufactured on the order of milligrams. To realize a nanoNewton of force, it would be necessary to use deadweight on the order of one tenth of a microgram. This stumbling block has led the Microforce Realization and Measurement Competence project to search for alternative methods of force realization. In order to circumvent the deadweight problem an electrostatic force balance has been built to realize forces using the meter and the derived units the Volt and the Farad.

The Microforce project is also exploring transfer standards compatible with accurate small force measurements. This talk will detail the characterization of an atomic force microscope cantilever using the electrostatic force balance as a link to the SI unit of force. The procedure and its development will be discussed as well as the results of the project. So that the complete lifecycle of a transfer standard is explored, the calibration of a nano-indenter against the cantilever will be related.

Santa Monica College

The Cell General
Derrik Asher

The primary objective of my research is to create a polymeric surface that allows specific cells to 'believe' that they are adhering or binding to a biological site to which one of the cells functions is performed. Co-polymers were synthesized using the atom transfer radical polymerization technique with a methyl methacrylate backbone and polyethylene glycol combs. The compositions and molecular weight distributions of the co-polymers were characterized using NMR and GPC. Films of the polymers were cast onto silicon wafers by spin coating and the surface properties were characterized using contact angle measurements. The created surface will then have a peptide, a specific amino acid sequence, grafted onto the pMMA backbone as the PEG was. With the PEG blocking most of the area on the backbone, the peptide will be added in low concentration to bind the backbone in random positions. The peptides will then bind to the cells, and the cells will perform their function as if they were in an actual biological system.

Limitations on Scaling of Silicon Dioxide as Gate Dielectric
Maria Kim

As the sizes of complementary metal-oxide-semiconductors (CMOS) keep decreasing, the gate dielectric capacitance has to be increased to keep at least the same drive current. This has been accomplished by reducing the thickness of silicon dioxide (SiO2) in the devices. However, as this thickness is reduced, we are approaching a limiting point at which SiO2 is not very reliable as the gate dielectric. The interface state density (Dit) of the gate dielectric strongly affects the device drive current, and thus is directly related to its performance and reliability. One of my projects was to extract the Dit from some wafers using different techniques. One set of wafers was made of MOS capacitors, so the Dit was measured using the conductance technique. Another set of wafers had MOS field effect transistors (MOSFET), therefore the Dit was extracted using the charge pumping technique. These data provide information about the quality of the gate dielectric in these wafers. This part of the project is done in collaboration with SEMATECH.

My other project was to fabricate MOS capacitors using a 2-level mask set and perform physical and chemical measurements of the major films and process steps. Once the MOS capacitors are finished, the electrical properties (e.g. capacitance-voltage to extract thickness) will be measured. Then a comparison will be made between three different measurement techniques: (1) CV on MOS capacitors, (2) ellipsometry, (3) transmission electron microscopy (TEM).

Effects of Delay Mismatch in MPLS Networks with 1+1 Protection
Liliya Krivulina

High-capacity optical-fiber backbone networks protect information flows belonging to their premium customers by routing two copies of the customer's data over disjoint paths. This scheme, known as 1+1 protection, ensures that the customer will experience no service interruptions even if a fiber cut occurs somewhere in the network. A protection scheme based on this concept was proposed for Multi-Protocol Label Switched (MPLS) packet flows at the Spring, 2002, meeting of the Internet Engineering Task Force (IETF) by a team from Lucent. The Lucent proposal will require the MPLS routers located at the ingress and egress edges of the MPLS network to protect certain data flows by creating two disjoint label switched paths (LSPs). Packets using the 1+1 protection service are duplicated at the ingress router, assigned an ID number, and sent to the egress router over the two LSPs. The egress router retrieves the least-delayed copy of each packet and forwards it to the destination, discarding the more-delayed copy. A sliding window allows the egress router to function even when packet losses occur. This scheme allows data to flow even if a link failure occurs on one of the LSPs, but a sufficiently large difference in the propagation delays associated with the two protection LSPs can cause performance degradations that may reduce the protected flow's quality of service (QoS) below what is acceptable to the customer. In this project we use discrete event simulation in Java to examine the impact of delay mismatch on the probability of packet loss and on packet jitter, and we show that both of these metrics are adversely affected by large LSP delay differences.

Polarimeter Using Photoelastic Modulator
Han Kyu Lee

When the spectroradiometer is polarization sensitive and comparing two sources which have different polarization properties, the expected value from a simple equation that describes the relationship between the measurements of a spectral radiance standard, which used to calibrate the radiometer, and the unknown source is invalid. Consequently, polarization correction factor is applied into the simple measurement relationship; polarization corrector factor involves two variables: radiometer polarizance or the degree of linear polarization by the radiometer, and Stokes component from unknown source.

In the past, linear polarizers have been used in a motorized rotating mount to determine the polarizance from 200 equations characterizing the polarizer and radiometer. In addition, measurements are required at various wavelengths due to the characteristic of the polarizance that varies at different wavelength. The characterized polarizer and radiometer are then used to measure the polarization properties, Stokes components, of the unknown sources in order to determine the correction factor.
My project is to develop the procedure that determines the radiometer sensitivity dependence on a polarized source using a Photoelastic Modulator, PEM. PEM is an instrument used for modulating the polarization of a beam of light based on photoelasticity, the property of materials that acoustic deformation can cause the material to become birefringent. Birefringence is the property of a material that has different index of refraction for linearly polarized light in either direction. In a way, PEM works like a retarder, which serves to change the polarization of an incident wave. Therefore, by setting the retardation of PEM to be the half wavelength, the polarization of source light can be analyzed by modulating the polarization to shift periodically about orthogonal to each other at twice the frequency of the PEM. Using Mueller matrices, radiometer polarizance and Stokes component of the unknown are determined.

Southern Methodist University

Estimating the Work of Integer Partitions
April K. Andreas

For a given set of numbers, the integer partitioning problem is to divide the numbers into two groups, so that the sums of the numbers in each group have a difference of zero or one, or to decide it is not possible. We also have the constraint that each group has nearly the same number of elements. Finding such a partition is useful for allocating computing resources, in some thermodynamics problems, and in theoretical computer science as an example of a provably hard problem. We have developed a new method to estimate not only the work required for finding the optimal partition, but to also estimate the number of partitions that satisfy the constraints exactly. In the process of developing this method, it is also possible that we may have discovered a new test for random number generators.

Southern University and A&M College

That's Good, But You Can Do Better
Cari Bershell

Many radioactivity measurements are made on an annual basis within the United States to support environmental monitoring, nuclear waste remediation and occupational health. The reliability of these measurements are assessed for the laboratories participating in inter-laboratory comparisons, where the laboratories measurement performance is tested with

known but undisclosed concentration level. These inter-laboratory comparisons include the following matrices, which are all relevant to the environment: synthetic urine, synthetic feces, air filters, acidified water, and soil. Within these five matrices laboratories are to test for the following radionuclides: Am^{241}, Pu^{238}, U^{238} and Sr^{90}. Year after year these comparisons are ran, and we answer the question; are the quality of measurements consistent with the national standards. However, we have yet to answer the question; are these laboratories improving with time? We have evaluated the results of NRIP participants and have found them to be in general agreement with NIST values and some that indicate improvement over time. There are instances however, where the results may indicate: 1) matrix dependent differences in measurement capability; 2) constant positive or negative measurement bias; 3) systematically changing bias; 4) poor analytical reproducibility; and 5) poor evaluation of measurement uncertainty. The participating laboratories, should evaluate potential problems in their measurement system that may include, but are not limited to: 1) unstable isotope dilution standards; 2) incorrect calibration of the isotope dilution standards; 3) incomplete uncertainty evaluation; and 4) operator training.

Laser Tracker Calibration for Acquiring the Values of Alignment Parameters Through A New Technique of Using Distance Measurement with the Lieca LTD500 Laser Tracker

Brandan J. Darensbourg

The Leica LTD500 Laser Tracker is a coordinate measuring machine that can track and record the 3-D position of an optical target anywhere inside the instrument work volume. The laser tracker is a native spherical coordinate measuring system that uses a laser interferometer to measure the range and two rotary encoders to measure the angular position of a spherically mounted retro-reflector target. However, laser trackers are not perfectly constructed. Small geometrical errors in the position and orientation of their optical components lead to systematic errors in the measured coordinates. These errors can be described by 15 scalar values or alignment parameters. The manufacturer specifies a compensation procedure that is designed to determine the values of each of the alignment parameters so that each measured coordinate can be correctly compensated. This project presents the results of an alternative procedure, developed at NIST, for estimating the values of the alignment parameters using point-to-point length measurements and a global least squares fit algorithm.

Characterization of the Water Calorimeter
Rachel McKinsey

External radiation beam therapy is one method used in the treatment of cancer. The water calorimeter is the primary national standard used for the calibration of these external beams. The water calorimeter measures the energy imparted to water, in the form of heat, by radiation. In the late 1980's, Steve Domen invented the water calorimeter. New technologies led to the development of a second-generation water calorimeter. The focus of this project has been to characterize the second-generation water calorimeter.

