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News Briefs

General Developments

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NIST LAUNCHES ECONOMIC TOOLS FOR HOMEOWNER DURABILITY DECISIONS

NIST economists have developed a decision model that helps homeowners select the most cost-effective level of durability. The model has been incorporated into a suite of Internet decision tools called National Economic Service-life Tools (NEST) that is available at www.PATHNet.org.

The initial public release of NEST in September 2003 features the first two tools, NEST Builder and Durability Doctor. NEST Builder lets users specify the details of their house including its location, size, layout, and the materials they have for the major components of the external shell: roof, siding, windows, and garage doors. Durability Doctor allows users to compare different building materials based on cost and durability. The tool lets users analyze and compare different views of their virtual house with materials based on three criteria: the greatest durability, the lowest installation cost, and the lowest monthly life-cycle cost. After studying these views, homeowners can customize their house with the materials they prefer.

Tools planned for future releases of NEST will let users budget for future replacements of major housing elements, predict when major housing elements are likely to fail, and learn about the risk of significant natural hazards in their location.

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NIST RESEARCHERS DEVELOP NEW MICROWAVE MIXER THEORY; AID INDUSTRIAL DEVELOPMENT OF CALIBRATION PROCEDURE

NIST researchers, along with a foreign guest researcher, developed a mixer theory based on a set of simple rules for transforming multiple-frequency mixer problems into equivalent single-frequency problems. The theory is significant because it allows a number of system problems involving mixers and frequency conversion to be solved analytically and because it demystifies this rather esoteric subject.

The theory has found immediate application in the development of vector-network-analyzer algorithms for image-mixer characterization. Working from a rough draft of a manuscript describing the theory, an industry partner was able to immediately apply the simple rules outlined in the theory to understand and develop a calibration algorithm for testing image mixers. The new algorithm already has been implemented in the firmware of a popular commercial network analyzer. The algorithm soon will be available to engineers in the new network analyzers offered by the company, as well as in a software upgrade.

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NEW MICROFLUIDIC DNA ANALYSIS SYSTEM FOR FORENSICS APPLICATIONS DEMONSTRATED BY NIST

Modern forensic DNA analysis systems are currently based on the separation of DNA fragments by capillary electrophoresis, a process which typically takes 40 min. Unfortunately, there is a large backlog of DNA criminal tests in the United States, prompting the need for the development of new methods. Using a microfluidic device, researchers at NIST have demonstrated a separation of a DNA ladder with fragments ranging from 50 to 550 base pairs in 4 min.

This effort to develop a rapid DNA analysis system for forensics using microfluidic systems is being sponsored by the Department of Justice (National Institute of Justice, Office of Science and Technology, Investigative and Forensic Sciences Division's Program on DNA Research and Development). Microfluidic technology is a promising alternative to capillary-based techniques due to its great potential to miniaturize, simplify, integrate, automate, and multiplex the analysis with higher throughput and speed. Although DNA analysis systems based on microfluidics technology recently have been commercialized for DNA sequencing applications, these systems do not meet the specific needs of the forensic community due to poor separation resolution of the relatively long fragments (order 100 bps to 400 bps) as well as incompatibility with standard test procedures.

The team involved in this effort includes NIST, the National Institutes of Health, Northwestern University, and a private company.

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STUDIES PERFORMED OF ACOUSTIC LOSS IN LANGASITE, LANGATATE, AND LANGANITE

Langasite and its isomorphs, such as langatate and langanite, have attracted significant attention in recent years as materials for improved electronic oscillators and filters. The potential advantages of these crystals over quartz include higher piezoelectric coupling, which enables devices to be made smaller; lower acceleration sensitivity; and higher Q, which reduces phase noise and enables higher-frequency operation. However, higher Q has been observed only in a few crystals, and acoustic properties usually vary significantly within a single boule.

In order to identify physical mechanisms responsible for degradation of the performance, researchers at NIST have performed a series of studies of the acoustic loss Q^{-1} in langasite, langatate, and langanite as a function of frequency and temperature, using a unique noncontacting acoustic-resonance system. The results show that, in each material, anelastic defect relaxations are the dominant contributions to the loss at all temperatures where measurements were performed (100 K to 750 K). The intrinsic loss (arising from phonon-phonon scattering) is not apparent in any of the measurements, which suggests that the maximum attainable Q may be significantly greater than values reported thus far.

