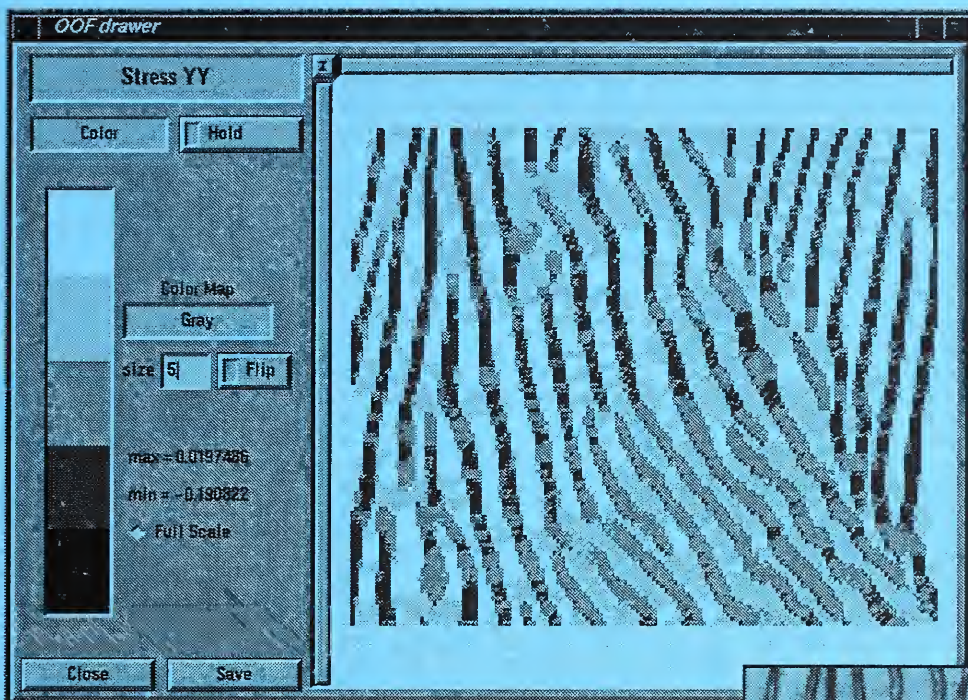
NIST
PUBLICATIONS

MSEL

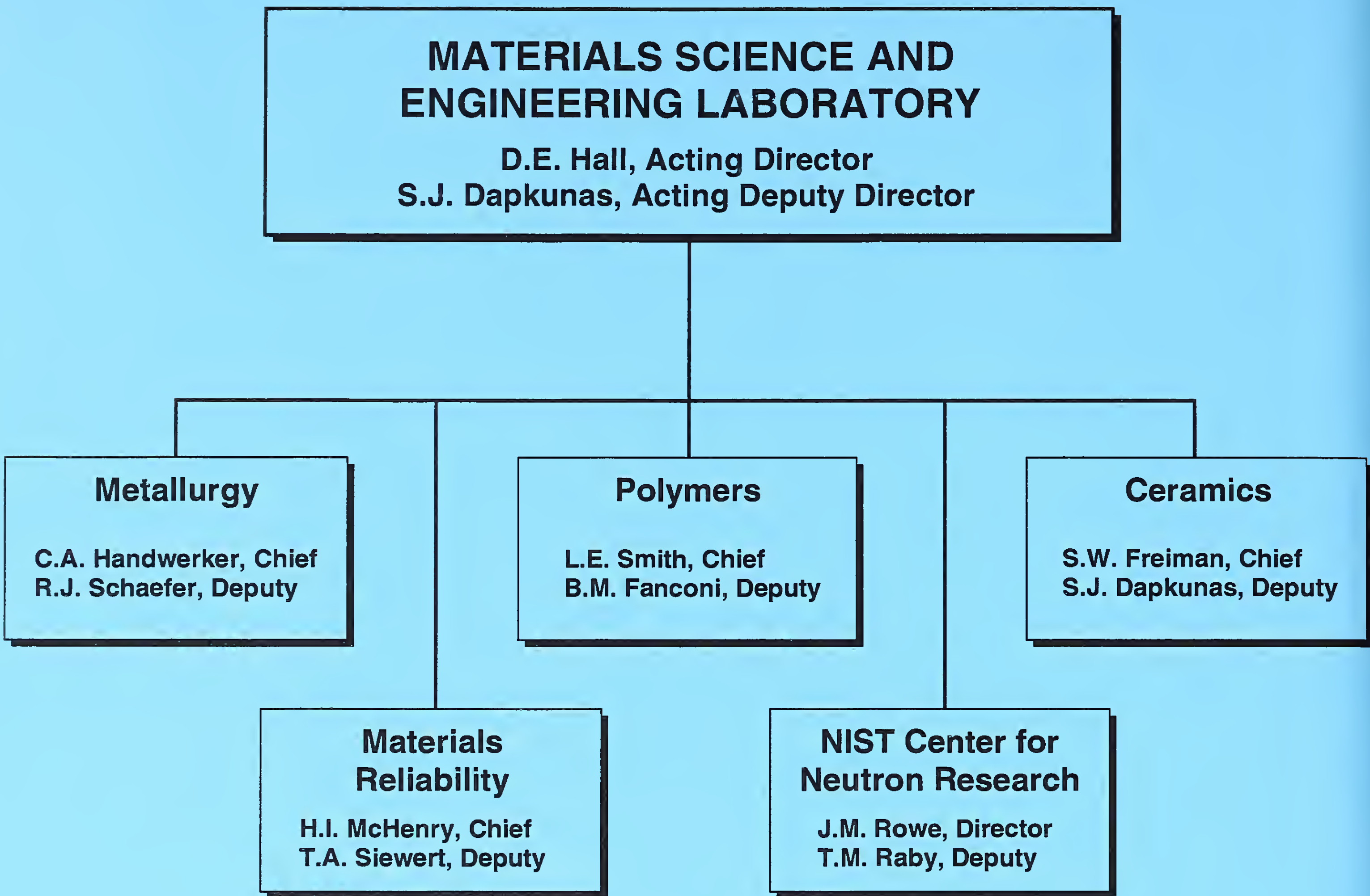
Materials Science and Engineering Laboratory

ANNUAL REPORT



NISTIR 6062
U.S. Department of Commerce
Technology Administration
National Institute of Standards
and Technology

Technical Activities
1997



The cover figure illustrates the use of the Object Oriented Finite (OOF) analylsis--a public domain software program created in collaboration with researchers from MSEL and the Information Technology Laboratory. Materials scientists use this software program to explore and calculate the macroscopic properties of real microstructures. Microstructures are scanned into a graphics file and then the user specifies material properties for the constituent parts of the microstructure.

In the illustration, the microstructure for pearlite (lower figure) is used an example of how OOF works on a two-phase microstructure. Thermoelastic coefficients were specified for the iron-carbide and iron phases and a virtual tension was then applied in plane strain conditions. The upper figure illustrates graphically the partition of stresses in the phases.

More information as well as software is available at: http://www.ctcms.nist.gov/~wcraig/oof

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D.E. Hall, Acting Director
S.J. Dapkunas, Acting Deputy

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Technical Activities 1997

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William M. Daley, Secretary
TECHNOLOGY ADMINISTRATION
Gary Bachula, Acting Under Secretary for Technology
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
Robert E. Hebner, Acting Director

TABLE OF CONTENTS

	Page
PREFACE	I
OFFICE OF THE DIRECTOR	iii
OVERVIEW	1
Introduction	3
Organization of Technical Staff	3
Organization of Technical Activities	5
RESOURCES	7
MSEL 1997 Total Funding by Source (FY 1997)	9
MSEL Staff Profile by Materials Class	10
NIST/NRC Postdoctoral Research Associateships Program	11
TECHNICAL PROGRAMS	13
THE CENTER FOR THEORETICAL AND COMPUTATIONAL MATERIALS SCIENCE	41
SELECTED CUSTOMER IMPACTS	49
TECHNOLOGY TRANSFER	57
Summary of CRADA Activities	59
Active CRADAs FY 1997	61
Patents Granted	69
Patents Pending	71
FY 1997 SRM's in Production	75
FY 1997 SRM Projects Under Development	76
Standard Reference Databases	79
APPENDICES	81
Honors and Awards	83
Standards Committees Memberships	85
Caption for Figure on Cover 1	Cover 2
MSEL Organization Chart	Cover 2
NIST Organization Chart	Cover 3

PREFACE

The National Academy of Sciences-National Academy of Engineering-National Research Council (NAS-NAE-NRC) Board on Assessment of the National Institute of Standards and Technology (NIST) Programs, and in particular, the Panel for Materials Science and Engineering, performs an important role in support of the programs and success of the Materials Science and Engineering Laboratory (MSEL). The Panel is one of our most effective means of technical peer review by counterparts in the scientific and engineering communities of U.S. industry and academe. Each panel member is selected by the National Research Council on the basis of expertise and extensive experience in the areas of research and technology conducted by the Laboratory. In addition to this Laboratory-wide Panel, we also have an Assessment Panel for the NIST Center for Neutron Research (NCNR).

The 1997 Annual Report was organized to assist the NAS-NAE-NRC Board on Assessment and is intended to be used as background information at the annual review meeting. This report provides general information about MSEL in addition to describing the activities, accomplishments, output and impacts of MSEL during the period of Fiscal Year 1997 (October 1, 1996, to September 30, 1997). A second series of reports on detailed technical activities are published separately as the National Institute of Standards and Technology Internal Reports (NISTIR) for each Division and Center within MSEL. All FY 1996 reports are available upon request or may be found by accessing MSEL's website at http://www.msel.nist.gov. This report, which summarizes MSEL's FY 1997 activities, will also be electronically available shortly after its date of publication.

In addition to the NAS-NE-NRC Panel this report is also made available to those in industry, academic institutions, and government agencies who wish to know more about our technical activities. MSEL appreciates hearing comments from the Panel and our customers about the information contained herein and its value in identifying ways in which we may more effectively serve your needs. We look forward to working with you in the future.

Dale E. Hall

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OVERVIEW

INTRODUCTION

The Materials Science and Engineering Laboratory provides technical leadership and participates in developing the measurement and standards infrastructure related to materials critical to U.S. industry, academia, government and the public. MSEL's mission is to *stimulate the more effective production and use of materials by working with materials suppliers and users to assure the development and implementation of the measurements and standards infrastructure for materials.* Materials science and engineering programs at NIST cover a full range of materials issues from design to processing to performance.

Separate research initiatives address ceramics, metals, polymers, composites, superconductors and the theory and modeling of materials structure and performance. This research supports efforts of U.S. industry to develop reliable, low cost manufacturing methods for producing tailor-made materials and products with superior properties.

Through laboratory-organized consortia and one-to-one collaborations, NIST's materials scientists and engineers work closely with industrial researchers. Examples include modeling and measurement based research on improved processing of rapidly solidified metal powders, polymer composites, ceramic machining, casting of aerospace alloys, and materials property sensors for aluminum and steel manufacturing. The laboratory is also strengthening its relationships with both the manufacturers of high-technology products and the major users of advanced materials.

MSEL's technical staff seeks to leverage its resources to effect the greatest impact on the Nation's measurement and standards infrastructure. Many mechanisms are employed to assess the most important measurement and standards needs for U.S. industry. Once these needs are identified, suitable planning is critical to accomplishing the Laboratory's mission. MSEL's Strategic Plan, revised in 1996, is considered a living document which must be concurrently critiqued to keep pace with the changing needs of materials suppliers and users. In FY 1997 the MSEL management team participated in an offsite meeting which focused on identifying issues of concern in program management and managing for impact. Such meetings enable MSEL to more effectively meet the needs of U.S. industry. This report summarizes MSEL's technical activities for FY 1997. More specific information about these activities may be obtained by reviewing the annual reports from our five technical divisions.

ORGANIZATION OF TECHNICAL STAFF

The Materials Science and Engineering Laboratory is one of eight Measurement and Standards Laboratories of the National Institute of Standards and Technology (NIST). MSEL's fiscal year 1997 budget totaled $47.3 million. An additional $25.6 million dollar budget covered special procurements and operating costs for the Reactor Operations and Research Facility Operations of the NIST Center for Neutron Research (NCNR). MSEL's staff totals 354 FTE's - "full-time equivalents" - of which 88 percent are engaged in scientific or technical support positions. Also during fiscal year 1997, 130 visiting scientists and engineers working onsite at NIST for a minimum of 2 weeks, collaborating on materials research projects with MSEL scientists and engineers.

The Laboratory consists of five technical divisions, including the three material specific divisions of Ceramics, Metallurgy, and Polymers, the interdisciplinary Materials Reliability Division, and the NIST Center for Neutron Research (NCNR). Each of the five units has the generic mission of fostering the economical processing and safe and efficient use of materials and products incorporating advanced materials by improving materials quality, manufacturability, and reliability. This mission is accomplished through developing and disseminating standards, measurement methods, predictive models, evaluated data and reference materials, and the scientific, quantitative understanding that is fundamental to the synthesis, processing, characterization, properties, and performance of materials.

