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News Briefs

General Developments

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NIST ANNOUNCES APPROVAL OF ADVANCED ENCRYPTION STANDARD

On Dec. 4, 2001, the Secretary of Commerce announced approval of Federal Information Processing Standard (FIPS) 197, Advanced Encryption Standard (AES). The new standard will be widely used to protect sensitive computerized information such as financial transactions. The announcement marked the culmination of a 4 year effort by NIST computer scientists, who organized an international competition in a drive to develop this strong information encryption formula to protect sensitive information in federal computer systems into the 21st century.

The AES incorporates the Rijndael encryption formula which was developed by Belgian cryptographers. Products implementing the AES are expected to be available in the marketplace shortly. FIPS 197 and information about its development are available at http://csrc.nist.gov and http://www.nist.gov/aes.

The AES replaces the Data Encryption Standard (DES) which NIST adopted as a FIPS in 1977 for federal agency use in the protection of sensitive, unclassified information. Private industry, especially the banking and financial services sectors, uses DES and Triple DES to protect vital electronic transactions. A recent NIST analysis (http://www.nist.gov/director/prog-ofc/report01-2.pdf) of the economic impact of DES states, "As a result of NISTs efforts, the market for encryption hardware and software expanded, developers of these products faced lower technical and market risks, and users of encryption systems (banks in particular) enjoyed operational efficiencies for their enhanced ability to substitute secure electronic transactions for more costly paper-based and face-to-face transactions . . . Assuming that industry would have reached a consensus on a data encryption standard three to six years after initial publication of DES, the economic impact results . . . indicate that it was far more effective and efficient for NIST to develop and implement DES than it would have been to wait for the results of industry cooperation." Assuming a 6-year lag in the development of DES without NIST's efforts, the savings realized by the banking industry are estimated at more than one billion dollars (net present value in 2000).
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CRITICAL DATA FOR INTEGRATED-CIRCUIT MANUFACTURING

The next generation of microlithography tools under development utilizes deep-ultraviolet radiation near 157 nm. This wavelength is characteristic of molecular fluorine lasers and is refracted (focused) by special materials such as CaF_2 and BaF_2. However, the index of refraction of these materials varies rapidly with wavelength, requiring precise determination of the lasers' actual spectral lines for engineering purposes.

Scientists at NIST have performed very accurate measurements (uncertainties of ± 0.0001 nm) of six wavelengths of a molecular fluorine laser of the type to be used for production of integrated circuits. Three of the lines were newly observed. They used the NIST 10 m vacuum spectrometer to record the spectra, which were calibrated by spectral lines from a platinum hollow cathode lamp. Accurate wavelengths for this lamp had been determined previously for the calibration requirements of the Hubble Space Telescope and included among the Physical Reference Data on a NIST website.
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UNDERSTANDING PROPERTIES OF POLYMER THIN FILMS

Polymer thin films have important applications in many industries. They are found, for example, in semiconductor devices, automobile coatings, and construction materials. The molecular structure at both the free and buried interfaces of thin films are critical to their performance, as they can determine characteristics such as adhesion and wear resistance. However, very few analytical techniques have both the sensitivity and selectivity to adequately study polymer interfaces.

NIST has developed procedures to study the interfaces of thin polymer films using vibrationally-resolved sum-frequency generation (VR-SFG). Recently, NIST has been developing a novel broadband approach to VR-SFG based on state-of-the-art femtosecond lasers. This technique has been shown to be a probe of molecular structure at polymer surfaces.

Most recently, by employing the optical interferences in thin films and by systematically varying film thicknesses, NIST has acquired spectra that selectively probe the buried interfaces between polymer and glass films. VR-SFG is now being applied to determine the relationship between interfacial molecular structure and adhesion. Results of this work may be found in the following reference: Appl. Phys. Lett. **80** (17), 3084-3086 (2002).
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FURTHER IMPROVEMENTS TO NIST-F1

NIST scientists have made several improvements to NISTs primary frequency standard, the cesium-fountain clock NIST-F1. The result is improved reliability of operation and improved accuracy. Reliability is important since the value of NIST data submitted to the BIPM is substantially higher if data are submitted at regular intervals. Furthermore, the achievement of highly regular operation offers the opportunity to use the data from this standard directly in the NIST time scale.

The improvements include: installation of new light shutters of substantially higher reliability; implementation of a servo-control system on the number of atoms tossed in each ball; a lower noise quartz-crystal local oscillator; and new software for the main line-center servo-control system. A completely new laser system (Ti:sapphire) has been acquired, and it will replace the current system as soon as final acceptance testing has been completed.

With these changes, the uncertainty of the standard has been improved from 1.7×10^{-15} to 1.3×10^{-15}. This is the best yet reported to the BIPM. Furthermore, quantum-projection noise has now been observed at a level of 30 atoms. This is lower by a factor of two to three than had been seen previously in a fountain frequency standard.
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COHERENCE BETWEEN NODES OF A DUAL MULTIPLEXED TRAP

In order to build a multiplexed quantum computer based on trapped ions, coherence must be maintained as ion qubits are transferred between traps.

This was recently demonstrated at NIST by a variation of a Ramsey experiment. In a three-step process on a single ion, a $\pi/2$ pulse was first applied to the ion as it sat in trap 1. The ion was then shuttled to trap 2 where it was subjected to a pi pulse. Finally, it was shuttled back to trap 1 where another $\pi/2$ pulse was applied to it. This sequence of pulses was similar to that typically applied to an ion in a single trap to achieve Ramsey interrogation, but here the ion had been shuttled between traps during the experiment to determine whether coherence was lost in the process of shuttling. The three-pulse ("spin-echo") technique is relatively immune to slow drifts in magnetic field over the averaging time of the experiment, but it is sensitive to the coherence between traps 1 and 2.

The observed high level of the Ramsey-fringe contrast demonstrated that coherence was maintained.
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ADVANCING THE THEORY OF THE HYDROGEN ATOM

The hydrogen atom is the most basic atom from the point of view of atomic structure theory. Historically, efforts to understand its detailed properties have led to many advances in understanding fundamental physics. This atom is important not only as a model system that tests the limits of atomic theory and experiment, but it also provides information on fundamental physical constants, such as the Rydberg constant. In the past decade, the precision of the experiments has been improving rapidly, and improvements in the theory have been necessary to keep pace.

Over the past several years, a NIST-led project has carried out a precise calculation of the most basic quantum electrodynamic (QED) effect in the spectrum of hydrogen, namely the radiative process in which the atom emits and then reabsorbs a photon (the quantum of electromagnetic radiation). This process results in shifts of the atomic energy levels, which, in turn, affect the

frequencies of light that are emitted and absorbed in experiments. The NIST work has led to a reduction of the uncertainty in the one-photon QED effect by over three orders of magnitude.

This accomplishment was made possible by a number of factors, including the high-performance computing resources at NIST and new developments in numerical analysis. The calculation required months of intensive, high-performance parallel computation.