This work was partially supported by a grant from the U.S. Army Research Laboratory.

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NIST RESEARCHERS USE "FRUSTRATED" OPTICAL TECHNIQUE TO MEASURE FORMATION OF NANOCOATINGS

Additives are frequently mixed into polymeric materials in minute quantities in order to make them processable into the typical products well known to consumers, such as plastic sheets, pipes, and wire insulation. However, the reason behind the effectiveness of these additives had remained mysterious because the existing tools available to measure their behavior in the manufacturing process were rather crude. Now, re-searchers at NIST have utilized the optical phenomena of frustrated total internal reflection to directly visualize the behavior of fluoropolymer additives when added to polyethylene.

Researchers discovered a continuous process in which the fluoropolymer droplets "rain down" on the internal surfaces of the extruder and form a nanocoating. Similar to the fashion in which a fluoropolymer-coated frying pan prevents eggs from sticking, this nanocoating allows the polyethylene to smoothly slide through the processing equipment with lower energy utilization and without defects. Based on the measured thickness of the coating, which ranges from 20 nm to 400 nm, a qualitative model of this process was developed and published in the current issue of the *Journal of Rheology.* A collaboration between NIST, a private company, The University of Minnesota, and the University of Maryland is currently using this technique to uncover the critical factors influencing the coating efficiency.

For further information, visit www.nist.gov/polymers and search for "frustrated," or read the article in the *Journal of Rheology* (Vol. 47, No. 6, pp. 1523-1545).

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IN SITU STRESS MEASUREMENTS DURING ELECTRODEPOSITION OF THIN FILMS STUDIED

Thin films of various metals are used by the microelectronics community to produce, for example, solderable surface finishes, magnetic recording media, and copper wiring in printed circuit boards and integrated

circuits. Such films tend to develop sizable mechanical stresses as they are deposited. Though not well understood, these stresses can result from the nucleation and growth process (e.g., lattice-mismatched epitaxial growth) or, in the case of the widely used technique of electrodeposition, from the use of solution additives and alloying elements needed to achieve desired deposition rates and mechanical properties. Often these stresses can approach or exceed the yield stress of the bulk material and can lead to loss of adhesion and the generation of bulk and surface defects. As feature sizes in microelectronic components continue to shrink, the stresses associated with the earliest stages of film growth raise serious concerns in the industry about device performance and reliability.

To address these concerns, NIST researchers have established a Class II (1 mW) HeNe optical bench dedicated to the *in situ* measurement of residual stress during electrodeposition using the wafer curvature method. The substrate is a 60 mm × 3 mm × 0.1 mm wafer of borosilicate glass onto which 250 nm of gold is evaporated. The curvature of the substrate is monitored during electrodeposition by reflecting the laser off of the glass/metal interface, through a series of mirrors and onto a position-sensitive detector. The average in-plane stress of a metal film electrodeposited onto the Au can be calculated from the deflection of the beam as a function of time. The apparatus can resolve surface stresses on the order of 0.3 N/m while the beam is in solution, thus allowing researchers to observe the stresses associated with the entire deposition process.

As a demonstration, NIST researchers have followed stress development in the first 50 nm of Cu deposited onto Au. This system is known to follow classical Stranski-Krastanov growth, where three-dimensional islands grow on top of one or more Cu monolayers. Researchers have quantified the surface stresses associated with the formation of the first Cu monolayer, as well as the formation and coalescence of discrete Cu nuclei. It is expected that measurements such as these will allow the researchers to determine the root cause of stress in electrodeposited thin films and to propose mitigation strategies.

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ONE- AND TWO-PHOTON PHOTOELECTRON SPECTROSCOPY USED TO STUDY MOLECULAR ELECTRONICS SYSTEMS

The drive to introduce organic molecular materials into electronic device applications, "organic electronics," is motivated by a number of potentially attractive features, such as ease of fabrication, ability to fabricate on flexible substrates, and the wide extent to which organic materials can be functionalized via organic synthetic methods. A range of applications is foreseen for organic field effect transistors and organic light emitting diodes including, for instance, flexible displays and other low-cost flexible electronics.

In addition to replacing inorganic semiconductors in more or less conventional device architectures, organic systems also are of interest in the more speculative, and potentially more revolutionary area of "molecular electronics." Here, it is envisioned that the non-linear characteristics of individual molecules, or small ensembles, will provide the required device functionality, allowing low-cost chemical synthetic methods to, at least partially, replace multibillion dollar semiconductor fabrication lines in the production of nanoscale device structures.