Directional Solidification of Eutectic Alloys in the Ag-Cu-Sn System
Shelli Pace

In the search for a Pb-free solder alloy, the eutectic alloy in the Ag-Cu-Sn system has shown much promise. Confusion however, still exists. The Ag-Cu-Sn system has a eutectic reaction, but produces a dendritic microstructure at the eutectic composition. Since the eutectic alloy in the Ag-Cu-Sn system possesses all the thermal properties of a eutectic, one would expect it to have similar microstructures as those of other eutectics. However, the eutectic in the Ag-Cu-Sn system does not. The microstructure consists mainly of (Sn) dendrites, raising questions as to whether it is indeed a eutectic. Normal soldering conditions do not provide the control necessary to systematically study this problem. Directional solidification provides better control of the growth conditions that, in turn, will improve understanding of the microstructure. In our experiments, the alloy composition and temperature gradient were kept constant. Several samples were grown at different velocities ranging from 0.83 μm/s to 500 μm/s. Standard metallographic procedures were used to prepare samples for observation. Samples were ground at 240 grit, 400 grit, and 600 grit. They were then polished with 6 micron, 1 micron, and 0.25 micron water-based diamond suspension. Then 0.5 silicon Mastermet ™ was used for each sample's final polish. Micrographs and image analysis techniques were then used in an attempt to determine why the alloy possesses a dendritic microstructure.

The Effects of Calcium, Phosphate, Light, and Time on the Stability of Peroxides
Kenya Danyelle Thomas

While hydrogen peroxide (H_2O_2) and carbamide hydrogen peroxide have been used to whiten the teeth, its instability has been a constant problem. As a compound, hydrogen peroxide is known to readily decompose into oxygen gas and water because of its somewhat unstable nature. In addition, this instability is more pronounced in the presence of certain chemical species; some compounds can initiate rapid, even explosive, decomposition of hydrogen peroxide, especially if the hydrogen peroxide solution is highly concentrated. The instability of the molecule can cause auto-decomposition simply by bumping or jarring the container, addition of heat, light, or opening the cap. This project investigates the effect of

calcium ions, phosphate ions, light, and time on the stability of hydrogen peroxide of different concentrations, as well as on the stability of urea hydrogen peroxide also known as carbamide peroxide. Furthermore, this project is a continuation of a previous project with the addition of the time and light factors. The methods used in measuring the peroxide content of solutions include permanganimetric, cerimetric, and iodimetric. In this part of the project, it was pertinent to discover which method produced the best results in precision while simultaneously being practical and relatively rapid.

Another part of the project is the synthesis and analysis of salts of peroxymonophosphoric acid (H_3PO_5). The synthesis of H_3PO_5 can be accomplished in a number of ways, some far more efficient than others. Once synthesized, the acid can be converted to a solid salt, then purified and analyzed by spectroscopic and crystallographic methods. This project analyzed the salts using the Greenspan and MacKellar method published in 1948. A goal of the project, which is in progress right now, is to measure the stability of such salts over time.

Third Order Discretely Sampled Constrained Trajectory Generation

Erica Walton

Researchers and scientists have long studied the computation of trajectories and its relationship to the robot system and machine motion. Trajectory can be described as the time history of position, velocity, and acceleration through a space. Many types of spatial shapes of potential paths of both joints and the end-effectors of robots and machines have been modeled mathematically. These models are used in machines to define and constrain their motion. However, in order to apply on a computer, the trajectory must be sampled. The goal of the robot is to move from an initial position to some desired final position in a certain amount of time. This motion involves a change in orientation along with a change in position. Additionally, to get to the target arbitrary position, a path description of sampled points is followed to ensure a smooth trajectory. Because the objective of this trajectory is to change positions in a smooth or continuous manner, curvature polynomials of cubic order that demand constraints on the sampled points have been sought because 3rd order polynomial motion equations have a continuous (linear) acceleration curve. The scope of this study is to figure a solution that will have these constraints work fittingly for third order trajectories with non-zero initial and final speeds.

State University of New York – Binghamton

Silicon Based Single Electron Tunneling Transistors
Paul Fleming

In my talk I will be discussing first the theory behind Single Electron Tunneling Transistors, then the applications for them, specifically in the field of metrology and finally how I attempted to construct the silicon version of the device over the course of my 12 week internship.

The theory section will start with a discussion of the driving fundamental concepts of the SET device such as electron tunneling and the Coulomb Blockade phenomena. These fundamentals will lead to a discussion of the device which makes use of the concepts: the tunnel junction. The talk will then proceed to a discussion of a circuit containing a tunnel junction, on to a configuration diagram for the SET transistor, then to the Single Electron Pump and finally to the multi-island Single Electron Pump.

After the workings of the SET transistor and pump have been explained I will discuss some of their uses in new technology. Examples being low power single electron circuits, and a constant current source for very low current values. The use focused on longest however will be the idea of completing the so-called "Metrology Triangle", i.e. the metrological relationship between the Volt, Ampere, and Ohm units. The electron pump can supply a current based on a known charge/second value, making it possible for us to obtain a very accurate quantum based Ampere to compare with the Josephson Volt and the Hall Ohm. A quantum standard for capacitance could be obtained similarly using the SET electron pump placing electrons onto a parallel plate capacitor.

The third portion of my talk (probably the longest portion) will focus on my personal work on this project. This was attempting to fabricate an SET transistor using silicon, to improve upon the current metal/insulator varieties, which are plagued by a troubling charge offset problem. A group in Japan derived a process, which they claimed did produce Silicon based SET transistors. They published their "recipe" for other scientists to attempt reproduction. My job has been to reproduce their steps and construct the device. My first 2-3 weeks were spent training to use the machinery in the NIST clean room, which is where the fabrication takes place, since then I have been repeatedly attempting to construct the device. I tried two different methods based on their publishing and to date have obtained only moderate success, but feel hopeful that there is a good chance for success before the internship program has ended. This section of my talk will discuss all the work I've been doing, what went wrong and right, how I've corrected, pictures of the devices and process, etc.

Probability Plot Correlation Coefficient Test for Lognormally Distributed Void Radii in Entrained Concrete
Sebastian J. Larrea

The performance of concrete in freezing and thawing environments has been linked to the presence of small, 5 micrometer to 200 micrometer, air voids entrained in the concrete mixture by the use of surfactants. Moreover, the performance depends intimately on the relative spacing between and among the air voids within the paste volume fraction of the bulk material. In the concrete research field, the air voids are characterized by one-dimensional probes over a random plane through the system. The statistical characteristics of these chord lengths are then used to estimate the three-dimensional characteristics of the air void system.

Although a number of parameter-free measures of different definitions of spacing exist, the most reliable ones depend on the statistical moments of the air voids radii. Unfortunately, these quantities can only be approximated from the moments of the one-dimensional probes. Further, for air void system modeling, an analytical description of the air void radius distribution would be extremely useful.

A study is performed on laboratory data to determine whether the air void radii are lognormally distributed. Assuming a lognormal distribution of air void radii, the chord distribution can be derived analytically. The cumulative distribution function (CDF) for the chords is then approximated numerically. The normal order statistic medians are calculated from the chord CDF and compared to sorted laboratory data. For a particular number of laboratory data, a Monte Carlo calculation is also performed to determine the distribution of the probability plot correlation coefficient in order to assess acceptance or rejection of the hypothesis that the laboratory data can be described by a lognormal air void radii distribution.

State University of New York – Oswego

Characterization of Sealant Formulations
Nathan Hoteling

This study describes the development of a working mechanical model for sealant behavior. The core of this working model is based on the fact that sealant behaves like rubber, which has a long history of research and development. Based on this long history, two important determinations were sought: the relative importance of the Mullins effect, and the type of constitutive equation to be employed. To evaluate the relative importance of the Mullins effect, stress-strain experiments were conducted in which the sealant was repeatedly stretched to fixed strain levels. Stress-relaxation after step strain experiments were conducted at specified strain levels. This addressed three important questions: 1) does modulus change with time, 2) does modulus change with strain level, and 3) is there time-

strain separability? No universal model was observed for the four-sealant chemistries tested, but individual analysis enabled rubber constitutive equation assignment to each. This is part of a study that will compare baseline behavior of specimens that have been exposed to various environmental factors, ultimately leading to the development of new service life prediction methods.

Texas Tech University

Nondestructive Evaluation of Fiber Reinforced Polymer Composites Bonded to Concrete

Tigist Belete

The Building and Fire Research Laboratory (BFRL) is conducting series of studies designed to develop the criteria for the use of infrared (IR) thermography for nondestructive evaluation (NDE) of fiber reinforced polymer (FRP) composites.

The project focuses on the use of infrared (IR) thermography for locating and characterizing subsurface defects in the FRP laminates. The project involves experiments combined with numerical simulations using commercial finite-element software. The objective of the BFRL study is to develop the technical basis for the development of standard test method.

My research has focused on both experimental measurements and numerical simulations. The experimental phase of my work involved heat flux measurements. The purpose of the tests was to evaluate heat flux homogeneity of the experimental apparatus used for quantitative IR thermography. The second component of my work involved numerical simulations using finite-element analysis (FEA). Using FEA, I simulated infrared thermography testing of various test objects containing delamination, debonds, and concrete spalls.