This project was a collaboration between NIST, the Technical University of Dresden, and the University of Regensburg, both in Germany. The results have received wide recognition. For example, the project has been described as a "spectacular success" in *Physics Reports,* Vol. 342, p. 63 (2001).

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NIST CONTRIBUTES TO DEVELOPMENT OF NEXT GENERATION MULTIMEDIA STANDARD MPEG-7

NIST actively participated in the development of the MPEG-7 Multimedia Content Description Interface standard, which was released at the Moving Picture Experts Group (MPEG) meeting in Thailand in December 2001. The MPEG-7 standard provides standardized, core technologies allowing metadata description of audio-visual data content in multimedia environments. A NIST scientist provided MPEG-7 schema and sub-schema validation for the ISO/IEC multimedia description scheme; MPEG-7 sub-schemas included description definition language, visual, audio, and W3C 1998 XML Namespace.

A new web-based NIST MPEG-7 validation service (http://m7itb.nist.gov/m7v) has been set up to help MPEG-7 developers validate their encoded MPEG-7 metadata online. Recently, the NIST scientist initiated new work in MPEG to develop an MPEG-7 interoperability test bed to provide a validation process for encoded MPEG-7 metadata for conformance and interoperability testing between MPEG-7-based applications and to verify applicability of MPEG-7 technology in a real application or production environment. The NIST scientist is the chair of the newly established MPEG-7 Interoperability and Profiling Group and co-chair of the MPEG-7 Applications and Promotion to Industry (MAPI) group within the MPEG standard body. In addition, the NIST scientist has recently been nominated to head as Vice President of the MPEG-7 Alliance an industry forum to help industry to transfer and adapt the MPEG-7 technology, and serves as the webmaster for the MPEG-7 website (http://mpeg-industry.com).

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NEW TEST METHOD TO DETERMINE THE CONSTITUENT CONTENTS OF POLYMERIC COMPOSITES

Researchers at NIST are proposing a modification of the standard burn-off test to characterize carbon/glass hybrid composites, ASTM D3171-99. Hybrid composites are increasingly being used in infrastructure, aerospace, and automotive applications. These hybrids use two different fibers to reinforce the resin, thereby gaining some of the advantageous properties of both fibers. Typically, carbon and glass are used since this combination provides high performance and low cost. Critical issues in such materials are the fiber mix ratio and the fiber and void contents. At present, there is no simple way to determine these features, although many techniques exist for measuring the components of single reinforcement composites.

The proposed amendment calls for heating the specimen in a muffle furnace in a series of steps designed to sequentially separate out the resin, carbon fibers, and glass fibers. In addition, void contents of these composites can also be calculated. Results obtained with the proposed method on both commercial and laboratory-prepared samples were found to be in excellent agreement with values obtained by labor-intensive microscopic examinations.

Knowledge of the constituents in hybrid composites is needed for the development of models that accurately predict composite strength and failure behavior. The ultimate goal of this work is to use parameters such as those determined by this new test to establish a mathematical link between micromechanics properties that initiate and control the modes of composite failure and the physics of composite failure behavior.

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HIGH NITROGEN STAINLESS STEEL ALLOYS PROVIDE NEW OPPORTUNITIES

During a project on the development of sensors for the powder metallurgy industry, NIST has developed a technique for production of nitrogenated stainless steel alloys with enhanced corrosion and mechanical properties. Discussions with metal powder producers are underway to develop commercial powder metallurgy alloys using the NIST process that will find applications in biomedical implant devices, light-weight armor plate, and other demanding environments. NIST developed this technique through work on a model for prediction of

nitrogen solubility and microstructure in modified 300 series stainless steel alloys.

The new powder metallurgy nitrogenated stainless steel alloys are single phase (austenite) with no tendency to form the embrittling nitride and sigma phase compounds often found in high nitrogen stainless steels. The unique microstructure results in consolidated parts with superior corrosion and mechanical properties compared to commercially available wrought alloys, and reduced costs compared to other powder metallurgy nitrogenated stainless steel alloys. Three NIST scientists were awarded U.S. Patent 6,168,755 for the development.

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INTERLAYER MAGNETIC COUPLING IN FERROMAGNETIC SEMICONDUCTORS FOR SPINTRONIC APPLICATIONS

Advancements in semiconductor circuitry have revolutionized data processing in recent decades. Simultaneously, developments in magnetic-based media have expanded capabilities for permanent data storage. An emerging technology called spintronics integrates magnetic components with semiconductor devices and has the potential to increase processing power by many orders of magnitude. In the ongoing search for materials combining properties of ferromagnets and semiconductors, researchers have discovered a promising new class of dilute ferromagnetic semiconductors that includes $Ga_xMn_{1-x}As$.

NIST researchers at the NIST Center for Neutron Research (NCNR) have begun to probe these structures with polarized neutron reflectometry and small-angle neutron scattering to determine the nature and relevant length scales of cooperative magnetic behavior in these materials. Polarized neutron reflectometry is ideally suited to the study of these structures because it provides depth-dependent magnetic profilometry of buried magnetic layers with sub-nanometer resolution. Since the equilibrium Mn solubility in GaAs is low (less than seven percent), the ferromagnetic transition temperature of the homogeneous alloy is limited to 110 K, far below feasible temperatures for device operations.

To stabilize a higher concentration of Mn, researchers at University of California Santa Barbara fabricated digital GaAs/Mn superlattices by molecular beam epitaxy techniques. NCNR and University of Utah researchers have probed digital structures with polarized neutron reflectometry to determine how the interaction between the Mn layers changes as a function of their separation distance. The experiments show that Mn layers spontaneously align parallel to each other after cooling in zero magnetic field. These early polarized neutron reflectometry measurements provide guidance for fine-tuning the structure to maximize the ferromagnetic order ing temperature as well as to establish other fundamental spintronic properties of these innovative semiconducting materials.

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NIST SUCCESSFULLY TRANSFERS X-RAY MICROCALORIMETER TECHNOLOGY FROM BOULDER TO GAITHERSBURG

The microcalorimeter energy dispersive x-ray spectrometer developed by NIST staff, has been successfully implemented on an analytical scanning electron microscope in Gaithersburg. The system improves the spectral resolution by one to two orders of magnitude compared to the semiconductor silicon energy dispersive x-ray spectrometer which forms the existing industry standard.

Such improved resolution combined with energy dispersive operation makes possible direct spectral separation of most overlapping peaks often encountered with silicon energy dispersive x-ray spectrometery in complex multi-element systems. The improved resolution of the microcalorimeter energy dispersive x-ray spectrometer also increases the peak-to-background ratio, which translates into more sensitive detection. Peak shape and shift can be studied to reveal chemical state information. The microcalorimeter energy dispersive x-ray spectrometer will be used initially by NIST scientists for a program of basic x-ray spectrometry to establish better values of weights of lines of complex L- and M-family x rays in the 200 eV 3 keV range. This improved spectral database is vital for the next stage in developing a systematic approach to low energy x-ray microanalysis.