In either application format, charge injection at a molecule-contact interface plays a vital role in controlling transport and, thus, potential device performance. Interfacial charge injection is dictated by chemical bonding and the resulting band lineup between the Fermi level of the contact and transport levels (HOMO and LUMO) of the molecule. Information relating to band lineup is difficult to obtain using conventional techniques in the case of the single-molecule length-scale systems of interest in molecular electronics.

Researchers at NIST have employed a combination of one-photon (He I resonance excitation) and two-photon photoelectron spectroscopy, using subpicosecond Ti:sapphire laser-based excitation, to determine the electronic structure, including injection barriers to both occupied and unoccupied levels, of 4,4′-bis-(phenylethynyl)benzenethiol self-assembled mono-layers, a system that has become a benchmark for theoretical and experimental studies in the area of molecular electronics.

Further work on the influence of chemical substitutions and measurements of electron dynamics are under way or planned for the future.

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NIST MICROFABRICATES ATOMIC VAPOR CELLS FOR CHIP-SCALE ATOMIC CLOCKS

A team of researchers from NIST have met a major milestone in the Defense Advanced Research Projects Agency's Chip Scale Atomic Clock (CSAC) program

by successfully microfabricating a cesium (Cs) vapor cell with a volume of less than 10 mm^3 using silicon micromachining techniques. Additionally, the researchers have developed vapor cell filling techniques and measured the effect of vapor cell buffer gas pressure on the intrinsic line width of Cs vapor atomic transitions. The cells developed by the team have volumes just under 10 mm^3, with spectral line widths less than 1 kHz for a 9.2 GHz Cs hyperfine absorption line. Other cells fabricated at NIST using the same process, and with volumes as small as 1 mm^3, have line widths only slightly larger.

Miniaturized atomic clocks (volume less than 1 cm^3) have military and civilian applications, including synchronization of encryption keys and communication networks and to help prevent jamming of global positioning systems.

Novel excitation techniques have been investigated by NIST, including coherent population trapping (CPT) resonances in which two optical fields are applied to a Cs vapor cell. The two fields are obtained by modulating the drive current for a vertical-cavity surface-emitting laser, thus generating laser sidebands separated by about 9.2 GHz. This eliminates the need for a resonating cavity and permits the cell size to be reduced to below the wavelength of the microwave radiation. At a critical frequency difference between the two laser frequencies, a dark-line or CPT resonance occurs, signified by a decrease in the Cs vapor optical absorption. This resonance then is used to lock the modulation frequency of the laser. The advantage of using the CPT method over conventional microwave excitation is that the clock can be made much smaller and simpler. Eventually, the goal of the NIST part of the CSAC Program is to develop a clock physics package (including laser, laser optics, vapor cell, vapor cell heater, photodetector, and magnetic shield) based on the CPT scheme with volume less than 3 mm^3.

Silicon micromachining methods currently being developed at NIST can be used to make vapor cells with dimensions well below 1 mm^3. In addition to a high level of miniaturization, other advantages include lower cost, higher reproducibility, and integration with control electronics and sensors.

The team has developed two methods for filling and sealing the micromachined cells: chemical reaction between barium azide and cesium chloride in an ultra-high vacuum system followed by anodic bonding of the silicon chip to a glass window in a nitrogen buffer gas ambient, and direct injection of liquid Cs in an anaerobic chamber followed by anodic bonding to a glass window in a nitrogen buffer gas ambient. In principle, both processes are scalable to wafer-level production.

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NIST PROVIDES KEY MEASUREMENTS FOR SUPERCONDUCTING MAGNETS FOR THE INTERNATIONAL THERMONUCLEAR EXPERIMENTAL REACTOR

Superconducting magnets are used in fusion energy projects, such as the International Thermonuclear Experimental Reactor (ITER), to confine and heat the plasma. The superconductors for the ITER's large magnet systems are all "cable-in-conduit conductors" (CICC), which provide both mechanical support for the large magnetic forces and a flow path for the liquid helium required to cool the cable. The superconducting magnet must be operated below the critical current of the cable, which is a function of magnetic field and temperature. Temperature is an important variable, and the local temperature of the conductor depends on the mass-flow rate of the coolant and the distribution of the heat load along the CICC.

