1. Metrology for Tissue Engineering: Test Patterns and Cell Function Indicators

Newell Washburn and Scott Kennedy

The ultimate goal of tissue engineering is to coax cells into regenerating missing or damaged tissue, such as bones, cartilage, or even organs. One strategy involves placing the cells on a biodegradable scaffold that will ultimately be replaced by new tissue. For example, a broken hip could be repaired by seeding bone-producing cells in a porous, biodegradable polymer in the shape of a screw that is used to fix the break. As the cells proliferate and produce new bone, the screw degrades so that eventually the break is repaired and only native bone remains. This project (a joint effort between the NIST Polymers Division, the NIST Biotechnology Division, and researchers at the National Institutes of Health) is focused on developing novel measurement methodology for assessing cell-biomaterial interactions, including tailored surfaces that induce gene expression associated with specific stages in cellular activity, and engineered DNA vectors that signal these responses in adherent cells. Measurement tools such as these, and the standards they would enable, are needed as the developing tissue engineering industry validates new materials and assures the integrity of the cell lines they manipulate. Efficient methods and tested standards are also critical to the fundamental research that will lead to better understanding of factors controlling cell growth and differentiation.

2. Structure/Property Relationships in Healthy and Diseased Tissues

Chris McCowan and Elizabeth Drexler,

We have been evaluating areas of opportunity for application of our expertise to the NIST strategic focus in health care. Recognizing that our focus for many years has been the testing and evaluation of structure/property relationships in metals and electronic materials, we have carried out an assessment of health care research areas in which this type of material measurement expertise is needed. The poster presents the results of this assessment and our initial experimental efforts. In this project, the materials are natural, diseased, and engineered tissues. We have targeted the cardiovascular system as our primary area for research, so arterial mechanics, stent, and heart valve issues are primary areas of interest. Our contributions to the cardiovascular research community are expected to include: (1) helping to increase the medical research community understanding of mechanical testing procedures, (2) development of new mechanical testing procedures for tissues and cells, (3) standardization of mechanical testing procedures, (4) quantifying structure/property relationships in cardiovascular tissues, (5) development of material models for cardiovascular systems, (5) supporting the development of medical devices for cardiovascular applications, (6) support of transluminal imaging and delivery systems. We have just begun our work in this area. We will outline our goals and rationale for the work and show some very preliminary results on two projects, a pulmonary hypertension study and a model of temperature distribution in the heart.

3. Damage Modes In Multilayer Structures For Biomechanical Applications

Brian Lawn and Yan Deng

The mechanics of contact-induced cracks in brittle coating on soft substrates are of interest because of potential failure of technological coating systems in concentrated loads. Important practical examples include such engineering applications as cutting tools, thermal barrier coatings, car windscreens, and electronic multilayer devices; and, especially, biomechanical systems, dental crowns, hip prostheses, and heart valves. We have conducted experiments on model brittle coating structures that simulate the essential features of practical layer structures, and yet allow direct *in situ* examination of fracture modes in the coating layer during stressing. In this work we characterize contact damage modes in model biomechanical layer systems, with a special (but not exclusive) focus on conditions that relate to dental crowns, using tungsten carbide spheres as indenters over clinically relevant loads. We observe the different transverse crack modes, and the critical loads required to initiate these competing modes. These studies allow us to derive functional analytical relations for the critical loads in terms of layer thicknesses, modulus mismatch, strength of brittle components and yield stress of deformable components, thereby enabling a basis for design of layer systems with optimal damage thresholds.

4. NIST On Dentistry's Cutting Edge

Fred Eichmiller

NBS/NIST has played a key role in assuring the quality of America's dental health. It started in 1918 when the War Department asked the National Bureau of Standards (NBS) to develop purchase specifications for dental filling materials used by the military. NBS scientists asked the American Dental Association (ADA) to collaborate in this effort. This soon evolved into a fruitful collaboration between NBS and the ADA to develop the first standards program for health care products. The Cooperative Research and Development Agreement that was established between NBS and the ADA in 1928 is still in place today, and the standards program has evolved into the ANSI certified ADA Standards Committee for Dental Products and the International Standards Organization Technical Committee 106 for Dentistry. The NIST-ADA program has proven to be a model of success for government-private collaboration. Much of technology used in the daily practice of dentistry has been developed in NIST laboratories and the ADA's close association with the dental industry and dental practitioners has greatly enhanced the ability to transfer new technology. Current programs carry on this tradition by focusing on improved filling materials, filling adhesives, cavity prevention technologies, bone repair, and standards for dental and medical products.