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SCREENING FOR NOVEL HYDROXYLATIONS BY P450 BIOCATALYSIS

Industries involved in manufacture of fine chemicals, pharmaceutical precursors such as the intermediates for Taxol or of high performance materials such as the polymers in bulletproof vests are searching for new synthesis routes to make relevant chemical building blocks. In many cases, these building block chemicals contain aromatic functionality or require specific

patterns of oxygenation along a chemical backbone. Oxygenated benzocycloarenes (fused benzenecycloalkane structures) are a class of such useful reactants that are hard to make by traditional organic synthesis routes. Biocatalysis is a particularly attractive alternative for making these compounds and has the additional advantage of doing so by green, environmentally friendly syntheses.

A project at NIST is focused on development of enzymes, tools for screening enzymes, and measurements of enzyme-catalyzed reactions that can apply to these industrial needs. The work builds on one of the human liver's principal drug-metabolizing enzymes, cytochrome P450 monooxygenase. Earlier work in the project showed that these enzymes are useful as biocatalysts for hydroxylation of benzocycloarenes to regio- and stereospecific alcohols. Now experimental and theoretical studies with wild type enzyme and an engineered mutant have shown that hydroxylation is regiospecific at the 1-position for a family of benzocycloarene compounds: benzocyclobutene, benzocyclopentene (indian), benzocyclohexene (tetralin), and benzocycloheptene.

A major scientific conclusion was that reaction energetics predominated over active site steric constraints so that quantum mechanical calculations comparing the energetics of all possible radical intermediates successfully predicted the hydrocylation patterns for all products. An important technological aspect was the development of a rapid spectroscopic assay for identifying potential targets of P450 catalysis in a high-through-put screening format. The work has been published in the *New Journal of Chemistry,* Vol. 26, pp. 35-42 (2002).

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PRISONS ACHIEVE FIRE CODE COMPLIANCE WITH ALARM, SAVING TIME AND MONEY

ALARM 2.0 is a software tool designed to help prison facility managers and fire safety engineers achieve cost-effective compliance with the widely-used Life Safety Code of the National Fire Protection Association (NFPA). Correctional facilities can use compliance with the Life Safety Code to receive accreditation from the American Correctional Association (ACA). ALARM, developed in NIST's Office of Applied Economics with the support of NIST's Office of Law Enforcement Standards, implements a goal-oriented or performance-based approach to achieving code compliance. This approach provides multiple alternatives to choose from when deciding how to achieve compliance by assigning varying weights to 13 safety features. By taking advantage of these alternative solutions, a user can compute the least-cost means of compliance to achieve significant savings compared with the rigid prescriptive solution.

Once the user specifies the current safety levels for the facility, the software designates potential safety improvements available to achieve compliance with the code. The user then enters dimensional data to find the least-cost combination of improvements and its estimated construction cost. The software generates a report detailing safety improvements to be made, broken down into tasks with cost estimates for each. A comprehensive manual and help system are included to answer questions about the software and the NFPA code. A tutorial explains all facets of ALARM and guides the user through the program.

ALARM 2.0 is based on earlier work in the Office of Applied Economics which was applied in the evaluation of 89 hospitals. An average of 41 percent savings was achieved compared with prescriptive solutions. ALARM is currently being distributed by the NFPA and the ACA.

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STANDARD SETS STAGE FOR GROWTH OF METROPOLITAN AREA NETWORKS USING FIXED BROADBAND WIRELESS

On Dec. 6, 2001, the Standards Board of the Institute of Electrical and Electronics Engineers, Inc. (IEEE) Standards Association approved the publication of IEEE Standard 802.16, *Air Interface for Fixed Broadband Wireless Access Systems.* The standard was created by the IEEE 802.16 Working Group on Broadband Wireless Access, initiated and chaired by a NIST scientist who also served as technical editor of the 355-page document, which specifies an advanced 10 GHz to 66 GHz radio system to provide interoperability between systems from various manufacturers. Details are available at http://WirelessMAN.org.

The 802.16 air interface standard is expected to form the basis of a global industry connecting buildings to public networks for data, voice, and video access without cables. Press coverage and company announcements of support have followed approval of the standard. One announcement stated, "The approval of the IEEE standard represents a turning point for the broadband wireless industry. Now, component, radio and systems suppliers can begin to implement the standard, and as this activity accelerates, the industry overall will benefit from more manufacturers entering the market, lower-cost designs and higher volumes. Ultimately, the number of businesses with access to broadband services will increase substantially around the world."

IEEE Standard 802.16 is primarily oriented toward business applications. However, the 802.16 Working Group, with 130 members, continues progress on extending its work to 2 GHz to 11 GHz with its 802.16a amendment project. At these lower frequencies, residential applications are the primary target.
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LOW-MELTING LIQUIDS IN HIGH-TEMPERATURE SUPERCONDUCTOR PRECURSOR SYSTEMS

NIST researchers are characterizing the phase equilibria of liquids in the BaF_2-BaO-Y_2O_3-CuO_x-H_2O system, in order to provide data essential for the reproducible processing of low-cost, second generation, high-temperature superconductor wire and cable. As concern increases about the supply of non-renewable energy resources and global environmental issues, high temperature superconducting materials remain attractive as part of potential solutions for improving the efficiency of energy distribution and utilization. Key is the availability of low-cost, long-length, high-performance wire and cable.

Commercial scale-up is beginning for fabrication of long-length cable using first generation materials based on Bi-Sr-Ca-Cu oxide (BSCCO) high-temperature superconductors. However, this is still a relatively high-cost process, which may limit large-scale application in the utility industry. Consequently, NIST researchers, sponsored by the Department of Energy (DOE), are investigating second generation high-temperature superconducting materials based on Y-Ba-Cu oxide (YBCO) coated metallic conductors.

These materials can be processed in tape form using thin-film deposition methods, potentially reducing the costs associated with the rather complex powder-in-silver tube process used for BSCCO. One of the most promising YBCO coated conductor processing routes is the fabrication of BaF2-containing precursor films which are then converted to oxide superconductor through reaction with water-vapor.

A relatively low temperature (<730 °C) liquid is thought to be involved, the control of which can greatly influence the kinetics of conversion and the resulting texture and transport properties of the superconductor. By studying the BaF_2-YBCO precursor system under carbonate-free conditions using specially constructed apparatus, NIST researchers have identified regions in multidimensional phase space where liquids occur at temperatures lower than 700 °C.
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CVD AND ELECTRODEPOSITION PHENOMENA LINK REVEALED

NIST researchers have quantified the link that exists between chemical vapor deposition and liquid solution electrodeposition for superconformal filling of high-aspect ratio, fine features. This recent work exploits the curvature enhanced accelerator coverage (CEAC) mechanism developed at NIST and used to quantify superconformal electrodeposition of copper (widely used for integrated circuit production), as well as superconformal electrodeposition of silver, also a recent NIST discovery.