Truman State University

Improving Beam Imaging of Synchrotron Radiation at SURF III (aka Size Does Matter)

Kevin Haworth

One of the many standards and calibration services performed at NIST centers around electromagnetic radiation. Using the Synchrotron Ultraviolet Radiation Facility (SURF III), NIST provides a continuous, broadband source stretching from infrared to soft x-ray radiation. This light source is used as a standard in calibrating items from photo detectors to satellite imaging systems. In order to provide the best services possible, it is necessary to perform numerous diagnostic tests on the radiation emitted. One of these tests maps out the vertical and horizontal beam dimensions, in addition to the intensity distribution along these

dimensions. This work is preformed on beamline 10. The original setup for this measurement is currently being replaced, by our group, to improve measurement of these values. Improvements in the method include installing an ultra-high vacuum beamline front-end with a copper mirror to absorb high energy radiation before reaching the camera, modifying the data acquisition software to increase the stability of the system in addition to increasing the number of frames processed per second, upgrading the frame grabber from an eight bit to ten bit camera, and replacing cables and power supplies to provide quieter data transfer. At the time of this talk it was not possible to complete setup due to external customer usage of SURF III. The original and improved setups for beam imaging will be discussed. In addition, separate work by the author done on beamline 3 dealing with reducing uncertainties in measurements of the angular distribution of the radiation to one-tenth of a percent will be briefly discussed.

Tulane University

Polarized Neutron Beam Characterization
Leah Broussard

The emiT II experiment is attempting to place limits on time invariance violation caused by the weak interaction by studying asymmetries in neutron decays. The focus of my project is the characterization of the neutron beam. Measurements such as the neutron polarization, energy, and beam profile were taken. A supermirror polarizer was used to measure the polarization of the neutrons. The neutron beam energy was measured indirectly using the velocity spectra taken by a time-of-flight spectrometer. Finally, the image of the beam showing the distribution of neutron counts was taken by exposing copper and dysprosium film.

University of California – Berkeley

Distributed Computing in Java: The Screen Saver Science Project
Jacob Scott

The growth of the Internet and of cheap, powerful, desktop computers has given rise to a new computing paradigm: distributed computing. The premier distributed computing project, Seti@Home, has over 3.5 million users and has more total processing power than ASCII White, the United States' most powerful supercomputer.

The Screen Saver Science project is an effort to create an generalized, task-agnostic distributed compute framework by leveraging the Jini network technology extension to the Java programming language. The basic idea is that when its screen saver turns on, a computer will automatically become a distributed computing client, helping make the world a better place instead of sitting idle.

I will start with an introduction to the basic concepts of distributed computing and some background on the state of the science. My talk will then trace over the path my summer research has taken, touching on the core components that power Jini. It will also cover JavaSpaces, a shared-memory built on top of Jini. Finally, I will relate the strengths and weaknesses of Jini, using my RemoteFileService as an example of programming with Jini.

University of California – Irvine

A Study of Behavioral Expectations and Consistency in Human-Robot Interaction

Siavosh Bahrami

As robots become more integrated in our everyday environments, people will interact with them without any formal training. The majority of the time the only "user-interface" to these robots is actual "physical manipulation." That is, the person does some action (a motion, saying a command, touching the robot, etc.) that causes the robot to behave in some manner. We are interested in looking at the difficulties that people interacting in a social setting with robots have in building a mental model of the robot's capabilities. Developing an accurate understanding of the behavioral properties of a robot that one has just encountered is very important in realizing the vision of humans and robots existing in the same space. People might have expectations of what a robot can do based on its appearance. People probably expect robots to act in some consistent fashion. In our study we are examining the factors of consistency and expectedness to determine the effect on a person's ability to construct a model of the robot behavior. Several behaviors were designed and implemented that either challenged or reinforced a person's behavioral expectations and notions of consistency. A pool of human subjects with no prior experience with our robot were asked a series of questions before and after their interaction with it in order to assess their experience. While these experiments are ongoing, the data from the initial set of studies run this summer at NIST will be presented in this talk. This is an exploratory study, which will help guide future research aimed at understanding the needs for effective and productive human-robot interaction.

The Accuracy of Current ACI Building Codes for Predicting the Effect of Carbon FRP on the Deflection of Concrete Beams

Heather G. Coman

Fiber-reinforced polymer (FRP) sheets are an efficient and competitive method of externally reinforcing structures.

One still unresolved issue is how to predict, by simple design formulas, the deflection of RC (reinforced concrete) beams strengthened externally with FRP. The present ACI (American Concrete Institute) formula is empirical, and based upon tests of steel RC beams.

Deflection data from seven RC beams reinforced with various sizes of reinforcing steel and externally reinforced with carbon FRP were compared with predicted deflections calculated with a modified version of the ACI deflection equation. The modification attempted to account for the effect of the FRP reinforcing as well as the steel reinforcing.

The preliminary results indicate that the ACI equation, even with these modifications, does not accurately predict the deflection of a beam reinforced with FRP sheets. Some work in calibrating the Tri-Axial Test Facility will also be presented.

Web-Based Database for NIST Electrical Standards Laboratories
Tam Duong

SURF intern Tam Duong (UC-Irvine) implemented the NIST Check Standard Database, which provides a research tool for the study of long-term behavior of reference standards. This database has users in research areas that include Resistance Metrology, Power & Energy Measurements, Impedance, and Ac-Dc Difference Measurements. Mr. Duong worked for 9 weeks in the NIST Electricity Division, with NIST staff physicists, engineers, and interns in the Fundamental Electrical Measurements group and Electronic Information Technologies group. He developed Common Gateway Interface (CGI) web methods similar to those used in the NIST-wide Information System to Support Calibrations (ISSC). Mr. Duong worked developing the data-input processes for the Power & Energy and Ac-Dc Difference Measurements projects, and greatly increased the search capabilities for data, based on the many diverse standards measurements in the laboratories. Each measurement project uses widely different classes of reference standards, and the Check Standard Database was designed both to accept and search for arbitrary data types, as well as store large blocks of data. The new web interface allows users to search for records on specific or general types of standards, and then retrieve the original measurement data in the form of spreadsheets or workbooks. Mr. Duong also helped create different types of output formatting specific to the measurement areas and measurement standards. This will help NIST staff study the processes that affect the behavior of electrical reference standards and improve the efficiency of critical measurement systems.

Graphical User Interface for Fire Fighter Protective Clothing Simulator
Hoang Minh Ho Dac

The goal of this project is to develop a graphical user interface in Java for a computer program written in Fortran 90, which simulates heat and mass transfer through fire fighter protective clothing. Previously, the input for the computer program was through an input data file and the output was text files that were subsequently post-processed using a graphical package.

The developed graphical user interface would provide a menu driven approach for entering the input for this computer program, for invoking its execution and for graphically displaying its output. The graphical display would create animation files for visualizing the time dependent output of the Fortran program. This interface is expected to be very useful for protecting fire fighter from burn injury and will be widely used in the fire industry.

Analysis of Conductivity in Mono-Crystalline Electrical Linewidth Structures
Puja Gupta

The measurement of linewidths on ICs is important for controlling the IC manufacturing process. Uncertainties of the physical linewidths of single-crystal linewidth reference materials that are now being calibrated at NIST by electrical measurements may be improved by a factor of 2 or more if a proposed explanation of the drift in electrical linewidth can be shown to be consistent with available measurement sets. The objective of the work to be undertaken is to investigate whether a model that attributes the drift of electrical linewidth to positive charge that accumulates in the features' native-oxide sidewalls after patterning and final rinse. This task will use available modeling tools, including charge transport theories and statistical methods to determine the nominal value of the linewidth.

Tunable LED Based Light Source
Mark Lawrence

Advancements in LED technology have provided commercially available LEDs with narrow spectral distributions across the visible spectrum. Using a number of different LEDs it is possible to simulate CIE standard reference sources such as illuminant A and D65, as well as produce a tunable source of pure colors ranging from the ultraviolet to the near infrared. A spectrally tunable LED source can then be used to calibrate colorimeters and spectroradiometers to a high degree of accuracy. Instruments calibrated using this method will be able to more accurately image sources that current calibration methods are not well suited for.

The focus of this summer's work is the development of an advanced LED source. This source incorporates a total of 60 LEDs with 40 independent current control channels. A spectrograph continuously marks and records the source spectral distribution. As part of the project, a computer program was written to control the current to the LEDs. This algorithm uses the spectral distributions recorded by the spectrograph to accurately match the source output to a sample spectrum. Another aim of the summer work is to test the spectrograph for accuracy and long-term stability.

In the future this project will move to 80 or more LEDs mounted radially in a larger integrating sphere. The LEDs will be switched to capless versions to eliminate instability due to the degeneration of the LED caps. We are investigating the necessity of temperature controlling the spectrograph or replacing it with a more accurate model.

Testing Disk Imaging Tools
Roshni Malani

In order for computer forensic evidence to be admissible in a court trial, the original evidence must not be tampered with and NIST is creating a standard to ensure that it is not. Computers, just like blood samples, must be handled with caution and care. For example, if you turn on the computer, then the original date at which it was last turned on will be overwritten and evidence will have been altered. Therefore, one of the first tasks after seizing a computer as evidence is to create an exact bit-for-bit copy of the hard drive, including all of its partitions, in a process called disk imaging. There are several commercial software products available for this purpose, including dd, SafeBack, and EnCase, but all of them have some particular situation in which they do not work as expected. To provide a measure of confidence in disk imaging tools, NIST has created a software package called the Forensic Software Testing Support Tools (FS-TST) that includes programs to initialize disk drives, detect changes in disk content, compare pairs of disks, and simulate bad sectors on a disk. In addition, most of the software is written in Borland C++ 4.5 for the DOS 6.3 environment and uses the interrupt 13h BIOS disk interface. However, some hardware devices, such as USB and Firewire, do not run in the DOS environment. Therefore, my project this summer has been to develop a similar software package that supports the testing of disk imaging tools in the Linux environment.