5. Folding Pathways of RNA by Cation Binding

Ursula Perez-Salas, Susan Krueger, Prashanth Ragan, Elena Georgieva, Sarah Woodson, Devarajan Thirumalai, and Robert M. Briber

Condensation of counterions around RNA reduces the phosphate charge by 75 – 95%. This reduction of electrostatic repulsion between phosphates after the counterions condense triggers a collapse of the chain to a more compact structure that contains some native as well as nonnative interactions. From a theoretical standpoint, the relationship between the extent of charge neutralization and the dimension of the RNA (radius of gyration, RG) leads to the prediction that the RG decreases proportionally to 1/(Z squared). Using small angle neutron scattering (SANS), it was observed tha the RG of the azoarcus ribozyme does indeed collapse to different compact forms using salts of various concentrations.

6. The Dynamics of Cytochrome – C

Adam Pivovar

In order to deepen our understanding of the molecular motions involved in protein folding, we have employed differential quasielastic neutron scattering (QENS) to measure the dynamics of *cytochrome c* in the native and several unfolded states. In a typical QENS experiment, neutrons exchange both energy and momentum with the sample, allowing one to surmise the characteristic time scale and length scale, respectively, of the molecular motions involved. Another fundamental property of incoherent neutron scattering is the extremely large relative scattering cross section of hydrogen relative to all other atomic species, that is, atoms other than hydrogen remain virtually invisible in the scattering process. Because the hydrogen distribution within a protein is nearly homogeneous, an incoherent QENS experiment reflects the ensemble dynamics of the protein, particularly motions of the non-exchangeable protons of the side chains. *Cytochrome c* is ideally suited for these preliminary investigations as it has several well characterized and easily accessible non-native folded states that, in comparison with the native state, permit rationalization of the dynamic behavior. Molecular dynamics simulations are currently underway that should, as it is possible to directly compare the QENS with the calculations, foster an intricately detailed picture of the molecular motions involved in protein folding.

7. Neutron Interferometry Studies of Vectorially-Oriented Single Monolayers of Membrane Proteins

Larry Kneller, Charles Majkrzak, and J. Kent Blasie

Vectorially oriented monolayers of membrane proteins such as cytochrome c may provide ideal model systems for the study of electron or ion transport. Yeast cytochrome c can be tethered to, and thereby vectorially oriented on, the soft surface of a mixed endgroup organic self-assembled monolayer (SAM) chemisorbed on the surface of a silicon substrate. Neutron reflectivities from such membranes were measured on the NG-1 reflectometer at the NCNR with different H20 and D20 hydrations to examine the water distribution within the layered structure.

8. Diffractometer for the Cold Neutron for Biology and Technology (CNBT)

Susan Krueger, Charles Majkrzak, Joseph Dura, Anne Plant, S. H. White, D. J. Tobias, Irvine, J. Kent. Blasie, H.W. Huang, T.J. McIntoshuke and J.F. Nagle

The CBNT consortium, funded by NIH in cooperation with NCNR, is dedicated to development of improved measurement methods and research in the study of biological and biomimetic membrane structure by cold neutron reflectivity and by neutron diffraction from related multiplayer specimens. New resources for computer simulation and biospecimen preparation are also a key to this research effort. The new diffractometer/reflectometer is designed to optomize the collection and analyze of neutron scattering data from layered film systems so that the maximum amount of structural information can be obtained.

9. Quantum Percolation

Jeff Lynn and Martin Greven

A combined substitution of Mg+Zn into the square planar La2CuO4 lattice has allowed for the first time neutron measurements up to and through the percolation threshold in the extreme quantum limit (S=1/2). Monte Carlo calculations combined with measurements of the spin correlations demonstrate that quantum fluctuations do not shifty the percolation threshold, and the non-linear sigma model provides a quantitative description of the system up to surprising high substitutions.

10. Dynamics of Rodlike Micelles Studied Using Neutron Spin-Echo

Steven Kline, Nicholas Rosov, and Sungmin Choi

Polymerized rodlike micelles with controllable surface charge provide a model system to study the interaction in dispersions of anisotropic particles. Neutron Spin-Echo (NSE) measurements provide a direct measurement of the inter-particle structure, S(q), a quantity which cannot be directly measured using small-angle scattering. Combining NSE measurements with small-angle neutron scattering (SANS) allows unambiguous identification of the inter-particle and intra-particle scattering contributions, giving a clear picture of both the structure and interactions.