The CEAC mechanism explains the link between the coverage of catalyst adsorbed on the surface of the growing metal and the changing area of that surface as it impacts the local metal deposition rate. Models based on this mechanism explain why deposition of metal occurs predominantly at the bottom of sub-micrometer dimension trenches and vias, leading to bottom-to-top filling of high aspect ratio features, an essential ingredient of integrated circuit fabrication in today's electronics. The newest NIST work explains experimental observations, published in the last year, of superconformal filling during chemical vapor deposition of copper. Based on these results, industry might one day be filling vias and trenches with a variety of metals using techniques in addition to electrodeposition.
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DAVE: DATA ANALYSIS AND VISUALIZATION ENVIRONMENT

NIST scientists at the NIST Center for Neutron Research have developed a new software tool for the reduction, visualization, and analysis of neutron inelastic scattering data. DAVE, short for Data Analysis and Visualization Environment, is an integrated suite of interactive software tools with a visual interface for treating and analyzing neutron inelastic scattering data sets. With a few clicks of the mouse, users can reduce their data from one of the inelastic spectrometers, make cuts through the scattering function, and fit them with the lineshape of their choice from a library of model functions.

The integration of these functions greatly simplifies moving among the different inelastic spectrometers. Moreover the software is designed so that users can easily add other instruments or more advanced analysis functions. DAVE is a stand alone executable application freely available for PC, Linux, and Mac platforms.
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NEW PHOTOMASK DESIGNED FOR SEM MAGNIFICATION CALIBRATION

In preparation for the issuance of a new batch of the successful scanning electron microscope (SEM) magnification calibration artifacts, Reference Material (RM) 8090 and Standard Reference Material (SRM) 2090, NIST scientists have completed design of a new lithography photomask. In the past, all individual samples of RM 8090 or SRM 2090 were made by direct write electron-beam lithography, because optical lithography did not have the required resolution. That limitation has recently changed with the implementation of 193 nm lithography.

The new mask designed for 193 nm lithography is the state-of-the art, and will provide 100 nm lines and 100 nm spaces and all the larger, up to 1.5 mm sized line pairs in *x* and *y* directions. The new design also includes areas for optical scatterometry measurements and a large field of patterns that can be used for geometry measurements in the SEMs at both low and high accelerating voltages. These samples can be used not only in SEMs, but also with any other microscopes. The new batch of samples will be made through cooperation with International SEMATECH. They will be individually much less expensive because they will be made using regular integrated circuit manufacturing processes.
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SHAPE-SENSITIVE MEASUREMENT OF NESTED LINES

In a scanning electron microscope (SEM), nested lines (lines with nearby line neighbors) image differently than isolated lines. This is because some of the electrons that otherwise would escape from the illuminated line to the detector have trajectories that intersect the neighboring lines. The extent of the effect depends upon the proximity and height of the neighboring lines, as well as the electric fields near the sample. The different appearance of lines that may, in principle, be the same width complicates linewidth measurement.

NIST scientists took these effects into consideration in calculations of the expected image for nested lines with varying sidewall angles. The resulting library of line shapes and their expected images was used to deduce the line shape, width, and separation of closely spaced polycrystalline silicon lines by comparison with top-down SEM images of the sample (the measurement configuration used in the semiconductor industry). This result was compared to an SEM image of the cross-sectioned pattern with good agreement. This is the first test of the library-based shape-sensitive linewidth measurement method on nested lines.
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STANDARD BULLETS—SOON A REALITY

In 1997, members of the law enforcement community approached NIST about developing physical standards for optical imaging systems used to match bullets and the criminals who use them. Originally, NIST scientists developed two prototype standard bullets. Based on the comments received from firearm examiners nationwide, these prototypes were developed into Reference Material (RM) 8240 bullets.

They are designed with six signatures from six master bullets of ATF and FBI laboratories and with the same material, color, shape, and twists as real bullets. The signature uniformity of these RM bullets will be tested first at NIST using a stylus instrument with a NIST-developed algorithm, comparing with a set of virtual bullet signature standards developed at NIST in 2001. These RM bullets will be further tested at ATF and a private Canadian company using the Integrated Ballistics Identification System. Twenty of the RM 8240 bullets are nearly done with another 20 planned for delivery in 2002. Before the delivery of these 40 RM bullets nationwide, a NIST workshop is planned for our future customers on how to use NIST RM standard bullets for the establishment of measurement traceability and quality control for the ballistics identification laboratories nationwide.
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NIST ASSISTS IN PERFORMANCE CHARACTERIZATION OF A NEW CMM

NIST engineers developed and delivered a modified version of the laser ball step gauge (LBSG) to a private manufacturing company. The system was designed and constructed at NIST to perform characterization tests of very large coordinate measuring machines (CMMs). The group also participated in the performance evaluation testing of the new CMM by performing difficult long length measurement tests.

The LBSG was designed specifically for establishing long reference lengths for large coordinate measuring machine performance evaluation. The private company expects to ship the LBSG system to Brazil, where their staff will use the system to perform acceptance tests on a much larger CMM.
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NIST RESEARCHERS TWO STEPS CLOSER TO ELECTRON-COUNTING CAPACITANCE STANDARD

A team of NIST scientists in collaboration with an intern from the University of Maryland, has made two advances in the development of cryogenic capacitors for use with the Electron-Counting Capacitance Standard (ECCS). The ECCS is being developed as a quantum-based representation of capacitance. It relies on pumping a precisely counted number of electrons onto the plates of a cryogenic capacitor and measuring the resultant charging voltage. About 100 million electrons are required to reach the desired voltage. Besides providing a "turnkey" primary capacitance representation, the ECCS will also provide an alternate route for experimental determination of the fine-structure constant.

Two recent advances have been implemented for the cryogenic capacitor. First, physical design changes have improved its stability and allowed an increase of its nominal value by an order of magnitude to 10 pF. This larger value makes the ECCS more attractive as a turnkey representation because it should support lower uncertainties for typical commercial capacitance calibrations. This increase in value was made possible by improved machining tolerances, which allowed fabrication of the device with a gap between the two capacitor plates of about 0.05 mm over a distance of about 10 mm. An additional benefit of the improved machining tolerances is that the capacitance value is within 1 % of nominal, which is important for use with much of our precision measurement instrumentation. The new device exhibits excellent stability; after equilibration at low temperatures, its capacitance drift is less than about 10^{-9} per hour.

The second advance was the performance of a preliminary measurement of the cryogenic capacitor directly against the NIST calculable capacitor. The calculable capacitor is a large mechanical capacitor that, through a fundamental theorem of electrostatics, provides the SI realization of the Farad through a measurement of displacement. Measurement against the calculable capacitor is crucial for the ECCS, both in terms of demonstrating its usefulness as a capacitance representation and for the measurement of the fine-structure constant. The stability of the cryogenic capacitor was an essential requirement for this measurement. The measurement noise in the comparison of the capacitor at low temperature against the calculable capacitor was roughly the same as observed in the routine measurements involving the calculable capacitor.

Some further refinements are needed. In addition to a full characterization of its performance and error budget, a more accurate means is needed for the course determination of the capacitance value; routine measurement against the calculable capacitor only yields capacitance values modulo 1.5×10^{-6}.