Ceramics Division

The Ceramics Division conducts programs pertinent to advanced ceramic materials through fundamental and applied research, the development of standard test methodologies, the preparation of standard reference materials, and the evaluation and dissemination of standard reference data. The participation of U.S. industry in all phases of the Division's research has been strongly encouraged as typified by the many research agreements between members of the technical staff and their colleagues from industry. Based on our continued assessment of measurement and standards needs of the U.S. ceramics industry, a shift in programmatic direction from materials and processes relevant to structural applications to those of primary importance for electrical, thermal, and optical functions, and, in turn, to expanded research in ceramic coatings and films has occurred.

Materials Reliability Division

The Materials Reliability Division develops measurement technologies which enable the producers and users of materials to improve the quality and reliability of their products. Measurement technologies are developed for process control to improve the quality and consistency of materials, nondestructive evaluation to assure quality of finished materials and products, and materials evaluation to assure reliable performance. Programs encompass developing on-line sensors to measure materials characteristics or processing conditions, characterizing of internal geometries of materials by ultrasonic methods, and developing measurements for evaluating the mechanical, thermal and magnetic behavior of materials on the micrometer-scale.

Polymers Division

The Polymers Division is responsible for providing standards, measurement methods, and fundamental concepts of polymer science to assist U.S. industries that produce or use synthetic polymers in essential parts of their business. Programs are planned primarily to develop improved measurement capability for broad sectors of the industrial community. The advice from industrial and technical communities is a key element in setting priorities. This advice stems both from workshops, and from extensive informal visits to customers. The Division has focused a majority of its resources on specific industrial sectors, thereby permitting an allocation of its resources that is appropriate with its mission and coincides with the technical strengths of its staff.

Metallurgy Division

The Metallurgy Division is working closely with materials suppliers and users to develop the measurement and standards infrastructure needed in diverse technological areas from steel making to the fabrication of nanostructured multilayers for magnetic recording heads. Both metals producers and users require measurements that enable more accurate predictions of materials performance, manufacturability and long-term reliability. The Division's program, thus addresses measurement-related needs within all industrial sectors using metals and alloys including: aerospace, automotive, electronics, and stationary power generation, as well as the needs of suppliers of steel, aluminum, nickel-based superalloys, and other specialty metals.

NIST Center for Neutron Research (NCNR)

The NIST Center for Neutron Research has three primary responsibilities: to operate the NIST Research Reactor (NBSR) as a NIST and national resource in a cost-effective manner while assuring the public safety; to conduct a broad program of materials research using neutron methods, while developing and maintaining state-of-the-art instrumentation to ensure the best utilization of the NBSR neutron scattering facilities; and to develop and operate the Cold Neutron Research Facility (CNRF) as a national center, providing unique measurement capabilities to U.S. researchers.

ORGANIZATION OF TECHNICAL ACTIVITIES

The Laboratory's technical activities are described in terms of research projects, research programs or strategic thrusts. Research projects are research and development activities having defined technical objectives, work plans, and planned outputs that address a specific technical opportunity or barrier in materials science.

Research programs are assemblies of research projects designed to collectively accomplish technical goals and objectives to overcome technical barriers in a specific technological area. Research programs are organized and managed as a collective set of projects and may reside within a single group, one division within MSEL or may extend to other laboratories within NIST.

Strategic thrusts are selected assemblies of research programs organized to collectively accomplish technical objectives in specific goal areas of MSEL/NIST. The MSEL strategic thrusts for FY 1997 and beyond are: Advanced Materials; Advanced Processing; and National User Facility. All strategic thrusts involve a measurements and standards underlying theme. Note that some programs may fit under more than one strategic thrust; a list of FY 1997 strategic thrusts and the programs which have their majority focus in that strategic thrust as follows:

ADVANCED MATERIALS PROGRAMS

Ceramic Coatings
Dental and Medical Materials
Electronic Packaging, Interconnection and Assembly
Evaluated Materials Data
High Temperature Superconductivity
Magnetic Materials
Mechanical Properties of Brittle Materials
Neutron Characterization
Polymer Characterization
Synchrotron Radiation Characterization
Theory and Modeling
Thin Film Measurements and Standards
Ultrasonic Characterization of Materials

ADVANCED PROCESSING PROGRAMS

Ceramic Machining
Ceramic Processing
Intelligent Processing of Materials
Metals Data and Characterization
Metals Processing
Nondestructive Evaluation
Polymer Blends and Processing
Polymer Composites

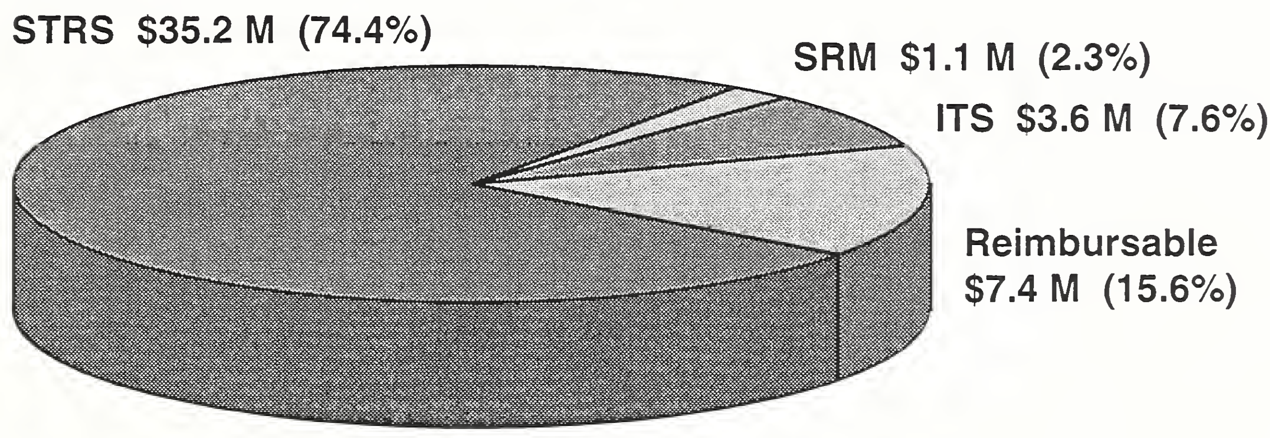
NATIONAL USER FACILITY

Neutron Facility Operation

RESOURCES

BUDGET RESOURCES

Total Expenditures by Source* ($47.3 million)
Fiscal Year 1997



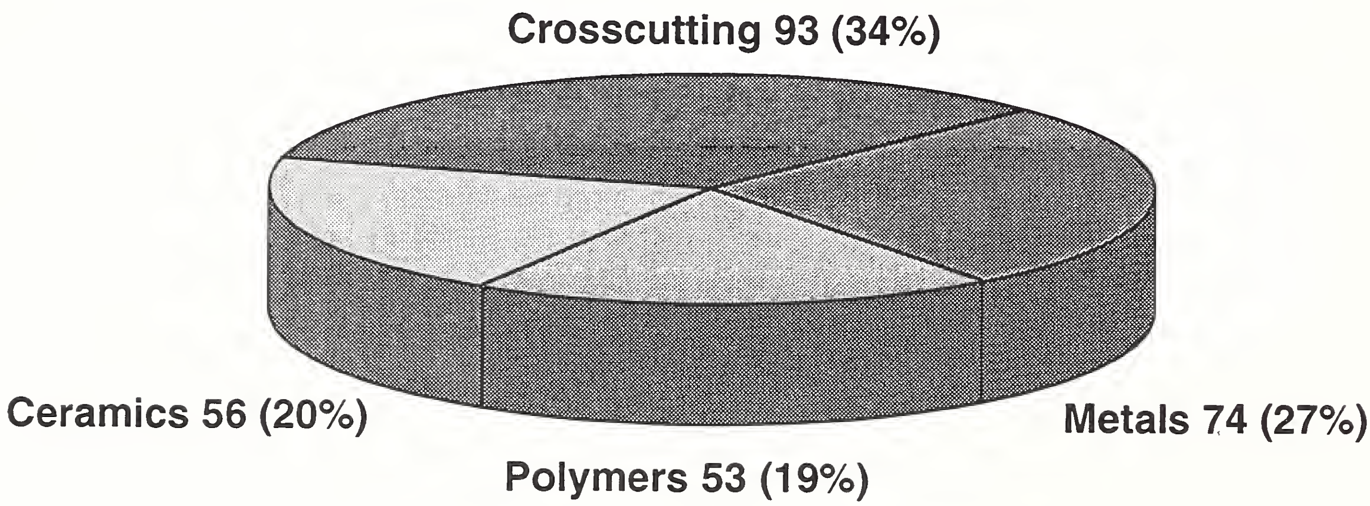
*Excludes $25 million STRS funding for operations and special procurements for Reactor Operations and the Cold Neutron Research Facility

Scientific and technical research and services (STRS) are congressionally appropriated funds. Reimbursable funds originate primarily from other government agencies and support MSEL's efforts to further the mission of those agencies where the unique expertise of MSEL's technical staff is needed. The percentage of other agency support represents a response to years of increasing STRS budget. MSEL's Standard Reference Material (SRM) Program funded at $1.1 million per year is the second largest SRM program in the NIST Measurement and Standards Laboratories.

Resources from the NIST Advanced Technology Program (ATP) are listed under ITS (Industrial Technology Services). It is noteworthy that MSEL leads all of the other six NIST technical operating units in supporting ATP's technical agenda. Since the amount of STRS and ITS resources represent a current and likely future budget scenario, the percentage of budget accounted for by reimbursables may increase.

STAFF RESOURCES

MSEL TECHNICAL STAFF PROFILE BY MATERIALS CLASS* (FTE)
Fiscal Year 1997



*Excludes reactor operations staff (30) and all non-technical support staff (49)

A profile of staff by materials class is shown above. The focus here is to show what we do rather than the academic discipline we came from. Clearly, staff resources are distributed fairly evenly over technical programs in metals, polymers and ceramics. Technical activities involving composite materials are found under each of the materials classes indicated in the pie chart.

Crosscutting activities include technical activities that support more than one materials class: research staff of the NIST Center for Neutron Research, the Center for Theoretical and Computational Materials Science, NIST Fellows, and the scientific staff of the Laboratory office. The large contingent of crosscutting expertise enables MSEL to apply state-of-the-art measurement methods to a broad array of technical problems that span materials classes.

Over the last five years, the total staff of about 350 full time equivalents as well as the ratio between technical and support staff have remained fairly constant. We see this trend continuing into the foreseeable future.

NIST/NRC POSTDOCTORAL RESEARCH ASSOCIATESHIPS PROGRAM

The NIST/NRC Postdoctoral Research Associateships Program provides two-year temporary appointments for outstanding scientists and engineers chosen through a national competition administered by the National Research Council of the National Academy of Sciences. These appointments provide an opportunity for the Nation's best scientists, mathematicians and engineers to engage in state-of-the-art research in association with senior research specialists of the Institute's staff, using the excellent and often unique research facilities at NIST.

This program provides an opportunity for concentrated research for outstanding postdoctoral level scientists and engineers with selected members of NIST's permanent staff. Program participants are sometimes offered permanent employment. Information on MSEL's FY 1997 postdoctoral research associates may be found in the following table.

Technical Activity	Name	Degree	Prior Academic Institution	Advisor
Polymer Blends and Mechanical Properties	Barnes, Kathleen	Poly.Sci	Michigan Tech U.	Nakatani
Transient Liquid Phase Bonding	Campbell, Carelyn	Matls. Sci.	Northwestern U.	Boettinger
Scattering and Polymer Solutions and Blends	Ivkov, Robert	Poly. Sci.	U. of Maryland	Amis
Model Based Ultrasonic Standards	Lerch, Terence	Engineering Mechanics	Iowa State U.	Fortunko
Crystallization Behavior of Polymer Near a Solid Substrate	Pochan, Darrin	Engineering	U. of Mass	Wu
Polymer Characterization	Proza, Ty	Poly Sci/Engr.	U. of Wisconsin	Barnes
X-Ray Absorption Measurements and X-Ray Diffraction on Ferroelectric Films	Ravel, Bruce	Solid State Phys	U. of Wash	Bouldin
Viscoelastic Flow in Composites Processing	Reiff, Andrea	Poly. Sci.	U. of Houston	Phelan
Super Mechanisms of Superplasticity in Zirzonia	Seidensticker, John	Ceramics	Penn State U.	Wiederhorn
Viscoelastic Property of Ultra Thin Polymer Films	White, Christopher	Pol Sci/Engr	U. of Wisconsin	Wu

TECHNICAL PROGRAMS

PROGRAM DESCRIPTIONS

MSEL carries out a variety of technical activities organized under the rubric of programs, projects, or strategic thrusts. Each program represents an array of research projects designed to collectively overcome a major technical barrier in a specific area of materials science. Projects are research and development activities having defined technical objectives and planned outputs addressing a specific technological barrier within a specific materials application of importance to MSEL's mission. Strategic thrusts contain an assembly of research programs designed to accomplish the major elements of both the MSEL and NIST missions. This year MSEL's strategic thrusts cover three focus areas: Advanced Materials, Advanced Processing, and National User Facility. Measurements and standards provide an overarching theme for these strategic thrusts.