11. The Magnetics of “Pixie-Dust” – do AFC Media Work as Expected?

Kevin O’Donovan, Julie Borchers, M.F. Toney

In magnetic recording technology, the equivalent of Moore’s law has the areal density increasing at 60 – 100% per year. To help maintain this trend, IBM, Fujitsu and others have recently developed novel AFC (antiferromagnetically coupled) recording media in which two ferromagnetic layers are separated by a thin Ru layer. The Ru layer thickness is tuned to antiferromagnetically coupled the ferromagnetic layers. Because a detailed understanding of the operation of this media is lacking, we have examined the magnetization reversal process of an AFC recording disk using polarized neutron reflectivity techniques. Our data provide some insight into the magnetic switching behavior of the two magnetic layers, suggesting that the antiferromagnetic alignment of the two layers, is imperfect in the field range of operation.

12. Nanoscale Cluster Formation and Dynamics in Relaxor Ferroelectrics

Peter Gehring and Gen Shirane

The lead-oxide class of perovskites Pb(Mg1/3Nb2/3)O3 (PMN) and Pb (Zn1/3Nb2/3)O3 (PZN), as well as solid dolutions mixed with PbTiO3 (PT), exhibit exceptional piezoelectric properties that can be used in high performance electromechanical actuators. Neutron diffuse scattering studies show that nanoscale ferroelectric regions form in the system, while the inelastic scattering reveals a concomitant dramatic softening of the lattice vibrations. These nanoscalar properties are directly tied to the high dielectric susceptibility of these materials.

13. Informatics for Neutron Crystallography

Brian Toby and Nick Maliszewskyj

Informatics is the management of information, e.g. scientific data. It covers how data are collected and analyzed, as well as how results are compiled in databases and are then extracted to form composite knowledge. Within the NIST Center for Neutron Research efforts are underway to improve all aspects of these processes. The poster will highlight our efforts, including new software web tools, and electronic communication standards with a focus on neutron diffraction capabilities.

14. Texture, Elastic Properties, and Residual Stress in Transportation Industries: Measurements and Modeling.

Hank Prask, Thomas Gnaeupel-Herold, Vladimir Luzin, and Stephen Banovic

The NCNR and the Metallurgy Division are engaged in a collaborative program aimed at elucidating approaches by which texture, residual stress, and elastic/plastic behavior can be better understood and fabrication methods improved for transportation applications. Neutron, x-ray and electron backscatter diffraction are utilized to characterize residual stresses, texture, and microstructure. Finite element models are being developed to describe key processes at the microscopic level. Results of residual stress studies and modeling will be presented for railroad rails. Residual stress results for friction stir welds in aluminum for aircraft will be given, along with results for spray-formed steel for automotive industry applications.

15. Evaluating Organclays for Nanocomposities by Small-Angle Scattering and Microscopy

Derek Ho, Charles Glinka, and Robert Briber

Polymer-clay nanocomposites have improved properties that are related to the degree of dispersal and exfoliation of the clay within the polymer matrix. Pretreating the clay to make the particles surfaces more organophillic generally enhances dispersion in polymers. We have used small-angle neutron scattering (SANS), wide-angle x-ray scattering (WAXS) and atomic force microscopy (AFM) to characterize the morphology of organclays dispersed in organic solvents as a first step toward comparison with their dispersal in bulk polymers.

16. Imaging Chemical and Molecular Nano Properties with Combinatorial NEXAFS

Daniel Fischer and Jan Genzer

NIST operates a soft-x-ray (C,N,O,F) materials characterization facility to study the structure and chemical nature of diverse materials at the National Synchrotron Light Source (Upton, NY). We utilize polarized soft x-rays as a searchlight for chemical bond identification, orientation and quantification by measuring Near Edge X-ray Absorption Fine Structure (NEXAFS). We describe a new parallel process combinatorial methodology for the production of NEXAFS chemical pictures and reaction kinetics movies of nanostructured materials. Possible applications include the surface orientation and chemistry of continuously graded polymer films and graded or patterned self-assembled monolayers that exhibit tunable surface properties of potential use in nanotechnology. A one dimensional chemical NEXAFS picture of a semifluorinated gradient monolayer is presented that illustrates our current ability to measure chemical bond concentration and orientation of molecules on surfaces.