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NIST REVIEWS IMPACT OF CONSERVATION VOLTAGE REDUCTION FOR ELECTRIC POWER INDUSTRY

The old debate about the possibility of reducing the peak power demand that electric utilities have to meet by lowering the system voltage level by a few percent (known as a "brownout") has been rekindled by the incidence of rolling blackouts in response to overloaded transmission and distribution systems. The state of California is considering this approach, now called conservation voltage reduction (CVR), which rests on the undisputed fact that constant-resistance loads—such as incandescent lighting—draw power proportional to the square of the supply voltage. It would appear that a systematic reduction of a few percent could significantly reduce the peak demand, reducing the possibility of overloads. Such overloads might otherwise make it necessary to arbitrarily cut-off the supply to some sections of the distribution system to avoid a collapse of the complete system.

Prompted by these CVR proposals, a NIST researcher has completed an objective review of their implications for publication by Electric Power Research Institute, the major electric power industry R&D organization, as a PQ Commentary.

The conclusion of this review, entitled *The Power Quality Implications of Conservation Voltage Reduction* (see www.epri.peac.com), is that while some peak demand shaving might be beneficial, sophisticated loads that are already sensitive to brief voltage reductions, known as sags, caused by incidents on the power grid would be even more vulnerable if these sags would occur during a CVR period. The report urges cooperation among equipment manufacturers and users, together with electric utilities and regulatory agencies, supported by an objective test program on the possible side effects of CVR. This report will serve to illuminate the old debate and help to raise awareness of the possible negative consequences to power quality before CVR is implemented.

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NIST STAFF DEVELOPS METHODS FOR ACCURATELY CHARACTERIZING ON-WAFER WAVEFORMS

Due to advances in integrated circut (IC) design, digital design engineers now need the ability to accurately measure electrical waveforms in high-speed digital integrated circuits. Unlike the larger ICs of the past, modern digital ICs are so fast, highly integrated, and sensitive to loading that no good strategy exists for waveform measurement on the IC.

Working in response to this need, NIST researchers developed frequency-domain mismatch corrections for non-invasive on-wafer waveform measurements. Conventional microwave two-tier characterization procedures fail for the non-invasive probes of interest to the digital industry. They not only developed an alternative microwave calibration capable of characterizing non-invasive probes, but they developed procedures for correcting waveform measurements performed with the probes to 40 GHz, adequate to characterize all but the most demanding digital circuits. While implementing the method is complex, the measurement apparatus required for the measurements is composed entirely of commercially available equipment, making the method suitable for advanced industrial laboratories. The group is working on methods for simplifying the calibrations for use in less well-equipped laboratories.

This is the first high-frequency electrical calibration suitable for correcting waveform measurements performed with non-invasive probes designed to allow the circuits to continue to function at the normal operating speed during electrical test.

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NIST HELPS SET THE STANDARDS ACROSS THE ELECTRONICS MANUFACTURING SUPPLY CHAIN

From telecommunications to personal computing, electronics manufacturers are no longer competing globally as individual companies but as partners within a complex web of suppliers. The ability of a company to recoup its investment costs depends on the speed with which it can get products to the international market, ramp up to volume production, and scale production back to meet changing demand. To facilitate entry in various markets and to keep costs under control, large manufacturers are outsourcing nearly every aspect of the production cycle, from design through assembly, to logistics, warranty, and repair.

Through the joint leadership of a NIST researcher and a private company manager, several standards to facilitate supply communication were released in November 2001. At a panel led by the NIST researcher at this year's IPC APEX conference, company representatives discussed how they are now building these new standards, including the IPC Product Data eXchange (PDX) suite and a number of RosettaNet Partner Interface Process (PIP) specifications into their outsourcing strategy. During the Spanning the Virtual Factory—Managing Supply Chain Communications forum in January, a telecommunications company revealed an information architecture with PDX at the center. While they've had to adapt some of their own applications to take advantage of the standards, many of their suppliers are already providing compliant products. As is the case with other major manufacturers, they are putting standard-based implementations into production.

For slides from the APEX forum, refer to www.nemi.org. To download the PDX standards, refer to http://webstds.ipc.org/. To download RosettaNet PIPs 2C1 through 2C10, refer to www.rosettanet.org.

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FIRST QUARTER RELEASE OF PROTEIN DATA BANK CD-ROMS

NIST has completed the production of the latest Protein Data Bank (PDB) CD-ROM set. The CD-ROMs are produced quarterly; currently there are 1200 subscribers. This set contains the 16 972 protein or nucleic acid structures in the PDB as of Jan. 1, 2002. Eight CD-ROMs are required to contain the compressed structure files and the corresponding experimental data files. The PDB is updated weekly with 50 to 70 new structures, and the data are available via the internet at http://pdb.nist.gov. Therefore, the CD-ROM distribution is intended for those researchers without good internet access and for industrial researchers who for proprietary reasons do not wish to work on-line.

Subscriptions are increasing by more than 100 each quarter. This quarter a new program was used to produce the CD-ROM masters. The new program allows for starting the processing from several different stages and automates the processing of tasks that had formerly been done by hand. This both shortens the process and makes it more reliable. NIST manages the Protein Data Bank in collaboration with the San Diego Super Computer Center and Rutgers, the State University of New Jersey, Biochemistry Department.

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CRYSTALLOGRAPHIC PHASE ANALYSIS OF SUBMICROMETER PARTICLES BY ELECTRON BACKSCATTER DIFFRACTION

The characterization and identification of small particles are critical to advanced manufacturing methods in semiconductor, pharmaceutical, metallurgy, and ceramics, as well as environmental monitoring and homeland security. The chemical compound identification of particles is essential to the understanding, improvement and control of electronic device yield, near-net-shape processes, drug effectiveness, environmental particulate health effects, and trace-explosive-particle forensic analysis.

In collaboration with Sandia National Laboratory, NIST is developing procedures for analyzing the crystallographic phase of individual sub-200 nm particles utilizing electron backscatter diffraction (EBSD) in the field emission scanning electron microscope. One of the difficulties in performing EBSD analysis of small particles is that the quality of EBSD patterns from particles less than about 200 nm in size, particularly particles with low average Z and or low density, is not sufficient to allow crystallographic phase identification.

Monte Carlo simulations of the electron trajectories from small particles indicate that most of the 20 keV beam electrons penetrate through these particles with minimum angular deflection. The vast majority of the transmitted electrons enter the mounting substrate where they are scattered diffusely, in the case of an amorphous substrate, and become a significant source of background noise in the EBSD patterns collected from these particles.

To improve the quality of EBSD images from sub-200 nm particles, NIST has designed an EBSD sample holder for mounting the particles onto a thin carbon film supported by a TEM grid. To significantly reduce the background signal from incoherently scattered electrons, the film is mounted over an electron trap so that the electrons penetrating through the particles also penetrate the film and are absorbed in the trap. Results show a significant improvement in the EBSD pattern quality from sub-200 nm Al_2O_3 particles. This new approach dramatically improves our sensitivity in identifying the chemical compounds that make up crystalline particles.