Development of a Liquid Chromatographic Method for the Analysis of Atmospheric Aerosol Samples
David Stout

Air pollution is one of the major environmental problems that exist, and thus it is critical to know its composition to understand the chemistry in order to help prevent it and clean it up. Aerosols are particles suspended in air that occur either naturally as from forest fires or by humans with the burning of fossil fuels. Normal phase, reverse-phase, and size exclusion liquid chromatography were used to develop methods to aid in the determination of the organic and water-soluble compounds that are present in atmospheric aerosols. Environmental aerosol samples are rather complex, containing numerous compounds in various and often times low amounts. Therefore, it is desired to have a chromatographic method that separates sample extracts into smaller fractions grouped by common chemical properties of compounds, which can then be further analyzed by gas chromatography mass spectrometry. Soxhlet extraction and sonication with different solvents were used to extract the compounds from high volume air sample filters into the liquid phase for analysis. It is

desired that the results found from this research will be able to be used in the development of a method for a quantitative analysis on aerosol samples taken from the environment.

Java Programming Support for Visualization Construction
Twie Le Tran

The Visualization of Building Structure Project is programming support for visual representation and simulation of steel structures. The Virtual Reality Modeling Language (VRML) is used for the visual representation of those functions. VRML is a scene description format to represent 3D interactive data on the Web. A VRML prototype is a method to create application-specific geometry such as beams and columns. The programming related to the VRML prototypes is used in JavaScript. My task is to rewrite them in Java so that they can provide significant improvements in processing time and memory usage. With my background of Java programming knowledge, I translated one VRML prototype of the building structure (Element2d) to Java from Java Script that works in a 1000 KB file. Now, I am working on another VRML prototype (Element) that allows viewing the construction in different ways such as solid, transparent, wire frame, or line. When rewriting the VRML prototype from Java Script to Java, some problems occurred due to the Java compiler, Forte. To run Java with the Forte Compiler, the Java zip file needs to be archived. Also, when programming, the Java variables, which declared on top of the class, have to be defined same type as the data types in VRML. Furthermore, VRML library also need to be imported and the Java class has to extend from the Script class for Forte to understand the VRML commands. In conclusion, while doing my research experience at NIST, I learned that real-world Java programming is much different than the projects I did in school. They are realistic because I actually interact with problems such as installing Java compiler version Forte 1.3 instead of 1.4. For instance, different compiler versions can cause the building structures not to display.

Vibration Isolation of the NIST Watt Balance
Kris Vaughan

The NIST Electronic Kilogram Project (EKG) can redefine the base unit of mass in the International System of Units (the kilogram) by an accurate determination of the Planck constant using a Watt Balance. However, a limitation to the NIST watt balance's accuracy is the introduction of noise from background vibrations. To reduce the vibration noise, a vertical active vibration isolation system is being directly implemented at the knife-edge of the watt balance. Using a "stand alone" balance identical to the NIST Watt balance, a feedback system consisting of three PZT actuators and two accelerometers was developed. Transfer functions and power spectral density measurements were made in the frequency domain using a dynamic signal analyzer enabling us to determine the system at different stages and develop the compensation filter. After the compensation filter was designed and included in the feed back loop, the loop was closed and maximized to performance.

University of California – Los Angeles

Elliptic Curve Digital Signature Algorithm (ECDSA) Validation Tests
Amarpreet Cheema

In today's business world, computer-based technologies have helped to replace paper-based transactions with their electronic counterparts. Along with the reduced costs and improved efficiency, electronic transactions can, unfortunately, make the financial community vulnerable to risks from accidental or deliberate alteration, substitution or destruction of data. To ensure that information has not been altered in transit, or to verify the originator's identity, we make use of public-key cryptography digital signatures. A digital signature is an electric analog to a written signature. Unlike written signatures, however, digital signatures can also verify the integrity of information.

The ECDSA is an algorithm used to create digital signatures and to establish secret keys securely. The ECDSA validation tests will be a part of the Cryptographic Algorithm Validation System (CAVS). This is a tool being designed by NIST for use in validating vendor's implementation of cryptographic algorithms. The CAVS tool records the passing or failing of each required validation test along with information indicating where the failure occurred. This information helps the vendor to identify problems with their implementations. This summer I added the ECDSA validation tests to the CAVS tool. I developed the user interface that lets accredited Cryptographic Module Testing (CMT) laboratories test and verify vendor's ECSDA implementations.

University of Maryland – Baltimore County

Quantitative Contrast Variation Analysis of MS2-Like Virus Particles For Future Use In Clinical Diagnostics
Ali D. Deyhim

A quantitative standard for an RNA bacteriophage MS2 was established by measuring and modeling the ratio of RNA to protein shell in the Armored RNA virus. Currently there is no convenient method for determining a concentration ratio between RNA to protein in Armored RNA viruses. The MS2 bacteriophage was an ideal choice amongst a family of Armored RNA viruses because it has an easy to model icosahedral spherical shape. Furthermore, it's convenient to attain recombinant forms of this non-infectious virus because they are commercially available for laboratory research. Our procedure consisted of calculating contrast variation found in the RNA and protein using Small Angle Neutron Scattering (SANS) measurements. These findings have useful implications because with an established percent of RNA to protein concentration we are able to determine an accurate molecular weight of the Armored RNA coat and nucleotide. Eventually, this extrapolated information will be used to develop an ultra- sensitive physical counting tool for Armored

RNA measurement. This counting tool can then be applied to improving clinical diagnostic procedures.

Photobleaching and the Damage of DNA During Fluorescent Detection
Elizabeth Humphries

Fluorescein is a fluorescent dye commonly used for many assays and detection applications. One disadvantage of fluorescent measurements is that the fluorophore fades during detection (photobleaching). One possible mechanism to explain photobleaching is oxidation of fluorescein by molecular oxygen. N-propyl gallate is a reducing agent that can be added to decrease the rate of photobleaching. We used a frequency domain technique to measure the rates of degradation of various solutions of fluorescein and the relative antifading effect of n-propyl gallate. Although the literature suggests a solution of at least 90 mM n-propyl gallate is needed to reduce photobleaching for some applications, the same antifading effect was obtained with concentrations of as little as 5 mM using our system. The protective effect of n-propyl gallate has important implications for many fluorescent applications. We plan to extend this work to detection of DNA in solution and on surfaces.

University of Maryland – College Park

Testing Random Number Generators Using the NIST Statistical Test Suite
Wendy Chou

The need for random and pseudorandom numbers arises in many cryptographic applications. For example, common cryptosystems employ keys that must be generated in a random fashion. Many cryptographic protocols also require random or pseudorandom numbers inputs at various points, e.g., for auxiliary quantities used in generating digital signatures, or for generating challenges in authentication protocols. Generators for such purposes often need to meet stronger requirements compared to other applications. In particular, their outputs must be unpredictable in the absence of knowledge of inputs.

To ensure the quality of these random and pseudorandom numbers, NIST developed a suite of programs, which tests 11 different generators for deviations from randomness. In this project, features of the test suite were investigated and enhancements to the usability of the test suite were made.

Automatic Table Generation for Values of Special Functions
Stuart Fletcher

This work is part of a larger project: the updating of the NBS Handbook of Mathematical Functions, published in 1964, into the NIST Digital Library of Mathematical Functions (DLMF). An important part of the old Handbook is its tables of function values for each special function.

However, in the present computing environment, printed tables are not the most suitable form for presenting data since, once in print, the tables are necessarily limited in range and precision, due both to space considerations in the printed book and to what was possible to compute at the time the book was published.

Since in its next iteration the special function data will be available online, the obvious alternative to archiving data statically is to use the current state of computing power and networking capabilities to allow the generation of tables according to user-specified parameters such as the desired range, precision, and any parameters specific to the function. It was decided the safest and most efficient way to do this is to arrange for computations to be done on users' workstations rather than a central server. Java was chosen as the implementation language since it has built-in facilities for taking advantage of this style of computation.
To assess the feasibility of this approach, this project has focused on writing a Java translation of a NIST Fortran 90 package that computes zeros and function values of the Airy functions. In addition to writing the code for doing the computation, a working prototype of a user interface has been developed that is a Web-based front end for dynamically generating tables. Some difficulties were encountered due to Java's lack of support for numeric computation, specifically the lack of complex and matrix data types. An extension to Java that adds complex numbers to the language was implemented as a preprocessor in order to alleviate some of these shortcomings.
The hope is that this work will serve as a starting point for implementing automatic table generation in the remaining chapters of the DLMF.