Earlier magnet systems that used CICC experienced unexpected degradation of their superconducting properties. To help determine the source of such degradation, NIST scientists measured variable-temperature critical current of a "witness" superconductor strand that was thermally processed along with the superconducting cables used to make the latest two ITER test conductors.

The results of NIST's unique variable-temperature measurements provide a comprehensive mapping of critical current as a function of magnetic field (0 T to 12 T) and temperature (4 K to 17 K), and form a basis for evaluating CICC and magnet performance. NIST scientists used the data to generate curves of electric field versus temperature at constant current and magnetic field. These, in turn, gave a direct indication of the temperature safety margin of the conductor.

NIST's results will be used by Lawrence Livermore National Laboratory, which will test CICC samples at the Plasma Physics Research Center in Villigen, Switzerland, with current up to 100 000 A and magnetic fields up to 12 T, while controlling the mass-flow rate of the coolant.

More information about ITER may be found at www.iter.org.

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NIST VALIDATES 100TH ADVANCED ENCRYPTION STANDARD IMPLEMENTATION

In October 2003, NIST's Cryptographic Module Validation Program (CMVP) reached a significant milestone by issuing the 100th Advanced Encryption Standard (AES) Algorithm Validation Certificate for hardware implementation of AES named 7814-W. This is an intelligent packet-processing chip that implements AES, Triple DES, integrated public key crypto-graphy, and compression. 7814-W implements the Electronic Codebook and the Cipher Block Chaining modes of operation for both encryption and decryption, and supports key sizes 128 bit, 192 bit, and 256 bit.

Federal Information Processing Standard (FIPS) 197, Advanced Encryption Standard, describes the AES algorithm as a symmetric block cipher that can encrypt (encipher) and decrypt (decipher) information. The AES is capable of using cryptographic keys of 128 bit, 192 bit, and 256 bit to encrypt and decrypt data in blocks of 128 bits. Since November 2001, AES has been the FIPS-approved symmetric encryption algorithm of choice.

The AES validation test suite consists of the Known Answer Tests (KATs), the Multi-block Message Test (MMT), and the Monte Carlo Test (MCT). The KATs are designed to provide conformance testing for the individual components of the AES algorithm. The MMT is designed to test the ability of the implementation to process multiblock messages, which require the chaining of information from one block to the next. The MCT is designed to exercise the entire implementation of the AES, as opposed to testing only the individual components. The AES validation test suite tests the Modes of Operation ECB, CBC, OFB, CFB (1 bit, 8 bit, and 128 bit), and CTR. For each mode implemented, selections are available for key sizes (128 bit, 192 bit, 256 bit) supported as well as the ciphering direction (i.e., encryption and decryption).

Successful completion of the AES validation tests is required to claim conformance to the AES as specified in FIPS 197. When applied to implementations under test (IUTs), the validation tests determine the correctness of the algorithm implementation. In addition to ascertaining conformance, the tests detect implementation flaws including pointer problems, insufficient allocation of space, improper error handling, and incorrect behavior of the AES algorithm implementation.

The AES validation test suite is part of NIST's CMVP, which encompasses validation testing for cryptographic modules and algorithms. Other cryptographic algorithms currently validated by the CMVP are the Data Encryption Standard (DES), the Triple Data Encryption Standard (TDES), the Digital Signature Algorithm (DSA), the Secure Hash Algorithm (SHA-1), and the Random Number Generator algorithm (RNG). In the near future, the Reversible Digital Signature Algorithm (rDSA), the Elliptic Curve Digital Signature Algorithm (ECDSA), SHA-256, SHA-384, and SHA-512, and HMAC validation suites also will be available.

The CMVP uses laboratories accredited by NIST's National Voluntary Laboratory Accreditation Program to test cryptographic products that conform to FIPS. A vendor contracts with an accredited laboratory to perform the tests. When testing is completed, the laboratory submits the results to NIST for validation. If the vendor's implementation of the specific algorithm successfully passes the tests, NIST issues a validation certificate to the vendor. The Web site is csrc.nist.gov/cryptval.