This section of the report contains program overviews for MSEL's 22 technical programs. One impact or accomplishment achieved for each program during FY97 is included directly after each overview. Technical activities for some programs, e.g., Polymer Composites, are carried out in one division of MSEL whereas programs such as Intelligent Processing of Materials have projects in two or more divisions. More complete information about these programs may be found in the annual reports from each of MSEL's divisions and centers.

ADVANCED MATERIALS PROGRAMS

CERAMIC COATINGS

The Ceramic Coatings Program is a measurement and characterization effort which addresses the processing reproducibility and performance prediction issues that are primarily associated with thermal-spray deposited ceramic coatings. The program focuses on plasma-spray-deposited ceramic thermal barrier coatings used in aircraft gas turbines and expected to be used in land-based turbines and diesel engines. Sales in the thermal-spray industry are currently valued at more than one billion dollars annually, a significant portion of which is ceramic thermal-barrier coatings. Collaborations have been established with industrial organizations including Pratt and Whitney, General Electric, Caterpillar, METCO, MetTech and Zircoa as well as the Thermal Spray Laboratory at the State University of New York at Stoney Brook and the Thermal Spray Laboratory at Sandia National Laboratory. The program includes collaboration with the National Aerospace Laboratory and the National Mechanical Engineering Laboratory, both in Japan, to examine functionally gradient materials. Collaboration is also underway with BAM (Germany) for the development of characterization techniques for thin, hard films. Research is conducted on the processing and properties of Physical Vapor Deposited (PVD) ceramic coatings in collaboration with Praxair, an Advanced Technology Program (ATP) awardee.

Participants in the NIST program are located in the Ceramics, Materials Reliability, and the NIST Center for Neutron Research of the Materials Science and Engineering Laboratory as well as the Chemical Science and Technology Laboratory.

The approach taken in the plasma-spray (PS) research has been to build on the analytical capabilities at NIST and the material processing capabilities of collaborators. The program has the following elements:

- development of techniques for characterization of physical and chemical properties of stabilized zirconia and tungsten carbide feedstock to provide data for increased processing reproducibility as well as data required for production of a Standard Reference Material suitable for calibration of light-scattering size distribution instruments used in industry for analysis of PS powder;

- development of scattering techniques to determine the quantity, size and orientation of porosity and microcracks in PS ceramic coatings suitable for use in modeling the thermomechanical behavior of these materials;

- development of methods to measure chemical, elastic modulus, and thermal properties on a scale suitable for use in microstructural models of behavior;

- development of techniques to model thermomechanical behavior of thermal-barrier coatings to enable more reliable performance prediction;

- development of techniques for accurate measurement of the thermal conductivity of PS coatings, by use of the guarded hot-plate technique suitable for incorporation in ASTM standards and by the pulsed laser heating technique, to provide a method for comparison with routine industrial techniques; and

- development and refinement of more sensitive methods for accurate analysis of oxide phases and residual stresses which affect performance and durability of coatings.

Research on chemical mapping of powders and microstructures is conducted in the Microanalysis Division of the Chemical Science and Technology Laboratory. Thermal property research is conducted in the Materials Reliability and Metallurgy divisions and the NIST Center for Neutron Research participates in both the powder analysis and scattering projects. A strong attribute of the PS coatings research is the use of common materials for which complementary data can provide a more complete understanding of processing-microstructure-property relationships.

Improving Coating Performance

Measurements that determine the microstructure and properties of thermal spray feedstocks were performed in collaboration with engine manufacturers, spray equipment and instrument suppliers. As a result of this research, Pratt & Whitney modified their spray dried zirconia feedstock binder content specification to improve coating performance.

DENTAL AND MEDICAL MATERIALS

The Dental and Medical Materials Program provides basic materials science, engineering, test methods, and standards to sectors of the health care industry for the development of new or improved materials and delivery systems. The focus of this program is the development of improved dental restorative materials with greater durability, wear resistance and clinical acceptability.

Dental restorative composites are heterogeneous materials having three essential phases: (1) a polymeric matrix which comprises the continuous phase, (2) fillers of various types, sizes, shapes and morphologies which constitute the disperse phase and (3) an interfacial phase that, in varying degree, bonds the continuous and disperse phases into a unitary material rather than a simple admixture. While all three phases are important in determining the properties of the composites, this program is focused primarily on the interfacial and polymer matrix phases. Since the polymerization shrinkage that occurs in the matrix phase is one of the most commonly cited deficiencies of dental restorative composites, resources are allocated to develop high conversion, durable, low shrinkage polymeric materials for use in dental resin and composite applications. The polymeric matrix of a dental composite typically is formed by free radical polymerization of a resin which is one or more vinyl monomers, usually of the methacrylate class. Polymerization is started either by the formation of initiating radicals from chemical reduction-oxidation (redox) reactions or by photochemical redox reactions.

Although only a minor component of these composites, the interfacial phase that develops from the interaction of the silane coupling agent with the polymer matrix and the siliceous filler exerts a profound effect on the properties of the composites. Because these composites are used in an aggressive, aqueous environment that constantly challenges the vulnerable silane mediated polymer-filler bond, understanding of this critical interfacial phase is being acquired so that strategies can be developed for its improvement.

The occupational and environmental hazards associated with the use of mercury-containing dental alloys are a recurring source of public concern. Since dental amalgams have performed exceedingly well over more than one hundred years, the development of a direct filling material still based on the common constituents of dental amalgams, other than mercury, is desirable. This project is focused on acid-assisted consolidation of chemically precipitated silver powders and property measurements of hand consolidated test compacts prepared with the tools and procedures normally employed by dentists. The observed values of flexural strength for the silver compacts were equal or superior to mercury amalgams. Corrosion resistance, microleakage and marginal toughness values of the compacts were found to be superior to those of amalgams. Wear and biocompatibility studies on the hand consolidated compacts are in progress.

Dental research directions in support of the goals are established in collaboration with the American Dental Association (ADA), the National Institute of Dental Research (NDIR), and guest scientists from the U.S. Navy and the U.S. Public Health Service. NIST has hosted research associates from

ADA since 1928. Currently, the ADA Health Foundation sponsors 32 research associates at NIST. The collaborative relationship between that professional association and the federal government is unique, and continues to develop and transfer important new technologies to dentistry and medicine.

Consolidation of Mercury-Free Dental Restoratives
The American Dental Association has obtained an exclusive license for a NIST patent on silver-based filling materials. The patent resulted from developmental work at NIST supported by the National Institute of Dental Research to find an alternative to mercury-containing dental restoratives and a technique to place or consolidate the restorative using normal dental hand tools.

ELECTRONIC PACKAGING, INTERCONNECTION, AND ASSEMBLY

Today's U.S. microelectronics and supporting infrastructure industries are in fierce international competition to design and produce new smaller, lighter, faster, more functional electronics products more quickly and economically than ever before.

Recognizing this trend, in 1994 the NIST Materials Science and Engineering Laboratory (MSEL) began working very closely with the U.S. semiconductor packaging, electronic interconnection, assembly, and materials supply industries. These earlier efforts led to the development of an interdivisional MSEL program committed to addressing industry's most pressing materials measurement and standards issues central to the development and utilization of advanced materials and material processes within new product technologies, as outlined within leading industry roadmaps[1]. The vision that accompanies this program - to be the key resource within the Federal Government for materials metrology development for commercial microelectronics manufacturing - may be realized through the following objectives:

- develop and deliver standard measurements and data
- develop and apply *in situ* measurements on materials and material assemblies having micrometer- and submicrometer-scale dimensions
- quantify and record the divergence of material properties from their bulk values as dimensions are reduced and interfaces are approached
- develop fundamental understanding of materials needed for future packaging, interconnection and assembly schemes

With these objectives in mind, the program presently consists of nearly twenty separate projects that examine key materials-related issues, such as: electrical, thermal, and mechanical characteristics of polymer and metal thin films; solders, solderability and solder joint design[2]; interfaces and adhesion; electromigration and stress voidage; and built up stress and moisture in plastic packages. These projects are always conducted in concert with partners from industrial consortia, individual companies, academia, and other government agencies. The program is strongly coupled with other microelectronics programs within government and industry, including the National Semiconductor Metrology Program (NSMP)[3]. The NSMP is a national resource responsible for the development and dissemination of new semiconductor measurement technology.

More information about this program, and other NIST activities in electronic packaging, interconnection and assembly, is contained in *Electronics Packaging, Interconnection and Assembly at NIST: Guide and Resources*, NISTIR5817 (http://www.msel.nist.gov/epia1996/contents.htm). Copies may be obtained by contacting Michael Schen at (301) 975-6741 or michael.schen@nist.gov.

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[1] *National Technology Roadmap for Semiconductors*, Semiconductor Industry Association, San Jose, CA, 1994, 1997 (in draft); *National Technology Roadmap for Electronic Interconnections*, Institute for Interconnecting and Packaging Electronic Circuits, Lincolnwood, IL, 1995, 1997 (in draft); *National Electronics Manufacturing Technology Roadmap*, National Electronics Manufacturing Initiative, Inc., Herndon, VA, 1996.

[2] http://www.ctcms.nist.gov/programs/solder
[3] http://www.eeel.nist.gov/810.01/index.html

> ***Solder Interconnect Design for Microelectronics***
> The Solder Interconnect Design Team, organized by the Metallurgy Division and the Center for Theoretical and Computational Materials Science, is developing software that will facilitate the design of electronic packaging. The Design Team, which includes Motorola, DEC, Ford, and Susquehanna University, has used this software to determine equilibrium shapes of solder joints and resulting forces on the electronic package leads. The software has allowed electronic package designers at Motorola to improve product yields from 20% to 90%.

EVALUATED MATERIALS DATA

The objective of the Evaluated Materials Data Program is to develop and facilitate the use of evaluated databases for the materials science and engineering communities. Both research- and application-directed organizations require readily available evaluated data to take advantage of the large volume of materials information developed on public and private sponsored programs. This information, particularly numeric data, is available in an ever increasing number of publications published worldwide. The necessity to consolidate and allow rapid comparison of properties for product design and process development underlies the database projects.

Evaluated databases are developed in cooperation with the NIST Standard Reference Data Program Office and, often, coordinated with the activities of other laboratories and scientific/technical societies. Research consists of the compilation and evaluation of numeric data as well as recently initiated efforts directed at more effective distribution and use of data. Database activities reflect laboratory programs with scientific capabilities required for appropriate data evaluation. Database projects in MSEL include:

- Phase Equilibria Diagrams (PED), conducted in collaboration with the American Ceramic Society;

- the Structural Ceramics Database (SCD), a compilation of evaluated mechanical and thermal data for nitrides, carbides, and oxides of interest to engineers and designers;

- a ceramic machinability database, developed by the Ceramic Machining Consortium (see Ceramic Machining Program);

- a high T_c superconductivity database developed in cooperation with the Japanese Agency for Industrial Science and Technology (see High Temperature Superconductivity Program);

- development and implementation of the STEP protocol for the exchange of materials data, under the auspices of the ISO 10313 activity;

- the NACE/NIST Corrosion Performance Database developed by NACE and the Metallurgy Division to provide a means to select structural alloys for corrosive applications; and

- the Crystal Data Center developed by the NIST Center for Neutron Research which provides fundamental crystallographic data on inorganic materials.

Availability of Superconductor Data on the World Wide Web
The PC version of the NIST Standard Reference Database on High Temperature Superconducting Materials is accessible through the World Wide Web (http://www.ceramics.nist.gov/srd/srd.htm). This database provides evaluated thermal, mechanical, and superconducting numerical property data for oxide superconductors.

HIGH TEMPERATURE SUPERCONDUCTIVITY

A significant program in high T_c superconductivity is being conducted in MSEL and other Laboratories at NIST. The primary focus of the MSEL program is on bulk superconducting materials for wire and magnet applications. In carrying out this program, researchers in MSEL work closely with their counterparts in other NIST Laboratories, and collaborators in U.S. industry, universities, and other National Laboratories.

The primary thrusts of the program are as follows:

- Phase equilibria - Work is being performed in close collaboration with the U.S. Department of Energy (DOE) and its national laboratories to provide the phase diagrams necessary for processing these unique ceramic materials. A prime objective is the development of the portions of the phase diagram for the Pb-Bi-Sr-Ca-Cu-O system relevant to production of the high T_c materials.