University of Massachusetts – Amherst

Validation of the ebXML Business Process Catalog
Nathan Barr

The rapid growth of the Internet is driving business-to-business transactions to be moved to the World Wide Web for increased efficiency and reach. Many companies have substantially benefited from the conversion to an electronic form of conducting business. However, there are currently many specifications for conducting electronic business, and creating software to conduct ebusiness in the current formats is very costly. In fact, the entry cost is too high for all but the largest companies to successfully adopt ebusiness. ebXML (electronic business

using eXtensible Markup Language) —a joint initiative by the United Nations/CEFACT and OASIS—promises to create a standardized framework for electronic business. The scope of the project is to create specifications from which "compatible" software can be produced. If ebXML is eventually accepted by all enterprises around the world and allows them to all move at "internet time," then business will be revolutionized similar to the introduction of a monetary system to replace bartering.

A basic feature of the ebXML architecture, which separates it from other XML frameworks, is its emphasis on business processes. Business processes that are defined systematically can be used as the basis for defining common message sequences across industry boundaries, and offer a basis for achieving interoperability. Key to the success of the business processes is the ability of users to locate the appropriate business process from the business process catalog. An information model for the business process catalog was implemented in a relational database to validate its structure. A crucial aspect of this structure is the method used to classify the business processes. Classification systems and similar attempts at classification were analyzed for possible extensions that could be utilized by this catalog. The method of classification was also analyzed for usability in the catalog.

University of North Carolina – Chapel Hill

Effect of Suspending Medium and Particle Size on Dispersion of Fine Alumina Powders for Laser Diffraction Analysis
Vadas Gintautas

Determination of particle size distribution is a critical element in the characterization of ceramic powders used in electronic and structural applications. Low angle laser diffraction techniques, commonly used to measure particle size distribution, require that the powder be diluted and dispersed. Since laser diffraction cannot differentiate between primary particles and agglomerates, chemical and mechanical means are generally necessary to aid in dispersion prior to analysis. This study examines the effect of suspending medium, ultrasonication, and primary particle size on the accuracy and reproducibility of particle size distribution measurements for fine alumina powders.

University of North Carolina – Charlotte

Calibrated Micropyrometer Measurement of the Tool-Chip Interface in Machining
April Cooke

Quantitative insight into tool wear in machining is obtained through the measurement of the temperature distribution in the region of predominant wear, the tool-chip interface. This interface is about 500 μm wide, so a micropyrometer system was devised consisting of an InSb infrared camera, a 15x fully reflective objective, an infrared/visual spectrum beam-splitter and a camcorder. The beam-splitter and camcorder assist with the location and

alignment of visual targets. The spatial field of view and resolution of the micropyrometer were measured with a 1951 USAF Chromium negative image target. The micropyrometer's response to radiation from a well-known blackbody radiation source is combined with measurements of the machined material's emissivity to obtain the distribution of temperatures in the tool-chip interface. The investigation of the relationship between the tool-chip interface temperature distribution and various controllable machining parameters such as cutting speed, feed, and rake angle is in progress, and preliminary results are shown.

University of Puerto Rico

Real-Time Measurements of Clay Dispersion Using VIS Dye Probes

Xiomara Calderón Colón

Nanocomposites have a great importance for their physicals and mechanicals properties. Nanocomposites show extremely well enhanced properties as compared to the conventional composite structures, however characterization of nano-structure is a challenge in itself. In order to measure the degree of clay dispersion in a polymer material, the aggregation and dispersion spectrums have been used in the present study. The phenomenon of "metachromasy" is well established and we have attempted to apply the similar principle to determine either exfoliation or intercalation of clay.

OM-MMT clay have been synthesized using dimethyl di-octadecyl ammonium bromide (DMDODA-Br) and 1,1'- Diethyl-2,2'-cyanine iodide (CN-0) dye. Intercalation characteristics of 1,1'- Diethyl-2,2'-cyanine iodide dye on MMT and OM-MMT have been studied using TGA and XRD techniques. Absorption spectrum for various dye concentrations in aqueous solutions has been studied and the study of absorption spectrums of dye-clay solutions in chloroform is currently in progress. In future work add the polymer at the dye-clay system.

The need for this study, experimental details and results will be presented.

Characterization of Airflow in a Manufactured House

Yaireska M. Collado –Vega

The Indoor Air Quality and Ventilation Group at NIST recently received a manufactured house test facility to conduct research on ventilation and indoor air pollution in residential buildings. To prepare this house for these research projects it is important to create an airflow model of the house. We can then characterize the airflow through the envelope and the ventilation systems both experimentally and through modeling, in this case using a software program developed at NIST *CONTAMW2.0.* This is a multizone indoor air quality and ventilation analysis program designed to help determine: airflows, contaminant concentrations and/or personal exposure to contaminants. The house model contains different ventilation system components such as ducts, exhaust fans, and ventilation inlets.

Simulations were performed to predict the outdoor air ventilation rates into the house by infiltration and mechanical ventilation. These ventilation rates were also measured experimentally to validate the model. The model predictions and measurements will also help us evaluate requirements to provide adequate levels of outdoor air ventilation in manufactured houses. Results of these simulations will be discussed and presented.

Optimizing PID Algorithms Using Smart Sensor Control

Saylisse Dávila

The extent of sensor usage in the manufacturing sector ranges from production lines to the final product itself. However, what we now consider a sensor has gone way beyond our expectations. Today, manufacturing demands for information gathering and handling require "smart sensors" that report more than simply an "on" or "off" condition. Because of these demands, engineers are constantly seeking ways to implement more intelligence into sensors and sensor-based devices.

Implementing smart sensors into an industrial process requires the selection of a control technique. Proportional-Integral-Derivative control, or PID has been used for many years and is still the reigning technique for industrial applications, because of the simplicity of its control algorithm.

Notwithstanding, we wish to augment a standard PID algorithm with smart sensor characteristics in order to optimize its behavior. First, we will develop and implement a PID-based temperature control system to use as our experimental testbed. Next, we will augment the PID algorithm with "smart sensor" characteristics to refine its behavior. Finally, we will determine empirically if the enhanced "smart sensor" algorithm used in the temperature control system provides better performance than a standalone PID controller.

Our approach to implement this smart temperature control system is by using an engineering modeling software package called LabVIEW. By applying "smart sensor" characteristics such as autonomous decision making, deeply embedded intelligence, and localized data processing into a temperature control system; our goal is to create an experimental design that minimizes the reaction time of a temperature control system. This system coupled with the enhanced PID controller should maintain a specific setpoint more rapidly and consistently after a disturbance has been introduced into the environment.

Measuring the Diffusion Coefficient of Small Molecules on Different Polymer Films

Ángel G. Fuentes Figueroa

To further reduce the size of integrated circuits and improve the performance of computer chips, we have to explore the physical property changes that can occur in thin polymer films, like those used in photolithography, and understand how these property deviations affect our ability to produce better, smaller and faster semiconductor devices. Previous measurements at the National Institute of Standards and Technology (NIST) show that thin films absorb more small molecules penetrants (i.e., water vapor) as compared to thicker films. However, it is also important to understand the behavior of the diffusion coefficient of small molecules when the film thickness is reduced. The diffusion coefficient of small molecules will also affect the photoacid (H^+) mobility in the polymer film. Changes in the H^+ mobility are alarming for the photolithography community, as the H^+ diffusion must be stringently controlled to optimize the resolution of a photoresist formulation. In this presentation we try to find a relationship between the thickness of different polymer films and the diffusion coefficients of small molecule in these films using a Quartz Crystal Microbalance (QCM) device to determine the mass absorption of a solvent (in our case water). The QCM uses the piezoelectric effect to generate a harmonic oscillation in a quartz crystal on which the polymer film has been coated. When air saturated with water is passed over the crystal, the polymer starts absorbing water. This effectively increases the mass of the film and shifts the resonance of the crystal to a lower frequency ($\omega^2=k/m$). By knowing the mass uptake as a function of time, we can calculate the diffusion coefficient into the thin film. By understanding the kinetics of small molecule and/or photoacid transport in thin polymer films, these experiments will help implement thinner films in deep UV lithography, and therefore the production of smaller integrated chip devices.

A New IMPACT in Silicon Carbide Power Devices

Rafael S. García-Cortés

Recently, a new class of power semiconductor devices has begun to emerge that utilizes the advantages of silicon carbide (SiC). In order for circuit designers to fully utilize the advantages of this new technology, SiC power device models must be developed for circuit simulation. The objective of this research is to provide the software tools necessary to enable circuit designers to systematically develop SiC component models for circuit simulation. This will enable circuit simulations demonstrating the advantages of SiC power devices compared to conventional silicon (Si) power devices for different circuit application conditions.

The metal-oxide-semiconductor field effect transistor (MOSFET) and the insulated gate bipolar transistor (IGBT) will be among the first SiC switching components to be developed. IMPACT (**I**GBT **M**odel **P**arameter Extr**AC**tion **T**ool) is a NIST software package for extracting parameters to be used in advanced physics-based IGBT models. The parameter extraction software package consists of five programs that extract the 20 physical and structural parameters needed in the most recent version of the Hefner IGBT model. The package enables users of the simulation software products to extract model parameters themselves and thus permits the simulation of new IGBT part numbers as soon as they are introduced.

The subject of this SURF project is to extend the IMPACT software package to include the model physics and parameters necessary for the emerging class of SiC power devices. These enhancements enable the five IMPACT programs to be used for SiC power devices in addition to the traditional Si power IGBTs. The programs have also been modified to enable the extraction of parameters for the unique power MOSFET device structures required for SiC such as the vertical double diffused MOSFET (VDMOSFET) and the Accumulation-mode MOSFET (ACCUFET). The new software is being used to extract model parameters for prototype SiC ACCUFET devices pioneering the introduction of three-terminal SiC power device model libraries.