17. NIST Combinatorial Methods Center: Portal for Industrial Outreach

Alamgir Karim

The measurements, standards, and test methods developed by NIST, in partnership with other organizations, often help unlock the potential of new discoveries and budding technologies. Combinatorial methods are a textbook example. These emerging tools can speed innovation in many fields - pharmaceuticals, chemistry, and, most recently, materials. In the diverse realm of materials, combinatorial methods hold promise for all classes, including metals, polymers, ceramics, and biomaterials. NIST has established the NCMC as a model for collaboration, in order to share expertise, facilities, resources, and information thereby reducing obstacles to participating in this fast-moving and instrument-intensive area. Although collaborations with multiple partners can be difficult, the goal is to foster cross-fertilization of ideas and research strategies, and to spur progress on many fronts by crossing boundaries of organizations, disciplines, and interests. Members have access to technical workshops, short courses, data libraries, and electronic bulletin boards; they can participate in non-proprietary focused projects; and they can enter into specific cooperative research and development agreements with controlled intellectual property.

18. Equilibrium Structure of Vitreous Bonded Grain Boundaries in Al_2O_3

Sheldon M. Wiederhorn, Bernard J. Hockey, John Blendell, Jong-Sook Lee and Myung-Koo Kang

In this poster we discuss the structure of vitreous bonded boundaries in aluminum oxide. Using sapphire crystals that have grown through vitreous bonded aluminum oxide to form single grain boundaries, we explore the effect of crystal orientation on the equilibrium grain boundary structure. A simple theory of wetted boundaries that assumes no energy of interaction between the surfaces predicts our observation that three types of boundaries exist: fully wetted boundaries, dry grain boundaries made only of dislocation arrays and grain boundaries made of a mixture of the first two. When an interaction occurs between the two surfaces that constitute the grain boundary or between the surfaces and constituents of the vitreous silicate phase, then the theory has to be modified to account for the observed grain boundary structures. In this paper, we give examples of the structures that form as a consequence of interactions and discuss the theoretical modifications that are needed to explain the results.

19. Research at the Advanced Photon Source in Support of U.S. Technology and Security

David Black, Andrew Allen, Harold Burdette, Gabrielle Long, Jan Ilavsky and Pete Jemian

Our research at the Advanced Photon Source is focused on microstructure characterization, where NIST scientists, in collaboration with researchers from industry, universities and government laboratories perform state-of-the-art measurements on advanced materials. Two examples of NIST/MSEL research activities at the APS are shown here: 1. thermal barrier coatings (TBC's) for advanced gas turbines, and 2. single-crystal sapphire for antiballistic missile applications.

TBC's allow advanced gas turbines to operate at increasingly high temperatures and therefore, with higher efficiency. Different crack and void microstructures control TBC performance and reliability, but there is no single industrial technique that can completely characterize this complicated microstructure. We show results from ultrasmall-angle X-ray scattering (USAXS), high-energy SAXS and X-ray microtomography that provide a comprehensive microstructural characterization of TBC's. Generic links between processing and service life in these materials has also been explored. This research is now supporting the extension of TBC technology to dielectric applications such as solid oxide fuel cells etc.

A research effort relevant to national security is the application of X-ray diffraction topography to single-crystal sapphire. The superior physical properties of sapphire make it the material of choice for the infrared (IR) seekers for antiballistic missiles. However, surface damage can reduce the strength of these components so that in-service survivability is reduced. X-ray topography has proved to be an extremely sensitive tool to image strength limiting surface damage due to fabrication, handling and proof testing of sapphire IR windows and domes.

Future opportunities include the possibility of MSEL becoming a partner in an X-ray microbea capability for probing materials at the sub-micrometer level. High throughput parallel detection X-ray diffraction and X-ray fluorescence on this instrument offer a unique capability for combinatorial materials science. Additional advantages include characterizing sub-micrometer strain and stress such as occur around electrical interconnects, and selected interface structures or buried layers relevant to many areas of nanotechnology.