- Flux pinning - Use is made of a unique magneto-optical imaging facility to examine flux pinning in a variety of materials, with much of this work being conducted in collaboration with American Superconductor Corporation. In addition techniques for better interpretation of magnetic measurements are being developed. Structure and dynamics of flux lattices and melting phenomena, critical to applications, are investigated with small-angle neutron scattering techniques.

- Damage mechanisms - Work is being carried out under a joint CRADA (cooperative research and development agreement) with American Superconductor Corporation as part of the "Wire Development Group" which involves a number of DOE National Laboratories and the University of Wisconsin to elucidate the effects of strain on the loss of current in superconducting wires. The primary tool being employed is the use of microfocus radiography available at the NIST beamline at the Brookhaven National Laboratory.

- Database - A high temperature superconductor database has been developed in collaboration with the National Research Institute for Metals (NRIM) in Japan. The High Temperature Superconductor Database (HTSD) includes evaluated open-literature data on numerous physical, mechanical, and electrical properties of a variety of chemical systems. The first version of the database is now for sale by the Office of Standard Reference Data.

- Crystal structure - Thermal neutron scattering techniques and profile refinement analyses are being utilized to investigate crystal and magnetic structures, composition, dynamics and crystal chemical properties. This research is being carried out in collaboration with a number of industrial and university experts and researchers at National Laboratories.

Improving Processing of Superconducting Wires
The primary crystallization field of the five-component Pb-Bi-Sr-Ca-Cu-O (2223) high-temperature superconductor (T_c = 110 K) has been determined. These data will be used by companies to design processing temperature-composition paths that will yield optimum superconducting wires and tapes

MAGNETIC MATERIALS

Magnetic materials are pervasive throughout our society. They are used, for instance, in magnetic recording media and devices, in all motors, in all transformers, on credit cards, as permanent magnets, as magnetic sensors, on checks, in theft control devices, in automotive and small engine timing devices, in xerographic copiers, in magnetic resonance imaging (MRI) machines, in microwave communications, in magnetic separation, and in magnetic cooling. Magnetic materials include metals, ceramics and polymers at different size scales ranging from large castings to particulates, thin films, multilayers and nanocomposites.

In the present trend to make devices smaller, thereby reducing weight or increasing storage density, new magnetic materials are constantly being developed. One critical need for implementation of these materials is the development of the measurement science needed for their characterization, in terms of both material properties and performance. This is the focus of the Magnetic Materials Program. Proper measurements of key magnetic properties, determination of the fundamental science behind the magnetic behavior of these new materials, analysis of the durability and performance of magnetic devices and development of standard reference materials are key elements of this program. Some information is only obtainable by the use of unique measurement tools at NIST like the neutron diffraction facilities at NCNR, or the magneto-optic indicator film apparatus for observation of magnetic domain motion. Of particular interest is understanding the magnetic behavior of low dimensional systems, in which one or more characteristic dimensions have been reduced to nanometer sizes. For these new materials, however, it is not known whether their exciting novel behavior is due to new physics or to a logical extension of large-size behavior to small dimensions. Consequently, implementation of this new type of material into marketable products is significantly delayed. NIST is providing the measurement science to address this critical unknown.

Areas of present study include the following:

- processing of magnetic multilayers for optimal giant magnetoresistance effect
- observation and micromagnetic modeling of magnetic domains for understanding magnetization statics and dynamics in advanced and conventional materials
- measurement and characterization of nanoscale magnetic interactions in multilayers, nanocomposites, and low-dimensional systems, needed for understanding and applying the physics of these materials
- measurement and modeling of the enhanced magnetocaloric effect in nanocomposites
- structure and magnetic characterization of new superconducting materials
- nanotribology of magnetic hard disks, measurement of stiction, friction, and wear at the nanometer scale
- measurement and understanding the origin of magnetic exchange bias in conventional and advanced magnetic structures and devices
- development of magnetic sensors of mechanical properties for incorporation as *in situ* controls in a steel mill
- development of a measurement system for the preparation of an absolute magnetic moment standard

By experimentally addressing important issues in magnetism, by bringing together the industrial and scientific communities through the organization of workshops and conferences in the area, and by the development and preparation of appropriate standards, NIST acts to accelerate the utilization of advanced magnetic materials by the industrial sector, and to enable industry to take advantage of new discoveries and innovations. In addition, close linkage with the national storage industry consortium (NSIC) which consists of 38 companies and a score of universities allows industrial relevance and partnership. Additional collaborations with Xerox, General Motors, Hewlett Packard, IBM, Seagate, and Motorola Corporations, for example, enable NIST to leverage its activities with the much larger, but complementary, capabilities of other organizations.

Storage of Magnetic Information
Researchers have identified the processing conditions which lead to significant improvements in the properties of thin-film magnetic materials which are critically important for high density information storage. The materials are based on the giant magnetoresistance (GMR) effect and will be used in the next generation of hard disk drives. This work has shown how to fabricate films with higher GMR values than ever before attained, and how to improve the thermal stability of these materials to make them usable in electronic circuits which are processed at elevated temperatures.

MECHANICAL PROPERTIES OF BRITTLE MATERIALS

Mechanical properties are the source of the greatest benefits as well as the most severe limitations of ceramic materials. Owing to their high strength-to-mass ratio, their relatively inert behavior in aggressive environments, their high hardness and wear resistance, and their ability to withstand significantly higher temperatures than metals or polymers, ceramics offer the potential for major improvements in component design for a wide range of applications. On the debit side, however, ceramic materials typically exhibit statistically variable brittle fracture, environmentally enhanced subcritical crack growth, sensitivity to machining damage, and creep/deformation behavior at elevated temperatures. Additionally, a lack of techniques, which can detect and quantify critical flaws before failure ensues, severely curtails current uses of ceramics. Unpredictable failure behavior of ceramics stems from three sources: (1) limited data and a deficiency of basic understanding of failure processes in ceramics; (2) limited standard test techniques to permit interlaboratory comparisons of materials behavior and collection of engineering data; and (3) inadequate models and statistical techniques for life prediction and reliability analyses. The Mechanical Properties of Brittle Materials Program has components specifically addressing each of these issues.

Basic understanding of mechanical behavior of ceramics is investigated at both room temperature and elevated temperatures. At room temperature, mechanical properties and failure processes are investigated in fiber-reinforced ceramic matrix composites as a function of microstructural scale and in aluminum nitride substrates as a function of processing conditions, phase content, and microstructure. Microstructural stresses related to enhanced fracture toughness are measured via micro-Raman techniques in heterogeneous microstructures and correlated with micro-mechanical modeling. Micro-mechanical computer simulations are used to elucidate distributions of residual stress distributions in highly anisotropic ceramics as a function of crystallographic texture. At elevated temperatures, the basic mechanisms responsible for crack growth, creep and creep rupture are investigated for various silicon nitride compositions, and for membrane and fuel cell materials.

To improve interlaboratory comparisons and to increase confidence in generated data, new standard test techniques for hardness and toughness are being developed and tested in round-robin experiments. Research and interlaboratory studies in instrumented indentation address the use of this technique for measuring elasticity and hardness of thin films and coatings. Micro-Raman techniques are being developed and calibrated so that quantitative assessments of microstructural residual stresses can be mapped for heterogeneous microstructures. At elevated temperatures, new creep specimens were designed which permit higher stresses with reduced non-gage section failures. Intra- and inter-laboratory studies demonstrated the robustness of these geometries. International interlaboratory studies are underway to elucidate their relationship to alternate testing geometries.

Finally, techniques to predict lifetimes of ceramics under constant and variable loading conditions are being developed. A nonparametric bootstrap approach for assessing the confidence of lifetime predictions is investigated and compared with analytical techniques. Work includes applying these techniques to aluminum nitride materials for thermal management systems and to fused silica and other glasses for spacecraft window applications. A new experimental procedure was developed for characterizing time-dependent failure under static loads.

Software for Modeling Mechanical Properties of Materials
The beta version of an object-oriented finite element program (OOF), developed in collaboration with NIST's Information Technology Laboratory and the Center for Theoretical and Computational materials Science, was made available on the World Wide Web. More than 100 copies of this program, which represents a new paradigm for understanding physical properties of real, complex, microstructures, have already been downloaded by non-NIST electronic addresses.

NEUTRON CHARACTERIZATION

This program encompasses the basic and applied research efforts and neutron scattering method development centered on the Neutron Condensed Matter Science Group in the NIST Center for Neutron Research. Group scientists and visiting researchers lead broad-based mission research in chemistry, solid state physics, materials science and biology, often in collaboration with other divisions in MSEL in addition to the Building and Fire Research Laboratory, the Chemical Science and Technology Laboratory (Biotechnology, Surface and Microanalysis, Thermophysics, and Analytical Chemistry divisions), and with well over 100 universities and industries from all over the United States and the world. Group scientists also develop and maintain state of the art capabilities and instruments as a national resource for cold and thermal neutron scattering research, including scientific leadership and oversight in the development and use of 10 experimental stations in the Cold Neutron Research Facility.

Current areas of emphasis in the multidisciplinary research program include: studies of the structure and excitations of high technology magnetic and superconducting materials, thin films and multilayers; crystallographic analysis of the atomic and molecular arrangements in catalysts, ceramics, superconductors, ionic conductors, and fullerites; sophisticated neutron diffraction analysis of residual stress and texture which affect properties and performance of technology important alloy, ceramic and composite structures and components; studies by neutron reflectometry and small angle scattering (SANS) of macromolecular and microstructures in materials and of atomic, molecular, macromolecular and magnetic surfaces and interfaces; inelastic neutron scattering studies of molecular bonding states and dynamic processes in chemical catalysts, sieves, polymers and battery materials, and molecular scale curing processes in cements; and studies of biomolecular structure and dynamics in proteins, lipid bilayers and membranes.

Characterizing Cubane by Neutron Methods
Scientists at the NIST Center for Neutron Research and the University of Chicago have recently achieved a great advance in our understanding of the properties of solid cubane (C_8H_8), an immensely strained molecule that represents an atomic scale replica of a cube. Because of the strain energy, cubane and its derivatives have potential applications as superexplosives, and for biomedical applications. The NIST/U. of Chicago research has determined the structure of the plastic phase of cubane for the first time, and probed the details of cubane dynamics. It is hoped that this will yield valuable insight into the engineering of future cubane-based compounds for specific applications. This work has recently been featured in Physics News Update, the American Institute of Physics Bulletin of Physics News and in the Science Times section of The New York Times.

POLYMER CHARACTERIZATION

The Polymer Characterization Program provides measurement methods, data and standard reference materials needed by U.S. industry, research laboratories, and other federal agencies to characterize polymers for processibility, rheological and mechanical properties, and performance. Molecular mass and its distribution have significant effects on the processibility of polymers through dramatic effects on their rheological properties. Mechanical properties and performance are significantly affected by the solid state structure formed during processing. Importantly, unlike many other common engineering materials, polymers exhibit mechanical properties that exhibit time dependent viscoelastic and aging behaviors, even at low temperatures. As a result, the focus of the program is on techniques that measure molecular mass and its distribution, solid state structure, mechanical properties, and rheological behavior of polymeric materials.

Primary methods employed for molecular mass characterization are dilute solution light scattering and osmometry. Chromatographic techniques, which require calibration by standards of known molecular mass, provide information on molecular mass distribution. Recent activities exploit advances in mass spectrometry using matrix assisted laser desorption ionization (MALDI) to develop the method as a primary tool for the determination of the molecular masses of synthetic polymers. Solid state structure of polymers is elucidated using small and wide angle x-ray scattering, atomic force microscopy, electron microscopy, as well as spectroscopic methods such as solid state nuclear magnetic resonance (NMR) and infrared spectroscopy.

Adequate characterization of the time-dependent viscoelastic and aging behaviors of polymers requires large amounts of testing. For this reason, methods are developed that reduce the number of tests required to describe the nonlinear thermo-viscoelastic properties of polymers. The approach applies the frameworks of solid and fluid continuum mechanics to interrelate mechanical responses under different geometries of deformation and in varied deformation histories. Phenomenological models and underlying physical theories are tested using the NIST torsional dilatometer, conventional rotational rheometry, and servo-hydraulic mechanical testing machines.

The polymer industry and standards organizations assist in the identification of current needs for standard reference materials. Based on these needs, research on characterization methods and measurements are conducted leading to the certification of standard reference materials. Molecular standards are used primarily for calibration of gel permeation chromatographs, the principal method employed by industry for assessing molecular mass and molecular mass distributions. Melt flow standards are used in the calibration of instruments used to determine processing conditions for thermoplastics. Rheological standards are developed for secondary calibrations of rheological instruments in industry and academia.

Sample Preparation Techniques for Spectrometry on the Web
Nearly 100 different procedures for preparing samples of synthetic polymers for analysis by matrix assisted laser desorption ionization mass spectrometry (MALDI-MS) were taken from the literature and placed on the World Wide Web (http://www.nist.gov/msel/div854/maldi/) for use by practitioners of MALDI-MS.