Detectors Performance for Radiation Measurements for Home Land Security

Angélica Pérez-Andújar

Due to the latest terrorist attacks the awareness to measure Radioactive Materials has increased. Measurements of a great variety of radionuclides for a wide range of activity levels are necessary. Some of the radioactive sources that are of great concern do to the relatively easy accessible as they are used in industrial and medical applications are ^{60}Co, ^{137}Cs, ^{170}Tm, ^{192}Ir, ^{125}I, ^{99m}Tc, ^{241}Am and ^{266}Ra. These materials could be released by planes, "dirty bombs" in cities and in water or in food supplies. Information about the adequate equipment required for the measurement of these sources is of great importance.

To prevent and detect the handling or spread of radioactive material it is necessary to develop standards that can ensure the selection of the right equipment for radiological measurements. At NIST we are working on the characterization of CdTe, High Purity Germanium (HPGe) and NaI detectors for measurements of gamma ray emitting sources. To determine under which circumstances each one of these detectors could be used it is necessary to know the detector efficiency, detection limits and energy resolution .The efficiency of a detector is given by the ratio of the measured activity to the total activity emitted by the source. On the other hand the energy resolution can be use as a tool for determine the presence of particular radionuclides. Another relevant characteristic is the detection limit of the detector that gives a measure of the capability of the detector to detect the presence of a radioactive source above background radiation.

The use of these detectors depends on which circumstance it is going to be use, for example the NaI detector has a higher efficiency than the Germanium detector but on the other hand the Germanium detector has a higher energy resolution that makes it better suited for nuclide identification measurements. Another example is that the Germanium detector cannot be use at room temperature but the CdTe and NaI detector do, this ability makes these detectors a good instrument for field measurements.

Testing the Capacity of Manufactured Home Walls to Withstand Horizontal Loads
Rolando E. Vega Ávila

The Idaho National Engineering and Environmental Laboratory (INEEL) and the University of Wyoming are conducting experiments designed to increase industry understanding of the structural behavior, and to improve the durability, windstorm resistance, and energy efficiency of manufactured homes. As part of this research, NIST is conducting experiments to measure the resistance of wood frame shear walls that are used in manufactured homes to resist lateral loads from winds and earthquakes. The test results will be used to develop and calibrate models for the analysis of lateral loads in shear walls of manufactured homes.

Structural analysis of manufactured homes under lateral loads, especially those loads generated by high winds, is a primary design concern. The improvement of their performance requires dependable analytical and computer modeling of their behavior under horizontal loads. Based on this, the NIST project will include the testing of three types of manufactured home exterior wood studs walls under horizontal loads inducing shear, bending stresses and uplift forces in the walls.

The results of this research can lead to reducing annual losses of life and property by providing validated information to enable the improvement of building code requirements and develop engineering software that can predict and optimize wind resistance.

University of Rochester

IT Support of Nanoindentation
Ross Camara

Characterization of the material properties of a sample can be accomplished using nanoindentation provided that precise geometry of the indentation probe is known. The current method for determining this geometry is to indent reference materials with known properties. An alternative technique has been developed using the Atomic Force Microscope (AFM) to directly image the tip. However, the finite size of the AFM tip leads to an image of the indentation probe that is larger than the true geometry. To determine the true probe geometry, the geometry of the AFM tip must first be estimated and then its effects on the image of the probe are removed. A Windows version of computer algorithms (based on

mathematical morphology), previously developed at NIST for UNIX systems, were used to estimate AFM geometry from images of a "tip characterizer" sample and then to "erode" the AFM tip from the image of the indentation probe for several different probe geometries. An interface was developed to allow the user to perform these without the need to understand the mechanics of the algorithms or visualization software. Linear regression is then used to determine the probe's area function that is used by the nanoindentation software. Additional compatibility issues are also being explored.

University of Wisconsin – Madison

Investigations in Linear Motor Dynamics
Michelle Shah

Linear motors lie at the forefront of the manufacturing industry, however, unlike the traditional rotary motors, their performance characteristics are still unknown. There are also discrepancies as to whether the existing standards for rotary motors are directly applicable. The goal of the overall research project falls on two levels. First, to provide industry with performance standards precisely associated with the linear motor to allow for accurate comparisons of machine tools. Second, to investigate failure modes, remaining life, key performance characteristics associated with test procedures, and controller strategies. This study is a subset of the overall project and is intended to research and analyze the dynamic properties of the motor. The investigation involves a series of tests used to understand the motor's dynamic characteristics. The first test, modal testing provides a relationship between frequency response functions and their individual modal parameters. Modal testing in the form of impact testing can generate valuable frequency response functions used to study relationships in control parameter variation. The research examined the relationship between frequency response functions and controller parameters in the amplifier and through the PMAC interface. The PMAC parameters: velocity feed forward, acceleration feed forward, and proportional gain demonstrates linear relationships. However, the parameters for the amplifier: velocity gain, velocity feed forward, and velocity integral demonstrate unique relationships. After each set of parameters was investigated, a brief design of experiments was carried out to uncover any relationships between parameters. The testing the stiffness and compliance of the machine slide will be completed and analyzed as well.

Valparaiso University

Where No Man Has Gone Before
Steven Wolf

The theory behind gas-phase interactions of small molecules is a well-developed area of statistical rate theories. But, there is no current statistical rate theory governing condensed, large-molecule phases. Using the technique of Reactive Molecular Dynamics, we are

simulating the thermal decomposition of several polymers: poly(isobutylene), polyethylene, polypropylene, poly(methyl methacrylate), and polymethacrylate. From these simulations, we determine the backbone scission reaction rate and the de-polymerization reaction rate. From these data, we can determine the Ahrrenius activation energies for each of these reactions, which we compare to experimental results. This helps us develop a mechanistic understanding of thermal degradations in polymers at a wide range of temperatures and finally help us learn about these mechanisms at lower temperatures.

Vanderbilt University

Development of Crystallization Strategies

Melanie Bernard

The physical structure of a protein is critical to its function. One of the best ways to obtain a structural map of a protein is to measure and interpret the diffraction pattern resulting from directing an x-ray beam through a crystal of that protein. The repeated lattice in the crystalline form gives rise to a unique pattern of diffracted points that can be solved to reveal the protein's structure. However, only crystals of high quality can withstand the procedure. Growing crystals of such quality to be used in the x-ray diffraction process requires specific conditions that vary for every protein. There are many different factors affecting crystallization growth (i.e. temperature, pH, protein concentration, precipitating agent, etc.). Conducting an experiment for every combination of variables would exhaust a crystallographer's time, funds, and protein supply. Some screens have been developed in order to test the suitability of a range of crystallization conditions. These screens sample a small number of combinations out of the possible parameter space. Jancarik and Kim developed a protein screen based on sparse matrix sampling, which utilizes conditions known previously to have been successful and uses random combinations of factors to yield initial crystals. Carter and Carter developed a screening method using their incomplete factorial design. This method takes an initial set of conditions and randomly assigns combinations of these variables. The design is then balanced so that each possible first-order interaction matrix is filled with entries.

Based on observations, it has been hypothesized that similar proteins share similar crystallization conditions. If this is true, then specific screens can be developed for each protein family. This step could possibly contribute to a high rate of success without exhausting resources by eliminating tedious trial and error experiments. To test this hypothesis, we chose the hemoglobin/myoglobin family as a focal point. Crystallization information for this family was extracted from the Protein Database (PDB) and the Biological Macromolecule Crystallization Database (BMCD). This data was compared and the precipitants, temperatures, concentration ranges, and pH values found successful in previous experiments were used to build our screen. Using four precipitants, four concentrations for each different precipitant, and five buffers/pH values, it was possible to construct and balance an incomplete factorial table with twenty-four experiments based on Carter and

Carter's design. The hemoglobin screen was then implemented at 4°C and 20°C by hanging drop experiments and tested with seven different hemoglobin proteins. After a sufficient crystal growth period had lapsed, the results were analyzed and the screen was revised. Using this information, the next step is to explore screening options for other protein families and discover which properties of these proteins contribute to their crystallization conditions using bioinformatics.

Virginia Polytechnic Institute

Comparison of Sensor-Driven Fire Model Algorithms with Experiment
Kai Zuehlke

Fire protection is a key component of a cybernetic building system. Detectors throughout the building deliver room condition data to a computer that could detect and model fire. Such a sensor-driven fire model would be capable of monitoring fires in buildings in real time and could provide valuable ballpark figures of fire and non-fire conditions. This information would be invaluable to building managers and fire chiefs who would be able to make better-informed decisions.

Complex fire models exist today that are capable of tracking fire growth in great detail. However, the long run times that such models require prohibit them from being run in real time. A sensor-driven zone fire model makes some simplifications that allow it to run in real time and yet retain a reasonable approximation of room conditions. Each room is modeled as two distinct and homogeneous zones - the hot upper layer and cooler lower layer. The sensor-driven fire model runs in reverse of other computer fire models, in that the effects of the fire are input and the fire source is output. The model takes the raw data; tracks the location, interaction, and changes of these layers; and calculates a fire source.