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NIST IMMERSIVE VISUALIZATION ENVIRONMENT AVAILABLE

NIST has developed an immersive visualization environment that can be used to gain increased insight into large, complex data sets. Such data sets are becoming more commonplace at NIST, as high performance parallel computing is used to develop higher fidelity simulations, and combinatorial experimental techniques are used in the laboratory. Immersive visualization environments allow the scientist to explore complex data interactively.

Fully immersive computer graphics include one or more large rear projection screens to encompass peripheral vision, stereoscopic display for increased depth perception, and head tracking for realistic perspective. The NIST Immersive Visualization Laboratory is a Reconfigurable Automatic Virtual Environment (RAVE) from a private company. The two-wall RAVE is configured as an immersive corner with two 2.44 m × 2.44 m (8 ft × 8 ft) screens flush to the floor. The large corner configuration provides a very wide field of peripheral vision, with stereoscopic display and head tracking.

For more information about scientific visualization at NIST, see http://math.nist.gov/mcsd/savg/vis/.

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NIST STRUCTURAL DATABASE USED FOR PHASE IDENTIFICATION IN ELECTRON DIFFRACTION INSTRUMENTS

Researchers use crystallographic information on a daily basis to visualize, explain, and predict the behavior of chemicals and materials. The NIST Structural Database (NSD) contains crystallographic and atomic positional information for metallic crystalline substances, including alloys, intermetallics, and minerals. Under an agreement recently signed with an instrument manufacturer, the NSD has been incorporated into an electron diffraction instrument for automatic phase characterization and identification.

The new electron diffraction software searches the NSD by elemental composition, retrieves the full structural crystallographic information, and uses this to generate a calculated or simulated electron diffraction pattern. Unknown phases can then be identified automatically by matching the calculated patterns with the observed patterns generated using the electron backscatter diffraction technique, an increasingly popular scanning electron microscope-based technique used for the analysis of samples in materials science, geology, microelectronics and related research fields.

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NIST RESEARCHER'S FINDINGS INFLUENCE INDUSTRY ACCEPTANCE OF PHYSICAL MODEL FOR BREAKDOWN

A NIST researcher has played an important role in influencing the semiconductor industry to refute the previously accepted thermochemical model (or "E-model") of dielectric breakdown of reliability of ultra-thin silicon dioxide.

The correct physical mechanism for dielectric breakdown has been controversial for over three decades. Until recently, there were three models that give vastly different projections for oxide life: the thermochemical model, the anode hole injection model, and the hydrogen release model. It is crucial that the correct physical model be used when making reliability projections; otherwise large errors in lifetime extrapolation will result.

The NIST researcher's work on substrate-hot electron injection showed that tunneling electrons were necessary for thin oxides to break down. This is significant because the thermochemical model does not require tunneling electrons to damage the oxide (only the applied gate field is required). Therefore, the thermochemical model can not be correct. This research is recognized as one of the most convincing demonstrations of the involvement of tunneling electrons in causing breakdown.

The NIST researcher recently created holes in thin oxides to show that holes do not efficiently cause defects that would eventually lead to dielectric breakdown. These results are significant in that they strongly suggest that the anode hole injection model either is incorrect or must be significantly modified as a physical model responsible for dielectric breakdown in ultrathin gate dielectrics.

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NIST REDUCES UNCERTAINTIES IN FAST PULSE CALIBRATION SERVICE

The application of new test instruments, a new test procedure, and an improved uncertainty analysis has resulted in a significant reduction in the reported uncertainty for transition duration (i.e., rise time and fall times) provided by NIST Special Test 65200S, "Fast Repetitive Pulse Transition Parameters." The uncertainties have been reduced from –2.2 ps/+ 4.4 ps to ±1.5 ps. In addition, the parameters of overshoot and undershoot have been added to the list of parameters provided by the 65200S.

The addition of these parameters was possible be cause of the new uncertainty analysis. The 65200S calibration service is used by manufacturers of high-speed samplers, military calibration laboratories, and aerospace and computer industries to calibrate the output of high-speed pulse generators and the step response of high-speed samplers. The reduction in transition duration uncertainty is significant because of the increase in speed of commercial samplers and in the circuits that they are intended to test. With these improvements, there are no other national metrology laboratories that surpass the measurement capability of NIST in high-speed pulse parameters.

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34.6 GHz ACROSS-THE-ROAD CALIBRATOR/ SIMULATOR DESIGNED AND TESTED BY NIST

Across-the-road photo radars are increasingly used for speed limit enforcement on the nations highways. During the past 10 years, NIST has played an important role in developing new instrumentation that is to be used for type certification of these traffic radars. In February 2000, we completed an analog calibrator/ simulator designed for use with K-Band (24.1 GHz) radars and demonstrated its use in calibrating a commercial Doppler radar to an accuracy of ±1 mph at simulated vehicle speeds of 65 mph. NIST subsequently received further support from the National Highway Traffic Safety Administration (NHTSA) through the Office of Law Enforcement Standards to develop another unit capable of calibrating similar radar systems that operate at Ka-Band (34.6 GHz). The microwave design of the 34.6 GHz calibrator is identical to that of the 24 GHz calibrator, but is software driven. The flexible software controls the Doppler frequency shift and signal time duration, thereby simulating to a ±2 % uncertainty the radar return for different vehicles from motorcycles to trucks moving at speeds of up to 120 mph. Lab testing is complete. The units will be delivered to a NHTSA type-certification laboratory.

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NIST EXAMINES FUTURE DIRECTIONS OF FLUID PROPERTY RESEARCH

As advanced technologies emerge in the chemical and related industries, fluid thermophysical properties will be needed for their design, development and optimization. However, there is a growing concern that technology is being developed in "virtual" environments where it is taken for granted that the computer will produce reliable results; the dependence of these results on underlying property data is often unappreciated. Many people feel that the fluid-property research required to connect simulated results to reality is in decline (especially in the United States), and that industry suffers for lack of reliable data.

NIST has been working to raise awareness of these issues, beginning with a forum organized in June 2000 in conjunction with the 14th Symposium on Thermophysical Properties in Boulder. Many of the key issues raised at that forum are examined in a forward-looking article written by two NIST scientists for *Chemical Engineering Progress,* the flagship magazine of the American Institute of Chemical Engineers. The article, titled "Fluid Properties and New Technologies: Connecting Design with Reality," reviews some of the significant future opportunities for fluid-property research, including molecular simulation, combinatorial methods, microscale process miniaturization, environmental technology, unconventional mixtures and materials, and data standardization and exchange. It also discusses some of the challenges (many of them structural, such as the downsizing of the corporate engineering groups that used to serve as a "bridge" between researchers and industrial needs) that must be overcome if fluid property researchers are to be successful in providing information that meets the needs of industry.