SYNCHROTRON RADIATION CHARACTERIZATION

The availability of synchrotron radiation is resulting in major discoveries over a wide range of disciplines within materials science. The Synchrotron Radiation Program is a development and characterization effort which includes the operation of beam stations at the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory, construction of beam stations at the Advanced Photon Source in a Collaborative Access Team (CAT) arrangement with the University of Illinois, Oak Ridge National Laboratory, and U.O.P. Corporation, and a microstructural characterization effort in which NIST scientists, and researchers from industry, universities and other government laboratories perform state-of-the-art measurements on advanced materials.

The range of scientific problems currently being addressed at the NSLS includes: microstructure characterization of portland cement, ultrahigh molecular weight polyethylene, man made diamonds and diamond films, sapphire windows, and GaN films on sapphire. Most recently, an *in situ* investigation of the formation of dislocation structures has been initiated successfully. *In situ* microstructure characterization, using ultra-small-angle scattering, x-ray imaging, and ultrasoft x-ray absorption spectroscopy is a very active area. Other areas of intensive investigation include studies of bond lengths in strained semiconductor layers, tribochemical reactions on surfaces, the orientation of lubricants on hard disk magnetic media substrates, order and orientation of proteins bound to self-assembled monolayers, and the development of new catalysts.

A wide range of materials studies were carried out at NSLS during 1997. The ultra-small-angle scattering facility (USAXS), which is used to examine microstructures from tens of angstroms up to micrometers in size, has yielded significant results, for example, on the microstructure of ultra high molecular weight polyethylene, on portland cement and plasma-sprayed ceramics, on semi-crystalline polymers, on metal-binding by pseudomonas aeruginosa, on the structure of bovine bone, on additive dispersions in polycarbonate, and on the dislocation structure of single crystal aluminum under stress. The USAXS instrument fills the gap between visible light scattering and pinhole small-angle cameras. As one of the few SAXS instruments in the world for which a primary absolute calibration is available, the results from the X23A3 USAXS facility are typically quantitative rather than qualitative.

The high-resolution, monochromatic x-ray topography camera at the NSLS facility is the only dedicated monochromatic facility of its type in this country. In the past year, it was used in studies of a range of basic and applied materials including sapphire, superconducting YBCO crystals, CVD diamond, and single crystal Al. The hard x-ray microscope, which was designed and built by NIST researchers, offers unique opportunities to perform *in situ* x-ray diffraction imaging and high-resolution x-ray radiography measurements.

Research by NIST scientists during 1997 included:

- studies of the relationship between microstructure development in hydrating cement and the morphology of additives,

- fundamental measurements of dislocation formation as a function of strain in single-crystal materials,

- studies of defects in superalloy single-crystal castings and sapphire windows,

- studies of the chemistry and the orientation of lubricants on hard-disk magnetic-media substrates,

- studies of tribochemical reactions in nanometer lubricant films,

- theory and experiment on bond-length distortions in strained-semiconductor

Improving the Composition for Concretes
Small-angle neutron and x-ray scattering measurements carried out on cements and concretes have established a link between the coarse features in the particle morphology of silica fumes and the microstructural development of the hydrating cement blends. This information is expected to lead to improved cementatious materials for the Nation's roads and bridges.

THEORY AND MODELING

Materials science and engineering is on the threshold of a fundamental transformation. Spectacular advances in computer processor power, memory, and computational methodologies now allow researchers to simulate highly complex materials behavior and microstructures. In FY97, the MSEL Theory and Modeling Program's activities continued their focus on the behavior and properties of materials over length scales extending from atoms to bulk materials. For example, MSEL researchers performed molecular dynamics simulations to study relaxation and glass formation in supercooled liquids, employed mesoscopic phase field and reaction-diffusion models of alloys, polymers and liquid crystals to study phase behavior, stability, separation kinetics, and morphological evolution in these materials, designed cellular automata models to investigate solidification in alloys, and developed finite-element software tools to model solder drops in microelectronic interconnects, domain formation in micromagnetic materials, and mechanical properties of composite microstructures.

In FY97 MSEL's Center for Theoretical and Computational Materials Science (CTCMS) facilitated numerous interactions between industry, academia, NIST and other government labs in the development and application of state-of-the-art theoretical and computational science techniques to industrially important materials and materials processing problems. To use more effectively the nation's talents and resources, the CTCMS integrates ongoing research at various institutions by forming temporary multi-disciplinary and multi-institutional research teams as required to attack key materials issues. The CTCMS has three principal activities, all operating interactively: planning, research, and technology transfer. Workshops are held as the first step in defining technical research areas with significant technological impact, identifying team members, and in building and designing the infrastructure for collaborative research. NIST, in its unique position as a "third Party" liaison, is well suited to play a national role in this planning process. The CTCMS provides an infrastructure and support for its members, including an interactive World Wide Web information server, and modern computing and workshop facilities. In FY97, CTCMS researchers within MSEL developed powerful new materials modeling tools and addressed critical technical issues in the areas of microelectronic interconnect design, Green's functions and boundary element methods applied to mechanical properties, microstructure and dynamics of glass formation, standards in micromagnetics modeling, morphological control of polymer-based liquid crystal display materials, and object-oriented finite-element modeling of composite microstructures.

Interacting with Customers Through CTCMS

The Center for Theoretical and Computational Materials Science (CTCMS) maintains a World Wide Web server that provides information on Center activities, research results, and software. Each CTCMS working group has a Web page which describes its research agenda, publications, meetings, and advances. In some cases, the CTCMS server has become a tool for confidential information exchange among the participants of a working group. In FY 1997, new features, including a web-based calendar and search engine, were implemented.

THIN FILM MEASUREMENTS AND STANDARDS

Functional ceramics (*e.g.*, ceramics primarily intended for optical, electronic, or thermal management applications) are increasingly being used in film geometries. In response to this growing segment of the ceramics community, the Thin Film Measurements and Standards Program endeavors to provide improved measurement tools and data that are needed to evaluate advanced ceramic films and film systems. Increasingly critical film performance requirements (*e.g.*, reduced dimensions, increased purity, improved interface properties, increased production rates, and tighter control of properties) place stringent demands on film processing control, models, and characterization techniques. However, lack of measurement methods to monitor film processing and accurately characterize film properties as well as limited theoretical understanding of interrelationships between processing conditions and final film properties reduce most film processing to empirical procedures. The activities in this program are designed to address these measurement and modeling issues, both with regard to specific, near term industrial needs as well as to the development of a materials science knowledge base required for use of ceramic films in future applications. Near term and long range goals have been developed based upon both general discussions between Materials Science and Engineering Laboratory staff and representatives of industry and universities at professional meetings and consortia workshops as well as focused, collaborative research projects with specific organizations.

The film characterization techniques in use or under development include electrical, mechanical, optical, thermal, and x-ray measurements. Specific research activities include:

- investigations of the processing and microstructural features that control poling behavior and domain stability in ferroelectric films;

- development and utilization of spectroscopic procedures to evaluate film composition in $BaTiO_3$ and to detect defects in ferroelectric and semiconductor films;

- development of methods to measure and statistically analyze texture and texture distributions in films and to relate these data to processing conditions;

- development of measurement procedures, models, and standards to permit quantitative evaluation of thermal diffusivity in thin films and to relate thermal diffusivity to film microstructure and morphology;

- application of advanced x-ray measurement capabilities (*e.g.*, EXAFS, DAFS) to the analysis of film structure and composition and the construction of an in-house state-of-the-art x-ray facility.

A critical requirement for the projects cited above is the ability to generate model film systems. To this end, this program includes two film deposition capabilities: metalorganic chemical vapor deposition (MOCVD) and pulsed laser deposition (PLD). The MOCVD system is an integral part of the ferroelectric film research projects already listed and, during the past year, has undergone a major upgrade to provide more precise compositional control. In contrast, the PLD facilities, while providing films for investigation, has had additional responsibilities, the development of *in situ* measurement procedures to monitor the physical and chemical processes involved during the film deposition process and the formation of models to relate the measurements to the film formation.

A New Method for Pulsed Laser Deposition
A novel, real time, particulate reduction method based on deflection by a pulsed gas jet, timed to coincide with the appearance of particulates prior to deposition, has been demonstrated. The feasibility of this pulsed laser deposition (PLD) method has already been confirmed for at least a 90% reduction in the number of particulates reaching the substrate using barium titanate targets. This research will lead to a wider use and greater acceptance of PLD by industry.

ULTRASONIC CHARACTERIZATION OF MATERIALS

The Program on Ultrasonic Characterization of Materials is directed to the development of model-based methods of physical measurement which characterize the internal geometries of materials, such as defects, microstructures, and lattice distortions. Our goal is to convert these measurement methods into sensors suited for production line and in-service measurements of materials quality and serviceability.

A primary focus of the Ultrasonic Characterization Program is microstructural characterization of metals and alloys, composite materials, and engineered surfaces. The idea is that models relate microstructure and physical properties. Thus, by measuring quantities related to physical properties, the salient microstructural features can be ascertained. For example, sound velocity is related to elastic properties, and thus, ultrasonic measurements can be used to characterize fiber-orientation distributions in composites or texture in metals. These model-based measurements enable industry to replace microscopy with nondestructive methods for the microstructural characterization needed to assure the quality of advanced materials.

The Ultrasonic Characterization Program is making significant contributions to measurement technology and materials modeling. We have worked with industry to commercialize advances in non- contact ultrasonics, wave form based acoustic emission, composites nondestructive evaluation and nonlinear ultrasonics. Modeling advances include Green's function methods for wave propagation in anisotropic materials, obtaining elastic constants from resonance spectra, and determining texture based on ultrasonic measurements.

International Acceptance of Ultrasonic Standards
Precision velocity measurements were made on a series of ultrasonic tests blocks provided by ASTM. In collaboration with Germany's Federal Institute of Materials Testing (BAM), we are using these results to address problems with a draft European Standard (prEN12223), which is being considered for adoption by the International Standards Organization (ISO).

ADVANCED PROCESSING PROGRAMS

CERAMIC MACHINING

The Ceramic Machining Program was established in response to a comprehensive survey of the U.S. advanced ceramics industry indicating that the high cost of machining and, at times, uncertain reliability associated with machining damage are primary impediments to the widespread use of these materials. This program is designed to address generic industry needs related to measurement methods and standards in order to assist industry in the development of machining technology for the manufacture of reliable and cost-effective components made from advanced ceramics. The specific projects include: (1) effects of abrasive machining on mechanical properties of ceramics, (2) intelligent machining of ceramics, (3) chemical and chemomechanical effects of grinding fluids, and (4) abrasive finishing and wear of dental ceramics.

Ceramic materials studied in these projects include those ceramics intended for structural applications, such as silicon nitride, and the ceramics used for dental restorations, such as machinable glass-ceramics. The first two projects are conducted jointly with the 22 member Ceramic Machining Consortium with input from NIST's Precision Engineering Division, Statistical Engineering Division, and Standard Reference Data Program. The Consortium members, representing a broad spectrum of industry consisting of materials producers, machine tool builders, suppliers of expendables (such as grinding wheels and fluids), and end users participate by providing materials, testing, advice, and other in-kind contributions. The consortium members also provide input to the other two projects and assist NIST in formulating the scope of the research projects. The close working relationship developed between industry, academic institutions, and NIST not only ensures the relevance of the research projects but also promotes an efficient and timely transfer of research information to industry for implementation.

Reducing the Formation of Cracks in Dental Materials
As part of an NIH supported study of wear and machining of dental ceramics, measurements of surface damage have led to the conclusion that the use of dental burs with coarse diamond particles can produce large cracks which can reduce the strength and wear resistance of teeth and ceramic restorations.

CERAMIC PROCESSING

Ceramic products are primarily produced by powder processing, where raw material powders are mixed with forming additives and shaped by various means into green bodies, which are then fired to the final, hardened state. The processing costs can vary greatly depending on the reproducibility and reliability of the process operation. One key to reliable and rapid development of new products is having good test methods to analyze the material at its different stages of processing. Unfortunately, no satisfactory measurements infrastructure yet exists within the ceramics industry, and as a result, much processing relies largely on art and experience.

The program on ceramic processing focuses on measurement methods of generic value to all ceramic companies. Clearer definitions are needed as to what needs to be measured, how is it to be measured, and how reliable is the measurement. Also, the value of the measurement to optimizing the processing operations is needed.

All subsequent operations depend on the raw materials characteristics, and therefore the measurement of the physical and chemical properties of powders is an important component of the program. The reliability of various measurement techniques is being assessed in a cooperative international program under the direction of the International Energy Agency and its subtask on ceramic powder characterization which is being coordinated at NIST in the ceramic processing program. In addition, SRMs needed to calibrate the measurement instruments in use are being developed. An intramural ATP project on the mechanism of drying, using NMR imaging, is in progress and is providing direct insight on the moisture gradients formed during drying.