I am analyzing data from a series of tests run last summer in which different types of fuels (mattress, chair, and cooking oil) were burned in a trailer home. The types of data include thermocouple temperature readings, commercial smoke and CO detector signals, gas analyzer data, and smoke obscuration measurements. I am identifying useful test runs, inputting test data into the algorithms, and evaluating the results. It is hoped that this data set will help validate the algorithms that are the basis of the sensor-driven zone fire model.

Wellesley College

Liposomes as Microreactors
Alyssa Meyer

Due to their properties, liposomes are good candidates for use as micro-containers in performing small chemical reactions. Our goal is to study chemical reactions created through the fusion of two liposomes containing different reagents. Similar to cell membranes, liposomes are made of a lipid-bilayer membrane enclosing an aqueous solution. We used two different techniques to make the liposomes, evaporation and electroformation. To fuse liposomes we first trap them using a system known as optical tweezers. This system uses tightly focused infrared laser beams to trap and manipulate microscopic objects without actually touching them. There is also a pulsed ultraviolet laser that works as a scalpel to cut or puncture the membrane of the trapped liposome, which induces the fusion. This summer we worked on modifying the apparatus to improve the traps and make the scalpel more efficient. Using two mobile traps we can optimally arrange the liposomes for fusion at a common contact point, at which we puncture the membrane using the UV laser. We are working towards the fusion of two liposomes containing different reagents, thus realizing a microreaction.

Western New England College

Holding Next to Nothing
Craig Beal

The progress of nanotechnology depends on the development of new tools to manipulate objects ranging in size from atoms to cells. By harnessing the momentum of photons generated by high-power lasers, optical tweezers capable of trapping and guiding small objects have been prototyped. This discussion will cover the physics behind optical tweezers as well as the development of an instrument capable of controlling multiple, irregularly shaped nanocomponents which may be patterned using methods such as electron beam lithography. Preparations for an experiment exploring the interactions of individual strands of DNA with nanopores will be used to illustrate one potential application of optical tweezers.

Williams College

Two Beam Non-linear Optical Effects
Rachel Gealy

When a laser beam passes through a liquid crystal cell, a multiple ring fringe pattern is observed. As the beam traverses the cell, the index of refraction of the medium changes in proportion to the intensity of the light, producing the interference pattern. In this experiment, we split the beam of a doubled YAG laser into two beams of equal intensity and propagated both through a .2 um-thick cell of 4'-Pentyl-4-biphenyl-carbonitrile liquid crystal in the nematic phase. The crossed beams produce two copies of a circular single beam pattern when they intersect exactly at the cell. However, when the beams overlap only partially, vertical fringes appear, and the circular rings are truncated, producing a symmetric pattern of two "D" shaped fringes. I observed how this two beam pattern is affected by the horizontal and vertical beam separation, the temperature of the cell, the intensity of the laser, the type of liquid crystal, and the alignment, homeotropic or homogeneous, of the cell. In addition to taking data, I modeled this phenomenon using *Mathematica* and a three dimensional graphics program.

York College of Pennsylvania

An Analysis of Time-Dependant Degradation of Organic Additives in Gunshot Residue
Stephanie McLean

When a gun is fired, residues, or partially burned gunpowder, are ejected into the air and are consequently deposited onto the shooter as well as the victim and the surrounding area. These resides can be collected and compared in order to provide a possible link between a shooter and a victim. Currently, most gunshot residue analysis focus on metals in the powers, however, some companies are attempting to remove all metals from the powders, thus negating current techniques. These techniques are also labor intensive and costly. In response, NIST scientists have been attempting to prove the validity of using organic additives found in gunpowder to provide this link between the shooter and the victim. The additives that are often focused on are nitroglycerine, a propellant, and stabilizers, which keep degrading bullets from becoming unstable and self-igniting. These stabilizers include, among others, diphenylamine and ethyl centralite.

Little is known about the degradation patterns of these chemicals under natural conditions that might be encountered following a handgun crime. To gain insight into how these chemicals degrade, a 50-day aging study was done as a summer project. Samples were left to age in both outdoor and indoor conditions, both in the light and in the dark. Samples were analyzed using micellar electrokinetic capillary electrophoresis (MECE), which is a separation of neutral, hydrophobic compounds based on the interaction with a charged micelle, which migrate in a capillary due to an applied electrical current. Possible

applications for this study include the ability to determine how long residues have remained on a surface. Understanding the changes in residue composition with time might help investigators account for events following a handgun crime.

APPENDIX A. A QUICK CROSS-REFERENCE

SCHOOL	STUDENT	PROJECT TITLE	PAGE	NIST LAB
American University	John Patrick Casey	Realization of the ITS-90 Below 84K	11	CSTL
Appalachian State University	Matthew Cass	QCSim: A Quantum Computer Simulation	11	ITL
	Erin Robertson	Stability Under Shear Flow of Strings in Model Emulsions	12	MSEL
	Rebecca Stamilio	Verifying SURF III as a Standard for Source-Based Radiometry -or- Was $1.97 Million Really Worth It?	13	PL
	Sarah E. Thompson	Fire Pattern Re-Creation	13	BFRL/ EEEL
Bates College	Amanda Slocum	Crystallographic Orientation of Surface Facets	14	MSEL
Brigham Young University	Jacob Anderson	Qubit-Radiation Field Entanglement	14	PL
	Yenny Martinez	Towards Controlled Interactions Between Qubits	15	PL
Bryn Mawr College	Mary Kutteruf	Fourier Transform Terahertz Spectroscopy of Amino Acids, Peptide Chains and Frozen Solvents	15	PL
	Jessie Rosenberg	Preparation and Characterization of Nanostructures for Surface Enhanced Raman Spectroscopy (SERS)	16	PL
Bucknell University	Matthew Paoletti	Characterization of Derived Porous Silicates and Bioencapsulated Catalytic Proteins	17	MSEL
Calvin College	Michael Scholten	Two-Beam-Excited Conical Emission	18	PL
Carnegie Mellon University	Michael Polyakov	Displaying Fourier Maps in FOX Using the Marching Cubes Algorithm	18	MSEL
	Michael Vahey	Characterization of MEMS Microheating Elements	19	EEEL
Case Western Reserve University	Margaret Polinkovsky	Reference Value Estimators in Key Comparisons	19	ITL
College of William and Mary	Andrew Busch	Ballistic Magnetoresistance in Nanocontacts	20	MSEL
	Kathryn Keister	20-Bit Precision Electronics for the Electrically Substituted Bolometer (ESB)	21	PL
Cornell University	Eric Hsu	Quantum Computing Simulation Optimizations and Non-Gaussian Errors on a Gaussian Density Operator	21	ITL
Drexel University	Joe Kopena	Translation Inference in the Process Specification Language	22	MEL
Georgia Southern University	Lisa DeBeer	Swimming in a 3D Optical Lattice	23	PL
Grinnell College	Sarah Campbell	Reference Lines in the Optogalvanic Spectra of Thorium and Uranium Over the Wavelength Range 422 – 462 nm	23	PL
	Thomas Parr	Synthesis of $HSCH_2CH_2CH_2O(CH_2CH_2O)_{3\text{-}8}CH_3$ and Characterization of Their Self-Assembled Monolayers on Gold	24	CSTL
Gustavus Adolphus College	Chad Custer	Optimization of Portland Cement Pastes Containing Fly Ash: An Empirical Approach	24	BFRL
Hamilton College	James Baker	Spectral Narrowing of a High-Power Diode Laser Array for Spin-Exchange Optical Pumping	25	PL
Harvard University	Monika Schleier-Smith	The Production of Nitrogen-13 by Neutron Capture in Boron Compounds	26	PL
Jackson State University	Angela Fortner	Chemical and Electrochemical Synthesis of Gold-Polymer-Gold Nanowires for Multifunctional Sensor Investigation	26	CSTL
James Madison University	Evan Schwartz	X-Ray Microscopy with Multilayer Mirrors in K-B Configuration	27	CSTL
Kent State University	Violeta Beleva	Calibration and Evaluation of Prostate Brachytherapy Seeds at NIST	27	PL
Loyola College	Heather Begley	DNA Sequence Detection Through the Use of Peptide Nucleic Acids	28	CSTL
	Kerry Begley	Analysis of Ephedra Alkaloids in Dietary Supplements	28	CSTL
Massachusetts Institute of Technology	Alexandra Ford	Structure and Magnetic Properties of Electrodeposited Co and Co-Fe Thin Films on GaAs (001)	29	MSEL

BFRL – Building and Fire Research Laboratory, CSTL – Chemical Science and Technology Laboratory, EEEL – Electronics and Electrical Engineering Laboratory, ITL – Information Technology Laboratory, MEL – Manufacturing Engineering Laboratory, MSEL – Materials Science and Engineering Laboratory, PL - Physics Laboratory.