The article is in the February 2002 issue of *Chemical Engineering Progress,* pages 34-41. A more complete record of the forum (including essays from experts reacting to the issues raised) has recently been issued as NIST Special Publication 975: *Report on Forum 2000: Fluid Properties for New Technologies—Connecting Virtual Design with Physical Reality.* This Special Publication, and related information, can be found on the Web at http://forum2000.boulder.nist.gov.
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NIST REAFFIRMS COMMITMENT TO CEMENT INDUSTRY

NIST portland cement Standard Reference Materials (SRMs) have underpinned product quality for the cement industry for nearly 50 years. The cement SRM 1880 series has proven to be essential to laboratories which certify concrete products for performance and which evaluate mechanisms for concrete corrosion and failure. NIST has recently completed re-certification of the entire suite of 10 cement SRMs in the 1880 series in collaboration with a subsidiary of the Portland Cement Association, and the U.S. Geological Survey.

The replacement series of cement SRMs reflects newer cement types now being used; ordinary and blended portland cement products from around the world were selected, including blends with limestone, slag, and fly ash, low Fe white cement, and two calcium aluminate cements. These materials are certified for more components that cover a wider range of elemental composition than any prior series. Four of the certificates of analysis of the new SRMs carry a table of results from the Cement and Concrete Reference Laboratory Proficiency Sample Program operated by NIST, which summarizes proficiency test results from over 200 laboratories.

A key development of the project was a matrix-independent x-ray fluorescence method created by a NIST scientist, in which calibration standards are prepared from primary reference materials using borate fusion. Major, minor, and trace constituents can be determined without corrections for matrix effects, which typically lead to high relative uncertainties in the final results. This new high performance method consistently yields expanded relative uncertainty estimates below 1 %. In addition to cement, the versatile method has already been applied to zeolite compounds, low alloy steel, and aerospace alloys.
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THE ROLE OF THE GENE OF THE COCKAYNE SYNDROME IN THE REPAIR OF OXIDATIVE DNA DAMAGE

Cockayne Syndrome (CS) is a human genetic disorder with diverse clinical symptoms that include hypersensitivity to sunlight, severe mental and physical growth retardation, progressive neurological and retinal degeneration, and skeletal abnormalities. It has two complementation groups, CS-A and CS-B. The gene of CS-B encodes a protein (CSB protein), which is known to play a role in the cellular repair of DNA damage, but it may participate in other pathways of DNA metabolism.

NIST researchers, in collaboration with scientists at the National Institute of Aging, NIH Baltimore, investigated the role of the CSB protein in the cellular repair of oxidative DNA damage, which results from normal cellular metabolism and oxidative stress. Transformed human cell lines with site-directed mutations in the CSB gene were established. These cell lines were then used to study phenotypical changes affected by the mutations, including DNA repair by whole cell extracts and the accumulation of oxidative DNA damage in genomic DNA of cells after exposure to oxidative stress. Cells were exposed to low doses of ionizing radiation to cause oxidative stress.

Researchers found that the mutant cells and those with the deleted CSB gene had greater sensitivity than wild-type cells to ionizing radiation. The mutant cells had lower activity of DNA repair as shown by determination of activities of DNA repair enzymes. The results showed that the biological functions of the CSB protein in DNA repair might be mediated by distinct functional motifs of the protein. In addition, the accumulation of two well-known products of oxidative DNA damage in genomic DNA was measured using liquid chromatography-mass spectrometry. These products accumulated to a greater extent in mutant cells and in cells with the deleted CSB gene than in wild-type cells after exposure of cells to ionizing radiation at 2 Gray. Taken together, this study suggests that the accumulation of oxidative stress-induced DNA lesions in genomic DNA of the CSB cells may contribute significantly to the pathogenesis of the human disorder Cockayne Syndrome.

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NIST'S CRYPTOGRAPHIC MODULE VALIDATION PROGRAM ACHIEVES MAJOR MILESTONES

NIST's Cryptographic Module Validation Program (CMVP) recently achieved three major milestones. First, the CMVP accredited the programs sixth cryptographic module testing laboratory through the National Voluntary Laboratory Accreditation Program.

Second, the CMVP celebrated the signing of the 200th certificate with the validation of the Promail II (Simply Postage III). The Promail II is an electronic device that stores revenue and dispenses it to a host computer, under the control and direction of a customer. The revenue is dispensed from the Promail II in the form of a digitally signed indicium, a unique bit pattern that can be determined to have originated from a particular device at a particular point in time.

Third, the Communications Electronics Security Group of the United Kingdom announced on Dec. 28, 2001, that it "proposes the use of FIPS 140 as the basis for the evaluation of cryptographic products used in a number of UK government applications and encourages the setting up of accredited laboratories in the UK to perform these evaluations." This takes the CMVP beyond North America.

The FIPS 140-1 Validated Modules List has become a "Who's Who" of cryptographic and information technology vendors and developers from the United States, Canada, and abroad. The list contains a complete range of security levels and a broad spectrum of product types including personal digital assistants, secure radios, Internet browsers, virtual private network devices, PC postage equipment, cryptographic accelerators, secure tokens, and others. The recent validations impact federal agencies by further increasing the number of tested and validated cryptographic products available for use in securing sensitive information.

The CMVP is a joint effort between NIST and the Communications Security Establishment (CSE) of the Government of Canada. NIST's Computer Security Division and CSE serve as validation authorities for the program. The website is http://www.nist.gov/cmvp.

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NIST PUBLISHES INFORMATION TECHNOLOGY SECURITY RISK MANAGEMENT GUIDELINE

In fulfillment of NIST's statutory responsibilities to advise Federal agencies on IT security, NIST recently published two new security guidance documents. NIST Special Publication 800-30, *Risk Management Guide for Information Technology Systems* provides an overview of the risk management process, describes how it fits into the system development life cycle, and defines the roles of various personnel who support and use this process. It also describes a risk assessment methodology, the steps in conducting an information technology risk assessment, and a risk mitigation process. Additionally, it outlines some factors that lead to a successful risk management program.

NIST Special Publication 800-33, *Underlying Technical Models for Information Technology Security,* provides a description of the technical foundations, termed "models," that underlie secure information technology. The document provides, in a concise form, the models that should be considered in the design and development of technical security capabilities. These models encompass lessons learned, good practices, and

specific technical considerations. The documents are available at http://csrc.nist.gov/publications/nistpubs/index.html.
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NIST MEASUREMENTS IDENTIFY MECHANISMS THAT LIMIT POLYMER PROCESSING

NIST has developed visualization tools that allow processors to improve the way polymers are manufactured. Polymer processors have long battled against a manufacturing defect known as "sharkskin," which causes the surface of the extruded polymer to become rough. The defect limits the speed at which polymeric materials are extruded; the speed limitation adversely affects manufacturing costs. Studied since the Second World War, the precise nature of the instability remains widely debated. Central to the debate is the precise flow pattern of the polymer as it flows through and exits an extrusion tube.