A new consortium called the Ceramic Processing Characterization Consortium (CPCC) was formed in June, 1997. Its mission is to assist the U.S. ceramics industry in establishing a generic, powder processing measurements infrastructure. The goal is to assess the measurement needs in ceramics processing and to take all necessary and feasible actions to find viable solutions. Measurement procedures are generally non proprietary, so ceramic companies can work together to improve the measurement methods of common interest and benefit. The members of the CPCC are volunteers, from companies, instrument makers, universities, and national laboratories. Their contributions to the projects of the CPCC should result in rapid advances in the near future. The current projects are: (1) powder characterization; (2) green body characterization; (3) moisture measurements; (4) dispersion and rheology; and (5) microstructure development. Teams for each of these projects have been formed. The reliability and reproducibility of commonly used instruments will be assessed, new methods will be developed, and a better understanding of how the measured properties affect the behavior of the material at different stages of processing will be developed through basic research studies. All studies will be generic and nonproprietary. All members of the CPCC share in the carrying out the work in the CPCC project teams. The present number of members is 80 persons and represent 64 organizations (50 companies, 5 government laboratories, 10 universities).

> ***Formation of New Ceramic Processing Consortium***
> A new consortium called the Ceramic Processing Characterization Consortium (CPCC) was formed. The purpose of the CPCC is to develop a stronger measurements infrastructure for the U. S. ceramic processing industry.

INTELLIGENT PROCESSING OF MATERIALS

Research activities in the Intelligent Processing of Materials (IPM) Program investigate the conversion of materials into value added products using model-based control of processing variables. Information for real time process control is provided by on-line sensors which measure material characteristics and/or processing conditions. Intelligent processing will enable industry to economically produce materials with improved quality, consistent properties, and enhanced functionality. The IPM Program makes important contributions to three MSEL strategic thrusts: advanced materials, advanced processing, and National User Facility.

The IPM concept is the principal approach used to achieve the MSEL goal (1996 Strategic Plan) to "foster the development and implementation of technologies for advanced processing of materials." The central elements of IPM are (1) process understanding expressed in terms of a process model, (2) real-time information on processing parameters and material condition obtained with on-line process sensors, and (3) a model-based sensing and control strategy to achieve the desired characteristics in the finished product. IPM projects advance each of these elements, and joint projects with industry are integrating these elements into improved processing capabilities.

The IPM Program is an important contributor to the MSEL goal (1996 Strategic Plan) to "foster the use of advanced materials in commercial products." Advanced materials are materials with microstructures which are designed and controlled to provide superior properties and performance for specific functions. Microstructural control is perhaps the most important application of IPM. The idea is to model microstructural evolution during processing, sense microstructural changes in real time, and use a model-based control strategy to achieve the desired microstructure in the finished product. Microstructural consistency is essential to the commercialization of advanced materials because it assures reliable properties and performance of the material.

The IPM Program also contributes to MSEL's measurement technology goal. A major focus of the IPM projects is process sensors, which our industrial collaborators repeatedly identify as a crucial need. Sensor technology is a core competence of MSEL which has its roots in sensor development for nondestructive evaluation of materials. Unique MSEL capabilities are being used to measure thermophysical properties at elevated temperatures; these data are combined with model enhancements and then incorporated in industrial software for metal casting. In addition, specialized measurement capabilities such as nuclear magnetic resonance and small angle neutron scattering are used to understand microstructure/morphology evolution in ceramics and polymers.

Weld Sensing
As a part of a multiyear Cooperative Research and Development Agreement with Tower Automotive, advanced weld sensing technologies were evaluated on their production line. Results for several hundred welds confirmed the accuracy of the sensors for designed to detect unsatisfactory welds, and gave Tower an opportunity to evaluate the utility of this technology

METALS DATA AND CHARACTERIZATION

The performance of metals during use and their behavior during processing can be understood and predicted only with the availability of a detailed body of information on their physical properties and microstructure. The value of this information is greatly enhanced if it is developed within the context of models or theories which describe how the measured properties of a metal will vary with changes in composition, microstructure, temperature, geometry, or other parameters. The Metals Data and

Characterization Program includes activities which refine the technology for measuring the properties and behavior of metallic materials, and which correlate these properties and behavior to alloy microstructures.

The large majority of metals are used in applications based on their mechanical properties, with other applications based on electronic, magnetic, optical, or other functional properties forming smaller but nonetheless critical markets. Whatever the application, satisfactory long term performance of metallic components demands chemical and microstructural stability, sometimes in the presence of harsh environments. This program identifies those processing, microstructure, and properties characterizations which are critical to U.S. industry for both the processing and the performance of metals, and carries them out within the context of the NIST mission of providing data and standards. A significant part of the program is the use of advanced microscopy techniques to characterize the microstructures which form the basis of the measured properties.

The measurements of microstructural, mechanical, chemical, and optical properties carried out under this program have an impact in a number of different technology sectors:

- Standard test methods are being developed to support the automotive industry in its effort to improve fuel efficiency by shifting to lighter materials, a shift which has highlighted the critical need for improved understanding and control of sheet metal formability. The Metallurgy Division's effort is being carried out in collaboration with the Manufacturing Engineering Laboratory's NAMT program and with ATP-supported consortia of U.S. automakers and several universities.

- The accuracy of a high speed laser polarimeter technique for measuring the normal spectral emissivity of metals and alloys at high temperature has been demonstrated by measurements on a standard reference material (molybdenum). The millisecond resolution of the existing system is currently being upgraded to microsecond resolution, which should enable measurements extending to temperatures well above the melting point of refractory metals. These techniques provide industry with benchmark high temperature thermophysical properties measurements.

- Precision measurements of Rockwell Hardness, the primary parameter used to specify the mechanical properties of metals and alloys, are leading to the establishment of traceable national hardness standards. Calibrated test blocks, together with national standards for measurement and calibration procedures, will facilitate the acceptance of a wide range of U.S. products in international markets, as well as minimizing product-acceptance disputes in domestic trade.

- Computational micromagnetic techniques are producing results which are important for understanding magnetization reversal in devices incorporating thin magnetic elements. Micromagnetic head-to-head domain wall structures and energies in thin magnetic strips have been calculated, resulting in a "phase diagram" for transverse and vortex type walls.

International Hardness Intercomparison
After developing national hardness standards, NIST researchers are promoting the development of international agreement on hardness scales. An intercomparison study using the new NIST Rockwell C Scale SRM test blocks, conducted by NIST and the National Research Laboratory of Metrology in Japan, showed good agreement at all three levels of hardness for which the NIST standards are produced. An intercomparison of one hardness scale was also conducted with Japan and good agreement was found at four levels of hardness.

METALS PROCESSING

The properties of metals and their alloys depend strongly on their processing history. For example, the distributions of phases, grain structure, alloy compositional segregation, and defects in final commercial products depend on the conditions under which materials are processed and fabricated. These distributions in turn are crucial in determining the alloy strength, ductility, homogeneity, and other properties important for industrial applications. The Metals Processing Program focuses on measurements and predictive models needed by industry to design improved processing conditions, provide better process control, develop improved alloy and coating properties, tailor material properties for particular applications, and reduce costs.

Major successes in applying measurements and modeling to processing applications have been achieved in interactions with the aerospace, powder metallurgy, electroplating and electronics industries. Predictive models for solidification and microstructural evolution during processing have been incorporated by industry into design systems for casting of aerospace alloys and production of defect-free electronic materials, helping to reduce rejection rates arising from defective parts. Cooperative research and development projects with industry have resulted in significant improvements in process control for atomization of steel and superalloy powders. Standard reference materials, certified for coating thickness, microhardness or chemical composition, are being fabricated by electrodeposition techniques and powder metallurgy. Critical mechanistic, chemical and process variables controlling the structure/ property relationships of coatings and thin films produced by electrodeposition are being developed to take further advantage of this electrochemical process, which does not require high purity starting materials and is readily adaptable to large scale production.

Measurements and predictive models for processing being pursued in this program are of three kinds:

- Measurements and models are developed to help design materials production processes, such as measurements and evaluations to provide alloy phase diagrams, which are the roadmaps that alloy designers use to predict the alloy phases that can be produced under specific processing conditions. These evaluations are playing key roles in NIST collaborations with industrial consortia on electronic solders and casting of superalloys for aerospace applications.

- Measurements are made under dynamic conditions to monitor, in real time, properties of materials while they are actually being produced and to determine difficult-to-measure process parameters while the process is occurring. Special fast response sensors, simulations and imaging techniques have been developed for application to powder atomization and thermal spray processes, and workshops have been held to transfer these techniques to industry. Here, dynamic models of the process are important both for design of manufacturing procedures and for applications of real time feedback and control.

- To evaluate the adequacy of process models, it is important to measure the properties of the final materials and relate them to the process conditions. Current work in this respect includes evaluation of methods used to optimize properties of electrodeposited coatings and corrosion resistance of rapidly solidified nitrogenated steels.

In all of this work, the goal is to help U.S. industry apply measurements and predictive modeling to produce improved materials at reduced cost.

> ***Solidification Path in Multicomponent Aerospace Alloys***
> The NIST software for computation of enthalpy-temperature relationships appropriate for multicomponent alloy solidification has been incorporated into ProCAST™, a commercial software code, as part of the NIST Consortium on Casting of Aerospace Alloys. Such data will be used by the investment casting industry to shorten design cycles for production of turbine engine parts.

NONDESTRUCTIVE EVALUATION

Under NIST sponsorship, the Program for Integrated Design, Nondestructive Evaluation (NDE) and Manufacturing Sciences is underway at the Iowa State University Center for Nondestructive Evaluation and the Center for Quality Engineering and Failure Prevention at Northwestern University. Currently, the main projects include: Design for Reliability, Design for Inspectability, and In-service Inspectability of Manufactured Components. The program objective is to develop and incorporate quantitative NDE inspectability models, materials information, manufacturing considerations, and life cycle costing into component design considerations.

Measurement models with ties to computer aided design (CAD) have been developed for ultrasonic testing, eddy current testing, and radiographic (X-ray) methods. The measurement models have been combined with the effects of variabilities to produce probability of detection (POD) models for these techniques. Test beds for validating the POD models were developed and used to demonstrate a design strategy which combines POD and reliability models.

Projects are continuing to refine the inspectability/reliability models and design procedures. Improvements include the development of methods to incorporate new NDE modality into structure, system extension to include open CAD interfaces, and incorporation of new materials failure modes into the NDE models, particularly porosity in castings. Planning is underway to use the NDE models to address standards and calibration issues, with the goal of a standard with transferability among components with different geometries and materials.

Efforts are being made to transfer the technology to industry. Major interactions include: Chrysler, Ford, Electric Power Research Institute (EPRI), Lockheed Martin, Northrop Grumman, McDonnell Douglas, Pratt and Whitney, Westinghouse, General Electric, Allied Signal, Morton International, Boeing, and Babcock and Wilcox.

POLYMER BLENDS AND PROCESSING

Applications of polymer blends and multiphase polymer materials continue to enjoy growth in terms of market share, consumption, and employment within the plastics industry. This growth challenges the flexibility of materials suppliers to meet customer needs with new materials and reduced product development cycles. The futility of trial and error approaches to address these challenges led industry to solicit measurement tools and methods of analysis which enhance their efforts to understand and control resin compatibility, phase morphology, and material properties. These demands have been further sharpened by the advent of new methods which provide better control in polymer synthesis and more precise definition of material components.

The Polymer Blends and Processing Program began with clear scientific goals to establish expertise in static and kinetic aspects of phase behavior in polymer blends, effects of shear flow on mixing and separating, and reactive processing to promote compatibility. The focus on these areas furthers program objectives by accelerating development of new measurement tools, including specialized light and neutron scattering methods, and by applying those tools to expand the knowledge base for thermodynamics and kinetics of polymer blends. Work extends to the effects of additives in a blend system, the relative behavior of blends in bulk compared to in thin films at interfaces, and the effects of complex thermal and mechanical histories on the phase separation. Fundamental advances in theory and modeling continue to guide and interpret the measurements.

Current research in the program has four areas of emphasis: (1) measurement technology for on-line characterization of temperature, phase behavior, and shear deformation; (2) shear effects on phase diagrams and phase morphology; (3) activity of additives, compatibilizers, and fillers; and (4) control of interfacial effects in blends and during processing. In each of these areas the program works with industry to develop measurement methods using tools of fluorescence, light scattering, neutron scattering and reflectivity, x-ray scattering, birefringence, microscopy (AFM, TEM, phase contrast), and rheology. Industrial collaborators include: Aristech Chemical, Dendritech, DSM, Dow Chemical, Dow Corning, DuPont, Dynisco, Exxon, Kodak, GE, Goodyear, Mobil, Raychem, Rohm and Haas, and 3M.

In order to promote communication and technology transfer with an even broader range of industrial partners the Polymer Blends and Processing Center has been established. The focus of the Center is efficient adoption of measurement technologies developed at NIST and assessment of new research directions for the Polymer Blends and Processing Program. The Center also promotes initiatives which cut across research projects to improve opportunities for industrial collaborators to use NIST measurement capabilities.