SCHOOL	STUDENT	PROJECT TITLE	PAGE	NIST LAB
McDaniel College (formerly Western Maryland College)	Christopher Drupieski	Characterizing the Response of Thermoluminescent Dosimeters to Beta, Gamma, and Broad-Spectrum X-Ray Radiation	30	PL
Miami (Ohio) University	Kathryn Lee	Uranium and Thorium: Radioactive Refugees or Simply Irrestible?	30	PL
New Mexico State University	Derek Powell	Scalability and Performance Limits of Planar and 6D Parallel Cantilever Bi-Axial Micro-Positioner	31	MEL
North Carolina State University	Robyn Bloch	Synthesis and Characterization of Titanium Dioxide (TiO_2) Nanoparticles and Nanostructured Films	31	BFRL
Northeastern University	Igor Malioutov	Fusion of Face-Recognition Algorithms via Nonparametric Dependence Characteristics	32	ITL
Pennsylvania State University	Evan Pickett	BaO-ZnO-Ta2O5 and BaO-ZnO-Nb2O5: Phase Equilibria for Talking Ceramics	33	MSEL
Purdue University	Thomas Young	Effects of Surfactant Polymerization on Micellar Structure	33	MSEL
Radford University	Tim Dutton	Multi-Component, Three Dimensional, Viscoelastic Flow	34	MSEL
Rensselaer Polytechnic Institute	Kevin Bowers	An Adaptive Leasing Mechanism for Jini™	34	ITL
	Jack Damerji	Building a Multi-Biometric Authentication System	35	ITL
	Maureen Desi	Fire Pattern Re-Creation	35	EEEL/ BFRL
	Reza Hosseinzadeh	Temperature Control of the NIST Electronic Kilogram	36	EEEL
	Eranga Tyrrol Crossley Jayewardene	Design and Development of a Measurement and Control System to Calibrate Line Pitch Samples on the AMRAY Scanning Electron Microscope	36	MEL
	Mark Matarazzo	Wafer Inspection at Low Dimensions: Automated Resistivity Mapping System	37	EEEL
Rice University	Eliot Flannery	Speaker Verification	38	ITL
Rochester Institute of Technology	Matthew Aggleton	Magneto-Optical Indicator Film Imaging of Magnetostrictive Thin Films	38	MSEL
	Brad Conrad	2002: A Nanoparticle Sizing Odyssey	39	MSEL
Saint Mary's College of Maryland	Kevin Beanland	Comparison of Scanning Electro Microscope Simulation Programs MONSEL and Metrologia	39	MEL
	Jonathan Mulholland	Micro-Force Measurement with Piezo-Resistive Cantilevers	40	EEEL
Santa Monica College	Derrik Asher	The Cell General	40	MSEL
	Maria Kim	Limitations on Scaling of Silicon Dioxide as Gate Dielectric	41	EEEL
	Liliya Krivulina	Effects of Delay Mismatch in MPLS Networks with 1+1 Protection	41	ITL
	Han Kyu Lee	Polarimeter Using Photoelastic Modulator	42	PL
Southern Methodist University	April K. Andreas	Estimating the Work of Integer Partitions	43	ITL
Southern University and A&M College	Cari Bershell	That's Good, But You Can Do Better	43	PL
	Brandan Darensbourg	Laser Tracker Calibration for Acquiring the Values of Alignment Parameters Through a New Technique of Using Distance Measurement with the Lieca LTD500 Laser Tracker	44	MEL
	Rachel McKinsey	Characterization of the Water Calorimeters	44	PL
	Shelli Pace	Directional Solidification of Eutectic Alloys in the Ag-Cu-Sn System	45	MSEL
	Kenya Thomas	The Effects of Calcium, Phosphate, Light, and Time on the Stability of Peroxides	45	MSEL
	Erica Walton	Third Order Discretely Sampled Constrained Trajectory Generation	46	MEL
State University of New York – Binghamton	Paul Fleming	Silicon Based Single Electron Tunneling Transistors	46	EEEL
	Sebastian Larrea	Probability Plot Correlation Coefficient Test for Lognormally Distributed Void Radii in Entrained Concrete	47	BFRL

BFRL – Building and Fire Research Laboratory, CSTL – Chemical Science and Technology Laboratory, EEEL – Electronics and Electrical Engineering Laboratory, ITL – Information Technology Laboratory, MEL – Manufacturing Engineering Laboratory, MSEL – Materials Science and Engineering Laboratory, PL - Physics Laboratory.

SCHOOL	STUDENT	PROJECT TITLE	PAGE	NIST LAB
Texas Tech University	Tigist Belete	Nondestructive Evaluation of Fiber Reinforced Polymer Composites Bonded to Concrete	49	BFRL
Truman State University	Kevin Haworth	Improving Beam Imaging of Synchrotron Radiation at SURF III (aka Size Does Matter)	49	PL
Tulane University	Leah Broussard	Polarized Neutron Beam Characterization	50	PL
University of California – Berkeley	Jacob Scott	Distributed Computing in Java: The Screen Saver Science Project	50	ITL
University of California - Irvine	Siavosh Bahrami	A Study of Behavioral Expectations and Consistency in Human-Robot Interaction	51	ITL
	Heather Coman	The Accuracy of Current ACI Building Codes for Predicting the Effect of Carbon FRP on the Deflection of Concrete Beams	51	BFRL
	Tam Duong	Web-Based Database for NIST Electrical Standards Laboratories	52	EEEL
	Hoang Minh Ho Dac	Graphical User Interface for Fire Fighter Protective Clothing Simulator	53	BFRL
	Puja Gupta	Analysis of Conductivity in Mono-Crystalline Electrical Linewidth Structures	53	EEEL
	Mark Lawrence	Tunable LED Based Light Source	53	PL
	Roshni Malani	Testing Disk Imaging Tools	54	ITL
	David Stout	Development of a Liquid Chromatographic Method for the Analysis of Atmospheric Aerosol Samples	55	CSTL
	Twi Le Tran	Java Programming Support for Visualization Construction	55	BFRL
	Kris Vaughn	Vibration Isolation of the NIST Watt Balance	56	EEEL
University of California – Los Angeles	Amarpreet Cheema	Elliptic Curve Digital Signature Algorithm (ECDSA) Validation Tests	56	ITL
University of Maryland – Baltimore County	Ali Deyhim	Quantitative Contrast Variation Analysis of MS2-Like Virus Particles for Future Use in Clinical Diagnostics	57	MSEL
	Elizabeth Humphries	Photobleaching and the Damage of DNA During Fluorescent Detection	57	CSTL
University of Maryland – College Park	Wendy Chou	Testing Random Number Generators Using the NIST Statistical Test Suite	58	ITL
	Stuart Fletcher	Automatic Table Generation for Values of Special Functions	58	ITL
University of Massachusetts – Amherst	Nathan Barr	Validation of the ebXML Business Process Catalog	59	MEL
University of North Carolina – Chapel Hill	Vadas Gintautas	Effect of Suspending Medium and Particle Size on Dispersion of Fine Alumina Powders for Laser Diffraction Analysis	60	MSEL/ BFRL
University of North Carolina – Charlotte	April Cooke	Calibrated Micropyrometer Measurement of the Tool-Chip Interface in Machining	60	MEL
University of Puerto Rico	Xiomara Calderón Colón	Real-Time Measurements of Clay Dispersion Using VIS Dye Probes	61	BFRL
	Yaireska M. Collado-Vega	Characterization of Air Flow in a Manufactured House	61	BFRL
	Saylisse Dávila	Optimizing PID Algorithms Using Smart Sensor Control	62	MEL
	Angel Fuentes Figueroa	Measuring the Diffusion Coefficient of Small Molecules on Different Polymer Films	62	MSEL
	Rafael S. García-Cortés	A New IMPACT in Silicon Carbide Power Devices	63	EEEL
	Angélica Pérez-Andújar	Detectors Performance for Radiation Measurements for Home Land Security	64	PL
	Rolando E. Vega Ávila	Testing the Capacity of Manufactured Home Walls to Withstand Horizontal Loads	65	BFRL
University of Rochester	Ross Camara	IT Support of Nanoindentation	65	BFRL
University of Wisconsin – Madison	Michelle Shah	Investigations in Linear Motor Dynamics	66	MEL
Valparaiso University	Steven Wolf	Where No Man Has Gone Before	66	BFRL

BFRL – Building and Fire Research Laboratory, CSTL – Chemical Science and Technology Laboratory, EEEL – Electronics and Electrical Engineering Laboratory, ITL – Information Technology Laboratory, MEL – Manufacturing Engineering Laboratory, MSEL – Materials Science and Engineering Laboratory, PL - Physics Laboratory.

SCHOOL	STUDENT	PROJECT TITLE	PAGE	NIST LAB
Vanderbilt University	Melanie Bernard	Development of Crystallization Strategies	67	CSTL
Virginia Polytechnic Institute	Kai Zuehlke	Comparison of Sensor-Driven Fire Model Algorithms with Experiment	68	BFRL
Wellesley College	Alyssa Meyer	Liposomes as Microreactors	69	PL
Western New England College	Craig Beal	Holding Next to Nothing	69	MEL
Williams College	Rachel Gealy	Two Beam Non-Linear Optical Effects	70	PL
York College of Pennsylvania	Stephanie McLean	An Analysis of Time-Dependant Degradation of Organic Additives in Gunshot Residue	70	CSTL

BFRL – Building and Fire Research Laboratory, CSTL- ChemicalScience and Technology Laboratory, EEEL- Electronics and Electrical Engineering Laboratory, ITL- Information Technology Laboratory, MEL – Manufacturing Engineering Laboratory, MSEL- Materials Science and Engineering Laboratory, PL-Physics Laboratory.


SURF
Twentytwo