Utilizing a transparent extrusion tube and a custom-built high-speed microscope, researchers at NIST have been have been able to map out the flow in the necessary detail to settle the question of the flow behavior at the exit. This work will be published in the March edition of the *Journal of Rheology*. Armed with this knowledge, manufacturers will be able to understand questions relevant for the next generation of materials, for example how to reduce the prevalence of sharkskin while maintaining the physical properties and appearance of the final material.
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THE POLAR NANOSTRUCTURE OF NOVEL RELAXOR FERROELECTRIC MATERIALS

A renaissance in the field of ferroelectricity has taken place over the past several years ever since the finding of exceptional piezoelectric properties in the lead-oxide class of relaxor ferroelectric materials $Pb(Zn_{1/3}Nb_{2/3})O_3$ (PZN) and $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN). When doped with sufficient $PbTiO_3$, a conventional ferroelectric, these disordered perovskites can exhibit strain levels up to one order of magnitude higher than those attained using present day industrial PZT ceramics, making them highly promising candidates for the next generation of solid-state transducers and actuators. Part of this novel behavior has been attributed to the presence of a narrow monoclinic region in the phase diagrams for solid solutions of both PZN and PMN doped with $PbTiO_3$. But as even the undoped compounds exhibit a superior piezoelectric character, the underlying polar nanostructure, absent in $PbTiO_3$, is believed to play an essential role in these materials.

Scientists at the NIST Center for Neutron Research (NCNR) and Brookhaven National Lab have an ongoing collaborative program to study the lattice dynamics (atomic vibrations) in the PZN and PMN relaxor compounds. Recent neutron inelastic scattering measurements at the NCNR have demonstrated a direct relationship between the lowest-frequency transverse optical lattice vibration and the polar nanostructure, thereby resolving a long-standing discrepancy between prior x-ray and neutron results. In PMN this vibrational mode becomes overdamped at 620 K, which is the same temperature at which the polarized nanometer-scale domains begin to develop. Concurrently, an unusual broadening of the transverse acoustic vibrational mode begins at 620 K, and increases strongly with decreasing temperature. These results indicate that this optical lattice vibration condenses into the polar nanoregions, resulting in a non-uniform distortion of the crystal lattice.

Subsequent experiments to clarify further how the polar nanoregions are responsible for the novel piezoelectricity observed in these and other relaxor systems are underway.
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CLASSIFICATION TOOL DEVELOPED FOR PROCESS SPECIFICATION LANGUAGE

NIST researchers completed an initial version of the "twenty questions" tool for the developing international standard, Process Specification Language (PSL). This tool allows a domain expert who is not versed in formal semantic theory to quickly map real-world industrial concepts of process into rigorously specified definitions amenable to computerized manipulation. The work is based on an approach that uses invariants (properties of models of the core PSL theories that are preserved by isomorphism) to provide a rigorous classification of activities within PSL. The resulting classes of activities are being incorporated into the standards documents for Parts 41 and 42 within ISO 18629.
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NIST RESEARCHERS RECEIVE DARPA AWARD

At a recent meeting of principal investigators in the DARPA Active Networks program, the program manager announced the selection of a research team from NIST to receive the 2001 "Bytes for the Buck" award, given annually. The NIST team focused on developing a standard means to specify processor demands for mobile computer programs, also known as mobile code. Well-accepted standards exist to express resource demands for memory (bytes) and bandwidth (bits per second), but no accepted standard exists to express CPU demands. Success in this research would permit mobile code, arriving over a network, to declare CPU requirements in an accurate, quantitative form that can be understood on any computer platform. With such a specification, computers can better control CPU usage by mobile programs. For example, malicious or erroneous mobile programs could be prevented from using excessive CPU time, while valid mobile programs can run safely to completion.

During the 2-year project, the NIST team measured CPU usage in many mobile programs and virtual machines written for DARPA, and then developed and evaluated various models to describe CPU demands.

While the results obtained show substantial improvements over various naive approaches currently used in the Active Networks program, more research remains before the project can achieve its original goal. Based on the promising results, DARPA funded an extension to the project.

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MEASUREMENTS CONDUCTED WITH X-RAY CALIBRATION INTERFEROMETER

A NIST researcher completed the testing and analysis of several three-flat, five-position measurements with the X-Ray Calibration Interferometer (XCALIBIR) using 300 mm diameter flats. The XCALIBIR is a measurement system that was designed at NIST to have the flexibility to measure flats, spherical, and aspheric optics. The tests were successful and allowed two conclusions to be drawn.

First, the center of the XCALIBIR field of view is affected by substantial noise caused by diffraction in some parts of the XCALIBIR optics. Second, outside the center of the field of view, the repeatability of the flat measurements was between 0.5 nm rms and 1 nm rms. These results are very encouraging and make it clear that elimination of the noise at the center of the XCALIBIR field of view is of paramount importance for the system to meet its goal of 0.25 nm rms accuracy.

Additionally, as part of the analysis of the test data, NIST researchers built the foundation for a MATLAB-based toolbox for phase measuring interferometry (PMI). The toolbox incorporates functionality for all steps of the data analysis chain from phase measurement to visualization. This toolbox will become the only validated, documented, and open reference implementation for many numerical methods and algorithms that are used in PMI. New methods can be easily incorporated into the toolbox and it will be possible to estimate the uncertainty associated with critical data analysis procedures, such as phase unwrapping. Portions of the new toolbox, even in its current early version, exceed the functionality of commercial phase measuring software.

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Standard Reference Materials

NIST RELEASES AIR PARTICULATE ON FILTER MEDIA STANDARD REFERENCE MATERIAL (SRM)

Investigations into the amount and composition of atmospheric particulates are currently carried out in virtually every country. Large numbers of air particulate matter (APM) samples collected on filter substrates are being analyzed for trace element composition. These analyses are routinely made on APM that has been collected on polycarbonate or Teflon membrane filters. Of particular concern for both environmental and public health agencies is the fine fraction of air particulate matter, called $PM_{2.5}$. This consists of particles with aerodynamic equivalent diameters smaller than 2.5 μm. $PM_{2.5}$ particles are formed in many combustion processes, and are small enough to penetrate deep into lung tissues where they can directly affect respiratory ailments. They are also linked to the formation of haze resulting in loss of visibility in many parts of the United States. To meet the standards needs of the air particulate community, NIST initiated research on producing contemporary $PM_{2.5}$ SRMs. Such standards can serve as enabling tools to improve air quality and cost-effective mitigation efforts.

A first of its kind, SRM 2783 is a simulated $PM_{2.5}$ urban aerosol that has been deposited onto filter media

and is certified for elemental content. Collaboration with the International Atomic Energy Agency provided the base material.

Certified and reference values have been determined for 27 elements with amounts ranging from 1 ng (U) to 58 600 ng (Si) per filter. This marks the first time that a reference material consisting of actual atmospheric particles deposited on filter media and certified chemical composition has been made available in quantity. To further develop SRMs suitable for the National Air Quality Program and industrial mitigation programs, NIST has entered an agreement with the Environmental Protection Agency to collect $PM_{2.5}$ in large quantities for the development of additional standards for organic and inorganic pollutants in ambient aerosols. An ultra-high volume sampler located in Baltimore is currently collecting $PM_{2.5}$ from nearly 20 000 cubic meters of air per day.

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NIST Special Publication 330, 2001 Edition

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