> ***Improved Blends and Processing***
> The capacity of NIST developed on-line instrumentation, using light scattering and optical microscopy to measure *in-situ* domain size and shape during extrusion of incompatible and reactively compatibilized blends was demonstrated. In addition to morphology studies, the instrumentation can measure velocity profiles and characterize multiphase mixing. Industrial partners, including 3M and Rohm & Haas, have begun work using this instrument to investigate effects of polymer processing aids.

POLYMER COMPOSITES

The Polymer Composites Program seeks to facilitate the introduction of lightweight, corrosion-resistant composite materials into commercial applications by expanding the essential science base and generating test methods, reference data, and standard materials. The outstanding properties of composites lead to products that are superior and competitive in international markets. Industries as diverse as transportation, construction, marine, offshore oil, medical devices, and sporting goods have recognized those benefits and are beginning to make significant use of these materials. For this to continue, however, two significant barriers must be addressed: the lack of rapid, reliable, cost-effective fabrication methods; and the poor understanding of and predictive capability for long term performance. These barriers were identified in a series of industry workshops, exchange visits, and consultations. In response to these challenges, the composites program initiated two tasks: one on processing science, and the other on interfacial microstructure. The degradation of the interface over time is primarily responsible for the loss of mechanical properties. The automotive industry strongly influences the composites program since many of the processing and durability issues span many automotive applications, and solutions developed at NIST are expected to rapidly propagate throughout the industry. Additionally, the group interacts with companies interested in offshore oil platforms, infrastructure, aerospace, and a variety of other applications.

The goal of the Processing Science Task is to develop the technology required to monitor, model, and control the events that occur during composite fabrication. The program focuses on liquid composite molding (LCM) since this fabrication method is of great interest to all industry sectors and is the consensus choice of the automotive industry as the method with the most promise for making structural automotive parts. The approach in this task involves three steps. First, measurement tools are developed and used to characterize the material properties that control processing, for example, permeability. Second, sophisticated process simulation models are formulated to analyze the effects of processing parameters rapidly and inexpensively so they can be optimized. Finally, process monitoring sensors are developed and used to provide feedback for verification and improvement of the simulation models and to help develop the technology for on-line process control. The current activities in this Task involve five projects, including a major industry-university-government program sponsored by the Defense Advanced Research Projects Agency.

The work in the Microstructure Task focuses on developing test methods for assessing the resin/fiber interfacial adhesion, and the subsequent degradation of adhesion resulting from fluid attack, particularly moisture. The long term goals are to first develop effective test methods, and then to use those tests to identify the chemical and physical mechanisms of degradation, and finally formulate reliable predictive models. The program focuses on glass fiber materials since they are the primary candidates for automotive applications. In addition, the work is beginning to look at graphite reinforced composites since these systems are important for marine and infrastructure applications. Microscale tests such as the single fiber fragmentation test are currently being analyzed to determine if they can provide realistic estimates of the performance of the resin/fiber interface in composite systems. A variety of interfacial physical and chemical structures are generated during preparation of microscale test specimens by varying the coating chemistry on the fiber, the resin processing speed, and the moisture content of the material. Full scale composite specimens are also produced and tested with identical fiber coatings and processing conditions for comparison with the microscale tests and to provide, in conjunction with the microscale tests, realistic structure-performance relationships. There are currently four specific projects in this Task, including a collaboration with the Automotive Composites Consortium to determine the effects of processing conditions on the interface of polyurethane matrix composites.

> ***Permeability Database Developed***
> A database of permeability and other reinforcement properties was released in collaboration with the NIST Standard Reference Data Program. This data will aid the composites industry in designing liquid molding processes by providing critical input to mold filling simulation software.

NATIONAL USER FACILITY

NEUTRON FACILITY OPERATION

The NIST Research Reactor (NBSR) provides the basis of the NIST Center for Neutron Research (NCNR), the premier neutron research center in the United States in terms of breadth of capabilities, scope of projects, and number of users. The maintenance and operation of the NCNR may be divided into two major activities: 1) to operate the NBSR as a NIST and national resource in a cost-effective manner while assuring the public safety; and 2) to develop and operate the research facilities as a national resource, providing unique measurement capabilities to U.S. researchers. These responsibilities are allocated, formally, between the Reactor Operations and Engineering Group and the Research Facilities Operation Group.

Reactor Operations and Engineering activities include the safe and efficient operation of the reactor in order to provide a cost-effective national resource. This activity also includes sample irradiations, helping users to design and install new experiments, and monitoring many experimental systems (e.g. the helium refrigerator for cold source cooling). In addition to operation, upgrade and maintenance of the reactor, this activity also includes ensuring compliance with all regulatory requirements.

The Research Facilities Operations activity includes development and operation of the NCNR as a national resource to provide neutron measurement capability to a broad research and development community--including materials science, physics, chemistry and biology--which is drawn from industry, universities, and government agencies. This entails the development, operation and maintenance of cold neutron sources, a network of eight neutron guides, twenty-four experimental stations, and a full complement of ancillary equipment such as cryostats, furnaces and magnets. The NCNR, as a national facility, provides measurement capability to outside researchers, on the basis of scientific or technological merit of long-term programs or individual experimental proposals. The Research Facilities Operation activity is responsible for soliciting and evaluating proposals, and administering the allocation of requested experimental facilities and instrument time.

In summary, the maintenance and development of facilities, the development of new applications of neutron measurement technologies, and encouragement of their use by the broadest possible community in the United States, are the primary goals of this program. It is anticipated that new uses of the unique resources provided by the NCNR will lead to continued dramatic increases in utilization, as has been the case over the last decade.

NCNR Hosts Workshop on Neutron Methods

A Workshop on High Resolution Cold Neutron Spectroscopy, jointly sponsored by the National Science Foundation and the NIST Center for Neutron Research (NCNR), was held at NIST on August 13-15, 1997. About 40 participants were introduced to the basic principles and techniques of neutron spectroscopy, emphasizing the types of research that can be undertaken using the new, high resolution instruments at the NIST Center for Neutron Research, which are unique in the U.S. These offer U.S. scientists and engineers a wide range of new research opportunities in virtually all areas of materials research.

THE CENTER FOR THEORETICAL AND COMPUTATIONAL MATERIALS SCIENCE

THE CENTER FOR THEORETICAL AND COMPUTATIONAL MATERIALS SCIENCE

The interdisciplinary field of materials science presents researchers with rich, complex problems often of a universal nature. The theoretical underpinnings are relatively undeveloped, partly because it is a new field of research, and partly because the problems are quite complex. Indeed, these problems are often far too complicated to solve with pencil and paper. However, the revolution of fast information access, high speed computation, and widespread availability of computational resources has made possible new approaches to research in materials science and engineering. For example, previously intractable problems have become manageable through numerical simulation. Computer experiments allow fast, inexpensive, and nondestructive prediction of materials properties and behavior. It is now possible to study the physics of materials on all length scales using computer simulation, allowing researchers to verify and improve theories and propose more realistic models. Visualization of microscopic and mesoscopic phenomena give researchers new insights not previously possible through traditional experiments. These insights often lead to the discovery of new phenomena, and can serve as guides to experiments. With the advent of these new techniques NIST is in a unique position to bring together industry, academia, and government labs to form research collaborations. Thus, in 1994 MSEL created the Center for Theoretical and Computational Materials Science (CTCMS) to further computational materials science and promote its application to industrial problems.

The CTCMS is now a recognized national center of expertise in computational materials science. The Center's mission is to:

- investigate important problems in materials theory and modeling using new computational approaches;

- create innovative and productive opportunities for collaboration in materials theory and modeling;

- develop powerful new tools for materials theory and modeling and accelerate their integration into industrial research.

FY 1997 ACCOMPLISHMENTS

INFRASTRUCTURE

CTCMS members include researchers from industry, universities, national labs, and the NIST labs. Within MSEL, each CTCMS researcher is a member of one of the five MSEL divisions. Consequently, the research agenda of the CTCMS is coupled to division agendas. The scientific diversity of CTCMS researchers encourages communication between mathematicians, physicists, chemists, and materials scientists and engineers, and facilitates interactions and collaborations on a wide range of problems in materials and materials processing.

The CTCMS consists of a central hub in MSEL, and partnerships with other NIST labs, industrial labs, universities, and national labs. In FY 1997, the CTCMS expanded its network of powerful workstations and multi processor computers with advanced graphics, computing power, and data storage. The facility provides computational support, audio/visual capabilities, and teleconferencing for CTCMS working groups and workshops. The CTCMS maintains a World Wide Web server (http://www.ctcms.nist.gov) that provides information on Center activities, research results, and software. Each CTCMS working group has a Web page which describes its research agenda, publications, meetings, and advances. In some cases, the CTCMS server has become a tool for confidential information exchange among the participants of a working group. New features, including a web-based calendar and search engine, were implemented.

WORKING GROUPS

The CTCMS forms short-term multidisciplinary and multi-institutional research teams to attack key problems in materials and materials processing. As a first step, CTCMS holds workshops to (1) define technical research areas with significant technological impact, (2) identify team members, and (3) design and build the infrastructure for collaborative research.

This year CTCMS working groups added new members, held group meetings and new workshops, and made numerous, significant advances:

MICROMAGNETIC MODELING

In the area of micromagnetics, modeling efforts are hampered by the fact that different computational methods give different solutions to elementary micromagnetic domain-structure problems. Today's fast workstations now make standardization of methods and solutions possible, and easily accessible to the community. The CTCMS Micromagnetic Modeling group was formed in FY 1996 to address the need for accurate, standardized micromagnetic modeling tools.

In FY 1997, CTCMS co-sponsored researchers from MSEL's Metallurgy Division, NIST's Information Technology Laboratory, IBM, Kodak, and a number of universities continued their efforts to develop interactive computational tools for micromagnetic modeling, provide solutions to standard problems, and conduct benchmark verification. This past year, seven submitted solutions to the first µMAG standard problem were collected and displayed for comparison, both on the CTCMS web page, and at a major international magnetism conference. This was the first time that the solutions of independently developed micromagnetic codes had ever been directly compared, and the results were alarmingly different. As a result, preparations are underway for a second standard problem geared toward finding the borderline conditions where solutions start to deviate.

Significant progress was made in the design and implementation of micromagnetic code for public distribution. The software has been designed to allow the maximum amount of flexibility and modularity for comparing and updating computational techniques. The initial release of µMAG software, "mmdisp," displays and manipulates micromagnetic spin configurations. In January 1998 the group plans to release a full micromagnetic code, "Object Oriented MicroMagnetic computing Framework"(OOMMF). These public domain software tools are available through the CTCMS web server.

GREEN'S FUNCTION LIBRARY

Industrial designers and computational engineers need to reduce the time-cycle of the component design process to remain competitive in today's marketplace. An electronic database of region-dependent Green's functions would allow rapid design modifications of complicated material geometries and reduce the time cycle by weeks. Data storage and input/output capabilities of current computers now make such modern computational tools possible.

The CTCMS Green's Function Group formed following a CTCMS-sponsored workshop in late 1994 on Green's Functions and Boundary Element Analysis for Mechanical Properties of Advanced Materials. Co-funded by CTCMS and the National Science Foundation, the group formed partnerships between researchers at several universities, NIST, PDA Engineering, Gates Rubber Company, Ford, and Motorola. Gates Rubber Company dedicated an employee full-time to this project. Publications from the group can be found on the CTCMS Web Server. The workshop report is available to the public as a NIST special publication.

The group refocused its goals for FY 1997 to develop an interactive, electronic library tool consisting of Green's function and boundary element solutions for standard materials geometries arising in elastostatics, elastodynamics, acoustics and ultrasonics. Several Greens functions were constructed this past year. This tool will be available on the CTCMS web server in FY 1998.

PATTERN FORMATION IN MULTIPHASE LIQUID-CRYSTAL/POLYMER MATERIALS

The performance and properties of devices made from multiphase polymer/liquid crystal materials depend crucially on the microstructure that emerges during processing. Present understanding of the nonequilibrium physics of morphogenesis in these materials is weak. Numerical simulations that implement newly-developed theories of these materials and compare morphologies with experimental morphologies can improve processing and design.

In FY 1997, the CTCMS continued its collaboration with the NSF Science and Technology Center for Advanced Liquid Crystalline Optical Materials (ALCOM) in Ohio to model the kinetic and morphological phenomena arising during processing in these materials. NIST principal investigators include members of the Polymers Division and NIST's Information Technology Laboratory. General Motors, Raychem, IBM, DPix, and Phillips are regular workshop participants.

With sponsorship of the CTCMS, ALCOM and the Department of Library Sciences and Media Services at Kent State University continued development of an interactive web tool for communication and collaboration between participants. This tool now allows researchers to easily and confidentially post experimental and simulation data, images, and comments to the rest of the group. The tool is accessible from the LCP group's home page, and password authentication is required for viewing or entry.