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RECOMMENDED PRACTICE GUIDE ON DATA EVALUATION THEORY AND PRACTICE FOR MATERIALS PROPERTIES DEVELOPED

Data evaluation is the process by which collections of data are assessed with respect to reliability, completeness, and consistency. Based on more than a decade of experience, NIST has developed a *Recommended Practice Guide, Data Evaluation Theory and Practice for Materials Properties,* SP 960-11, to address the growing need for the evaluation of materials property data. The work approaches data evaluation as a scientific discipline that evolves from the formal underpinnings of materials metrology. A theoretical foundation for data evaluation is developed first, and then the application of the basic principles is illustrated by developing a practical operational protocol specifically for materials property data. An extensive collection of examples is used to examine, in succession, the issues of accessibility, reproducibility, consistency, and predictability. Distinctions are made among definitive relations, correlations, derived and semi-empirical relations, heuristic theories, and value estimates. Subtopics include the use of properties as parameters in models, the interpretation of ad hoc parameters, and the treatments of procedural properties, response dependent properties, and system dependent data.

This guide is the 11th practice guide produced by NIST. More information on the SP 960 series can be found at www.nist.gov/practiceguides.

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TECHNIQUE INVENTED FOR MEASURING THE RESIDUAL STRESS IN A STRUCTURE

NIST scientists are among the inventors of a new technique to measure the residual stress in a structure. The technique is based on the fact that residual stress changes the polarization and phase of shear horizontal (SH) waves sent through a structure. Using this prin-ciple, the inventors motorized an electromagnetic-acoustic transducer to measure the acoustic characteristics of the structure. After the stress changed, the structure was remeasured. Then, the signal was sent through an algorithm to extract the stress value from the changes in the magnitude and phase of the SH waves. The invention has been issued Patent Number 6,502,463.

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NIST HOSTS GROUNDBREAKING VOTING STANDARDS SYMPOSIUM

Over 280 computer scientists, vendors, voting rights activists, secretaries of state, and local election officials participated in NIST's First Symposium on Building Trust and Confidence in Voting Systems in Gaithersburg, Md., on Dec. 10-11, 2003. In addition, two newly appointed election assistance commissioners addressed the attendees.

Participants discussed and debated challenging computer security and usability issues related to the Help America Vote Act and the role NIST will play in the law's implementation. Thirteen vendors of election equipment and technologies—one traveling all the way from the Netherlands—demonstrated their systems.

NIST panel moderators briefed the attendees on relevant expertise available to the election community to improve public trust and confidence in voting systems. A NIST scientist chaired the fourth panel, which reviewed consensus issues and possible next steps. NIST Director Arden Bement closed the symposium, noting the common purpose shared by all in attendance: that every vote has to count and every eligible voter has to be able to vote. The Web site is vote.nist.gov.

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NIST HOSTS ROCKET PROPELLANT RP-1 WORKSHOP

On Dec. 11, 2003, NIST hosted a workshop at the Boulder, CO, campus of NIST on the thermophysical properties of the rocket propellant designated RP-1. Specialists in rocket fuels (from the National Aeronautics and Space Administration (NASA), the Air Force, commercial rocket engine manufacturers, and academia) convened with NIST researchers to hear about recent NIST work conducted to help better define the properties of this fuel and to plan future activities required to achieve consensus standards for the properties of fuels over the broad ranges of conditions The work at NIST was conducted primarily in support of NASA efforts to develop highly reliable reusable rocket engines for future launch vehicles in which the fuels may encounter higher pressures and temperatures. The rational design of such systems must be based on accurately known thermophysical properties, and it was apparent to the rocket designers that information on the properties of RP-1 was extremely limited. In one NASA study, it was concluded that property uncertainties account for 70 % of the uncertainty in a portion of the propulsion system design, and it was noted that the differences in RP-1 properties from different sources can amount to 5 % to 60 %.

NIST researchers reported new, high sensitivity compositional characterizations of RP-1 fuels and new metrological quality property results for density, viscosity, heat capacity, and thermal conductivity with temperatures extending beyond a decomposition limit (near 600 K) and pressures to about 70 MPa. These data were used to establish accurate preliminary property surfaces for this complex fluid. A software implementation of the preliminary models was delivered to NASA engineers and their contractors for testing and to assist in the resolution of current engine design problems. Participants in the workshop were eager to use the current results, and were very interested in continued NIST efforts to explore the effects of sample-to-sample variation and refined processing methods on fuel properties, to help establish new protocols for fuel characterization, and to expand the range of conditions and properties.

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