20. Materials Reliability: A History of Service to the Nation's Infrastructure

David McColskey

Since its inception, the Materials Reliability Division has had a history of providing materials research data and investigative services in support of the nation's infrastructure. This history has included research on materials for use in Navy ships and submarines, Air Force aircraft, NASA satellites and shuttles, refinery storage facilities and nuclear reactor materials for the nuclear Regulatory Commission. In addition, research has been conducted for the Defense Nuclear Agency on composite structures for use in superconducting applications and for the Federal Highway Administration in support of bridge inspection and monitoring methods. Failure analysis investigative services have been provided to the Department of Transportation's Office of Pipeline Safety for the Alaskan pipeline, to OSHA for a refinery explosion that claimed 17 lives and for a commercial chemical blender explosion that killed 5 workers and injured 4 others. In addition, investigative services have been provided to the National Transportation Safety Board for general aviation aircraft accidents, to NOAA for a propeller shaft failure on a research ship, and to the U.S. Bureau of Reclamation for the failure of a very large concrete and steel water conduit in the desert Southwest and for failure of a turbine wear ring in the Hoover dam. The Materials Reliability Division also provided a detailed failure analysis on the recent failure of the NIST WWVB tower in Ft. Collins, CO.

Current work includes the evaluation of electromagnetic acoustic transducer technology for determination of fitness for service of structurally damaged gas pipelines and railroad rails. The poster presents some of this history and describes our current activities, which are supporting the NIST homeland security efforts.

21. Nanofabrication with Lithography: Quantifying Material Factors Limiting the Production of Sub-100 nm Structures

Eric Lin and Wen-li Wu

The semiconductor industry reports that the development of lithography to fabricate ever smaller feature sizes is the key enabler and driver for the continued performance increases of integrated circuits. Although current technology is able to fabricate 130 nm features, numerous technical hurdles exist in the fabrication of sub-100 nm features. The development of lithographic materials applied at these length scales requires new measurement methods to characterize the final structures and to understand the physical phenomena that limit their fabrication. We are developing high-resolution metrology tools unique to the industry such as x-ray and neutron reflectivity (XR, NR), small angle neutron scattering (SANS), and near edge x-ray absorption fine structure (NEXAFS) to address fundamental problems in the materials and processes used in lithography. Research topics include the chain conformation of polymers in sub-100 nm films, the direct measurement with nanometer resolution of the reaction front marking a solubility switch required for patterning, the measurement of differences in the reaction rate and component segregation between the surface and the bulk, and the characterization of lithographically prepared structures. Our objective is an integrated program to correlate quantitatively fundamental material and transport properties with the ultimate resolution of fabricated structures. Our work is carried out in close collaboration with industrial partners to ensure that our work has a broad impact upon the industry and the development of next-generation lithographic materials and processes.

22. Nanomagnetodynamics

Bob McMichael, Doug Twisselmann, Andrew Kunz

To achieve GHz data rates, the magnetic recording industry will need to control the dynamics of magnetic devices and recording media on nanometer length scales and sub-nanosecond time scales, and Magnetic Random Access Memory (MRAM) under development will require reliable, rapid switching in memory elements. Key to both of these advances is the ability to control magnetization damping. The MSEL portion of the joint MSEL-EEEL nanomagnetodyanmics project is focused on the modeling and metrology of magnetization damping at microwave frequencies in materials with nanoscale defects. Our recent accomplishments include construction and automation of a 0.5 to 26 GHz broadband ferromagnetic resonance (FMR) spectrometer that has helped us determine the form of the magnetic damping in a nearly uniform magnetic thin film. Measurements on thin films with controlled defects show the close relationship between the FMR linewidth and the spin wave dispersion relation. Most recently, we have recognized the role of damping in determining the extrinsic linewidth. This new model predicts line widths greater than those predicted by the more traditional "two-magnon" model.

23. New Materials for Ultra High Density Storage

William Egelhoff

Giant magnetoresistance thin films (commonly known as spin valves) are of great technological importance in read heads for computer hard disk drives. We have investigated the deposition and processing of a variety of giant magnetoresistance (GMR) spin valves with the aim of optimizing their properties. We have found that many of the magnetic and magnetoresisitive properties of spin valves are strongly influenced by surface and interface effects, some of which occur during film deposition. Some of the most important effects are the balance of surface and interface free energies, surface diffusion, interdiffusion at interfaces, low temperature deposition, the use of surfactants to modify growth, and specular electron scattering at surfaces. In some cases, it is possible to control these factors or to use them to manipulate the growth or improve post-growth processing of spin valves to improve their magnetic and magnetoresistive properties. For example, specular scattering is particularly important for achieving the largest possible GMR values in simple spin valves. The best hope for improving spin valves appears to be increasing the degree of specular scattering and reducing the bulk defect scattering. Investigation of magnetic tunnel junctions by x-ray photoelectron spectroscopy indicates that when Al is deposited on Co or $Ni_{80}Fe_{20}$ approximately a monolayer of Al diffuses into the Co or $Ni_{80}Fe_{20}$. This effect means that the interface is neither atomically sharp nor flat, and that after oxidation of the Al film the Al_2O_3 film will not have uniform thickness. Low angle x-ray reflectometry measurements confirm this effect. Since grain boundaries are well-known to be more reactive than flat surfaces, it is very probable that these effects are more pronounced at grain boundaries. Thus grain boundaries are likely to be the site of device failure when the Al_2O_3 is too thin. It is demonstrated that pre-oxidation of the Co or $Ni_{80}Fe_{20}$ can act as a diffusion barrier to prevent Al interdiffusion. When the Al is deposited it takes oxygen away from the Co or $Ni_{80}Fe_{20}$ instead of diffusing into it. It is suggested here that by fine-tuning the extent of pre-oxidation (so that the deposited Al uses up all the available oxygen) an atomically sharp interface could be created. Such an interface should lead to a more uniform Al_2O_3 film thickness, which in turn should permit the use of thinner Al_2O_3 films without device failure.

24. Current-induced Fatigue in Chip-level Interconnects

Robert Keller, C. A. Volkert, R. Mönig, O. Kraft, and E. Arzt

We have begun a new effort addressing time-varying reliability studies in chip-level interconnects. RRK spent 9 months at the Max-Planck-Institute for Metals Research in Stuttgart developing testing and characterization methods for ac-cycled lines with one of the world's premiere groups in electromigration research. What began as an effort addressing what we initially thought was purely an electromigration phenomenon became one that involved studies of electric current-driven thermomechanical fatigue, with the added twist of diffusion-induced processes. Specifically, aluminum interconnects on silicon-based substrates were tested using high current density sinusoidal cycling. Joule heating within the lines induced temperature cycling over ranges of approximately 29-177 K during low frequency (100 Hz) testing at rms current densities in the range 6-14 MA/cm^2. Differential thermal expansion between the aluminum and the substrate resulted in a cyclic total strain amplitude in the range 0.06-0.35%, and corresponding biaxial cyclic stress amplitudes of approximately 61-368 MPa. This poster shows observations of damage and lifetime behavior in these interconnects that are partially consistent with conventional fatigue approaches to damage evolution. For instance, damage during early stages of cycling showed site selectivity, with surface offsets being confined to individual grains. Continued cycling increased the severity of damage, as well as the proportion of surface area damaged, with final failure occurring in the form of open circuit. This happened at locations where the interconnect thinned down excessively, presumably due to localized plasticity and melting. Some observations are not easily described by conventional fatigue concepts as applied to bulk metals, such as lack of lower energy dislocation arrangements after millions of cycles, absence of microcracking, and the formation of whiskers. Effects of current density, interconnect geometry, and encapsulating materials are shown. We suggest that thermomechanical fatigue may pose an important reliability problem for copper-low-k dielectric interconnect systems in the context of low frequency operation, energy-saving modes, and power cycling.

25. The Mechanism of Superconformal Deposition: Copper, Silver & ……

Thomas Moffatt, Daniel Josell and Daniel Wheeler

Superconformal filling means seam- and void-free filling of high aspect ratio features through a deposition mechanism characterized by bottom-to-top filling. The existence of superconformal copper electrodeposition for electrolytes containing particular combinations of additives has permitted the use of damascene copper in modern electronics. However, this has been accomplished through pure empiricism because the mechanism by which superconformal filling was unknown. We explain the mechanism, and then use this knowledge to predict and demonstrate superconformal electrodeposition of silver. We also show the generality of the mechanism, by explaining superconformal chemical vapor deposition of copper.

26. La_2O_3-CaO-MgO-TiO_2 Ceramics for Wireless Applications

Terrell Vanderah, Virginia Miller, and Igor Levin

Dielectric oxide ceramics with high permittivity, low dielectric loss and near-zero temperature dependence of resonant frequency are critical elements in components such as resonators, oscillators and filters for wireless communications. Currently, only a few ceramics exhibit the properties necessary for use in these devices. Phase equilibria diagrams are needed to prepare controlled, temperature-stable ceramic mixtures with tailorable and low-loss dielectric properties. A potentially useful ceramic occurs in the $LaMg_{½}Ti_{½}O_3$–$CaTiO_3$ perovskite-related solid solution, which occurs in the quaternary La_2O_3-CaO-MgO-TiO_2 system. Subsolidus relations in the sub-systems La_2O_3-MgO-TiO_2 and $LaMg_{½}Ti_{½}O_3$-$CaTiO_3$-La_2O_3 were determined in air, and regions with temperature-stable ceramics were located. Compound formation, crystal-chemistry, and dielectric properties will be described.

27. Optical And Structural Studies Of III-Nitride Thin Films And Heterostructures

Lawrence Robins, Charles Bouldin, Igor Levin, Mark Vaudin, Joseph Woicik, Albert Davydov, Leonid Bendersky, Daniel Josell, Norman Sanford, Anthony Birdwell, John Armstrong and Ryna Marinenko

Devices based on thin films of the III-nitride materials (AlN, GaN, InN and their alloys) are beginning to enable advances in several important technologies: (a) compact blue, green, and white non-laser light sources for full-color displays and solid-state lighting; (b) blue solid-state lasers for next-generation optical data storage systems; (c) efficient deep-UV emitters for chemical and biological sensors and secure short-range communications; (d) solar-blind UV detectors for space applications; (e) field-effect and bipolar transistors for high-power, high-frequency, and high-temperature operation. Compared to other device-grade semiconductors, currently available III-nitride films typically possess a higher density of defects, larger strains, and greater inhomogeneity. Device developers thus require metrologies to correlate the structural, optical, and electronic properties of the films; techniques with nanometer scale spatial resolution are especially needed. We will discuss several ongoing MSEL projects in the III-nitride metrology area.

(1) InGaN alloys, which form the active layers of blue/green emitters, are susceptible to phase separation and related compositional instabilities. Several InGaN films were examined by cathodoluminescence spectroscopic imaging (CLSI) with ~200 nm spatial resolution. Large spatial variations were observed in the CL lineshape, including the appearance of a split-off peak at higher energy than the main band-edge peak. The non-uniformity was greatest in films with 4% to 8% In mole fraction, which are not believed to show bulk phase separation. Possible interpretations, and plans to correlate these results with other measurements, will be discussed.
(2) Metal contacts to n- and p- doped GaN, which are required in electronic and optoelectronic devices, show problems with excessive contact resistance, poor uniformity, and thermal degradation. Metallurgy and Ceramics researchers are investigating the chemistry, atomic structure, and electronic structure of the GaN/metal interface. We will discuss the use of low-electron-energy, depth-resolved CL to examine electronic states near the interface, and correlation of the CL results with TEM microstructural characterization.

(3) Accurate data on the composition-dependent linear optical properties of AlGaN alloy films, including refractive index, index dispersion, birefringence, and absorption edge position and lineshape, are needed as inputs for device design and simulation. Normal-incidence transmittance and reflectance spectroscopy provides some of the needed parameters; by combining the transmittance/reflectance results with the complementary prism-coupling waveguide technique (performed by Optoelectronics, NIST Boulder), values of the optical constants are estimated throughout a wide spectral range.

28. NIST Materials Research and the Automotive Industry

Clare Allocca

For nearly a century, the National Institute of Standards and Technology has been supplying research results, tools, and services that help U.S. automotive companies improve their processes and products. Today, nearly 80 R&D projects under way in NIST's laboratories address the industry's technical needs, from coatings, lubricants and emissions control to machining, stamping, and supply-chain collaboration. The newly formed NIST Industrial Liaison Office (ILO) has developed a detailed inventory of these projects to allow our customers to have easier access to broad project information. In addition, the ILO is seeking feedback from industry in order to maximize the impact of NIST's work. About 40% of this diverse portfolio contains projects with Materials science aspects.

This poster depicts selected projects in several areas of Materials Science—metals forming, engineered surfaces, ceramics and polymers. Among some of the materials technologies being developed at NIST for use by the Automotive Industry are:

- Measurement methods, models, standard tests, and data that allow industry to predict the behavior of sheet metal being formed into automotive components, such as doors, thus shortening the development time for new body component designs and enabling the use of new lightweight materials to increase fuel efficiency
- Process models to enable the understanding of the fabrication of metal matrix composite materials, thus enabling these lightweight materials' use in the automobile, with a resultant increase in fuel efficiency
- Measurements, measurement methods, models, and standard tests for manufacturing processes and machine tool performance that enable faster, higher quality, cheaper, and more efficient production of parts using advanced materials
- Advanced methodologies, measurements and models to relate the properties of polymer coatings to behavior under the types of conditions that cause scratching and marring on a vehicle's surface
- Measurements and reflectance and rendering models for improved specification of appearance attributes (e.g. automotive paints)

The objectives, approaches, products, and industry relevance of these and many other projects are described.

29. OOF: Object-Oriented Finite Element Analysis of Material Microstructure

Stephen Langer

The structure of a material on a microscopic scale determines how it will behave on a macroscopic scale. This is especially true for composite materials with complicated microscopic geometries, but theoretical models for predicting the macroscopic behavior are limited to simple idealized geometries. Materials scientists in industry and academia have a need for software that can predict macroscopic behavior using the real microscopic material geometry as a starting point. OOF is a finite element program created at NIST, as a joint venture between ITL and MSEL, to address this problem. With OOF, a user loads an image of a microstructure (either from a micrograph or a simulation), identifies features in the image, assigns material properties to them, generates a finite element mesh that conforms to the material boundaries, and performs virtual experiments to determine the macroscopic properties of the specimen. The material properties and parameters can then be adjusted to determine their effect on the macroscopic behavior. OOF1, which solves elasticity and thermal conductivity problems, is available on the web, and won a 1999 Technology of the Year award from Industry Week magazine. OOF2, which will solve a much wider variety of problems, is currently under development.

30. The Center for Theoretical and Computational Materials Science

James Warren

The Center for Theoretical and Computational Science (CTCMS) is the focal point in MSEL for the development and practice of materials theory and modeling. The Center's mission is to (i) investigate important problems in materials theory and modeling with novel computational approaches; (ii) create opportunities for collaboration where CTCMS can make a positive difference by virtue of its structure, focus, and people; (iii) develop powerful new tools for materials theory and modeling and accelerate their integration into industrial research. By combining resources, tools, and knowledge under the same umbrella, the CTCMS provides the infrastructure necessary for MSEL to perform world-class theory and modeling that has an impact that extends beyond the sum of aggregate parts and fosters creativity.

31. Hardness Standardization

Sam Lowe, Christian Johnson, Douglas Smith, and George Quinn

Hardness is the primary test measurement used to determine and specify the mechanical properties of bulk products, coatings and thin films. Industry uses a wide range of indentation hardness tests, with applied forces ranging from micronewtons to kilonewtons. The Metallurgy and Ceramics divisions of MSEL are engaged in all levels of standards activities to assist U.S. industry in making hardness measurements compatible with other countries around the world. These activities include the standardization of the national hardness scales, collaborative development of new indentation tests, development and production of primary reference transfer standards, leadership in national and international standards writing organizations, and interactions and comparisons with U.S. laboratories and the National Metrology Institutes of other countries.

32. Polyolefins: Serving the Largest Market

William Wallace, Charles Han, and Kalman Migler

The polyolefins industry (primarily polyethylene and polypropylene) comprises the largest share of the U.S. market for polymers; specifically, polyethylene and polypropylene are the top two materials used in blow molding, and film and sheet production. It is estimated that in 2002, the North American polyethylene production alone will exceed 42 billion pounds. In addition to this, metallocene polyethylene and polypropylene demand is expected to grow 20 percent per year through 2006. For this growth to be sustained, a variety of characterization and processing tools are required by this large industry. The Polymers Division is therefore investing to meet the needs of these materials producers and materials processors. We are assisting them from their initial materials research to their final materials production. For the initial materials production, we are providing tools to characterize the molecular mass and molecular mass distribution of their polyolefins (through Standard Reference Materials and mass spectrometry techniques) and are then providing the theoretical framework needed to predict polyolefin blend miscibility for new classes of materials. In the final materials' production, we have developed tools for characterization of melt processing conditions through process monitoring and visualization. In this manner, we aim to accelerate the rate at which polyolefin products reach the market with support from cradle to grave.