> In collaboration with researchers and their students at UCLA, University of Maryland, and Kent State University, the LCP group implemented a new theory of nonequilibrium isotropic/anisotropic polymer blend materials, and developed software tools for modeling their microstructure and kinetics.

GLASSES AND GLASS-FORMING MATERIALS

Improved understanding of the microscopic physics of disordered and partially-ordered materials is required to make better glass. Recent advances in parallel computing now make previously intractable simulations of these materials possible. Following a workshop organized and sponsored by the CTCMS on Glasses and Glass-Forming Materials: Challenges in Materials Theory and Simulation, a group of researchers from various universities, national laboratories, and NIST formed the CTCMS Glasses group to measure and characterize the microstructure and dynamics of heterogeneities arising in liquids as they form glasses. CTCMS and the Parallel Computation Division at Sandia National Laboratories are co-supporting a postdoctoral researcher on the project. In FY 1997, the Glasses group conducted large-scale massively parallel simulations of standard models of glass-forming systems, and reported a number of startling results that may contribute to our understanding of anomalous structural relaxation and physical aging in glasses. Proceedings from the FY 1996 workshop were published in the journal Computational Materials Science.

SOLDER INTERCONNECT DESIGN

Inspection and repair of solder defects in electrical and optical interconnects is expensive and labor-intensive. As circuits become smaller, the importance of computational tools in integrating design and performance with manufacturing and reliability increases. The electronics industry wants to optimize solder interconnects but lacks tools to predict the performance and reliability of the wide range of geometries used.

In FY 1997 the CTCMS Solder Interconnect Design Team (SIDT) continued to develop and evaluate computational methods and software tools for modeling geometries that arise in solder interconnects. Problems identified by group members that are under current consideration include tombstoning (lifting of a small component off the circuit board), forces on the gull wing lead, solidification of the solder interconnect, reactive wetting (dissolution and the formation of intermetallics), and optoelectronic interconnects.

The group held workshops at the CTCMS attended by team members from the Edison Welding Institute, DEC, Motorola, BOC Gases, Ford Motor Co., Lucent Technology, AMP, Rockwell, Delco, Texas Instruments, Susquehanna University, University of Colorado, University of Massachusetts, University of Wisconsin, University of Loughborough, Lehigh University, University of Greenwich, Marquette University, RPI, University of Minnesota, Sandia, and, of course, NIST.

At the June 1997 workshop, work on a variety of topics was presented spanning the industrial concerns of AMP, TI, Ford, Motorola, and Lucent, as well as exciting new scientific work from many of the team's academic and government partners. A new modeling technology is currently being developed by at U. Greenwich to describe the stresses which develop during the solidification of solder interconnects. This effort also should improve the ease of use of the Surface Evolver, an NSF Geometry Center software tool that underlies the solder tools, and which currently requires substantial specialized expertise. A new model describing the dissolution and spreading of a solder drop over a reactive substrate was developed. CTCMS-supported researchers at the University of Greenwich are examining the buildup of stress during the solidification of optical interconnects, as well as the behavior of the solder-flux paste under reflow. A CRADA with Boeing was established in FY 1997 in conjunction with the ATP program in optoelectronics. It is expected that the research fostered by the SIDT will play an important role in modeling solder interconnects in optoelectronic devices, where solder is used solely as an adhesive.

Public domain software tools developed by the Solder Group are now available on the CTCMS Web server. These tools have improved development and implementation of industrial electronic packaging processes at such companies as Motorola and DEC, and are anticipated to greatly improve cost efficiency. In one case, designers at Motorola were able to prevent component "fall off" while soldering side two of a two-sided board, changing the yield from 20% to 90 %.

In one soldering challenge, a product suffered from “floating and twisting” of every battery contact during soldering, requiring each contact to be repositioned by hand. Using the software and insights gained at the semi-annual NIST Solder Interconnect Design Team meetings, Motorola solved this problem as well.

WULFFMAN: AN INTERACTIVE CRYSTAL SHAPE CONSTRUCTOR

Tools that allow researchers to construct and manipulate complex three-dimensional crystal shapes with varying surface energy anisotropy and arbitrary symmetry can facilitate materials characterization and design. Over the past two years, CTCMS researchers created such a tool, which they named “Wulffman.” This tool is a powerful, interactive module designed to be used with Geomview, a general public-domain software tool developed at the NSF Geometry Center.

Wulffman is available to the public on the CTCMS Web server, and is currently being used by researchers at DuPont to design materials for reflective paints.

OBJECT-ORIENTED FINITE ELEMENT MODELING OF COMPOSITES

Prediction of macroscopic properties from microstructures of composite materials remains a challenging problem in materials science. Interactive public-domain computational tools that enable researchers to calculate such properties from micrographs of real materials are being developed by NIST researchers from MSEL's Ceramics Division and the Information Technology Laboratory under co-sponsorship of the CTCMS. In FY 1997, CTCMS supported a combined experimental and computational program in collaboration with researchers at Northwestern University to investigate residual stresses in highly-textured microstructures in iron titanates, which exhibit very large residual stresses due to thermoelastic anisotropy.

SELECTED CUSTOMER IMPACTS

Advanced Materials

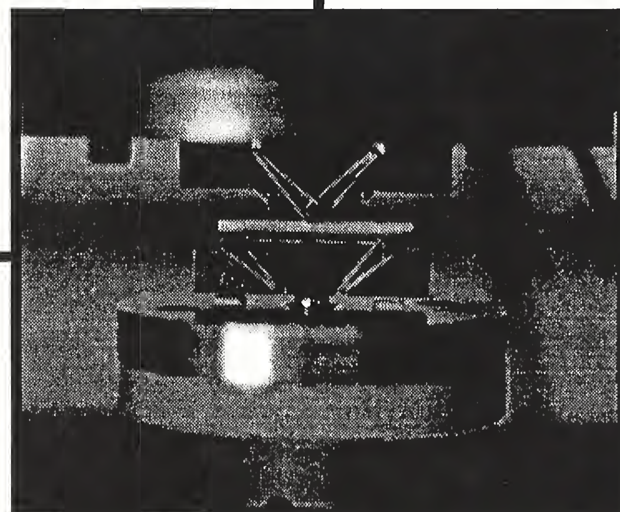
Determination of Flexural Strength of Advanced Ceramics

Problem:

The non-uniformity of existing flexural test methods in the ceramics industry causes problems in materials property data comparisons between companies.

Technical Description:

- Experimental and analytical work quantified sources of experimental error
- MSEL led the development of ASTM and draft ISO standard test methods



Need was determined by:

An interlaboratory round robin study that demonstrated inconsistent results.

Impact:

- Consistent data and testing procedures are available worldwide
- Cost savings in U.S. estimated \$0.8 M - \$1.6M annually
- Test fixtures readily available and at lower costs

Advanced Materials

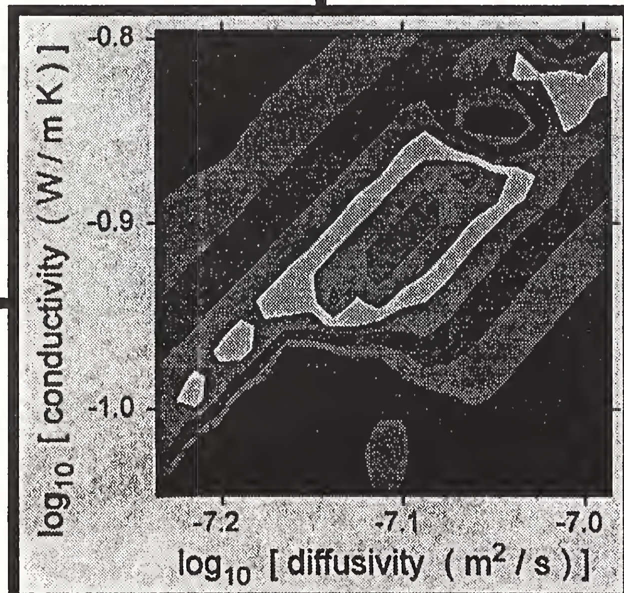
Data for Thermal Management of Polymer Thin Films

Problem:

The electronics and electronic materials industries need thermal property measurement methods for polymeric thin films of electronic packaging materials to meet the challenge of developing smaller packages.

Technical Description:

A method for reliable, simultaneous measurement of thermal conductivity, thermal diffusivity, and interface heat transfer coefficients by laser pulsed methods was developed.



Need was determined by:

Representatives of the microelectronics industry identified thermal property measurement as a key problem during workshops hosted by NIST and during visits to industry by staff.

Impact:

This method enables manufacturers to more accurately design for the dissipation of heat generated by integrated circuits. It also provides data for the transfer of heat across interfaces within electronic packages.

Advanced Processing

Advances in Optical Sensors for Polymer Processing Earns Fed. Lab. Consortium Excellence in Tech. Transfer Award

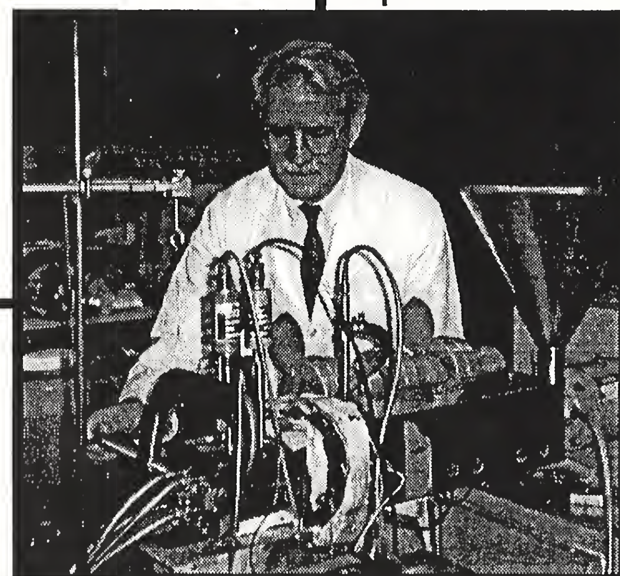
Problem:

Inadequate monitoring and control of polymer injection molding results in lengthy startup times and out-of-spec products.

Technical Description:

Develop a new class of on-line sensors based on optical and fluorescence measuring methods for:

- Resin Temperature and temperature profiles
- Molecular orientation
- Crystallization kinetics
- Heat transfer from the resin to the machine



Need was determined by:

- Workshops hosted by NIST and attended by industry scientists identified measurement and control needs in polymer processing
- Research plan jointly adopted by NIST and industry members of an MSEL-led consortium

Impact:

Sensor and measuring technology transferred to industry:

- 3M Co.- quality of mixing ingredients and temperature measurements
- DuPont Co.- resin temp. profiles
- Mobil Chemical Co.- molecular orientation
- Packard Electric - temperature and molecular crosslinking

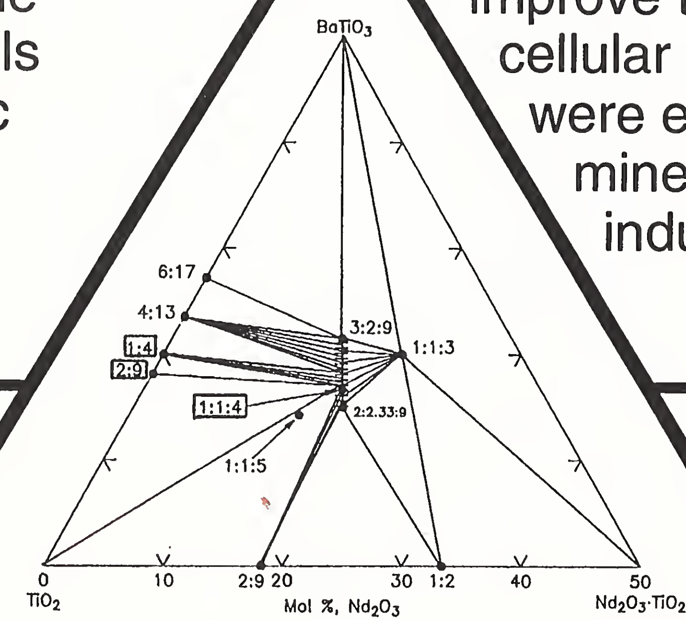
Advanced Processing
Phase Equilibria Studies of Ceramics for Wireless Communications

Problem:

Decreasing size of electronic devices requires phase equilibria data for the selection of materials with better dielectric properties.

Technical Description:

Phase diagrams of titania-based systems that are used to improve the fabrication of cellular circuit components were empirically determined and provided to industry.



Need was determined by:

1995 NIST workshop to identify and prioritize key R&D issues for the commercial wireless market.

Impact:

High-dielectric ceramic magnets are used as circulators and isolators in cellular telephones. Improved fabrication of these magnets increases product reliability.

Advanced Processing

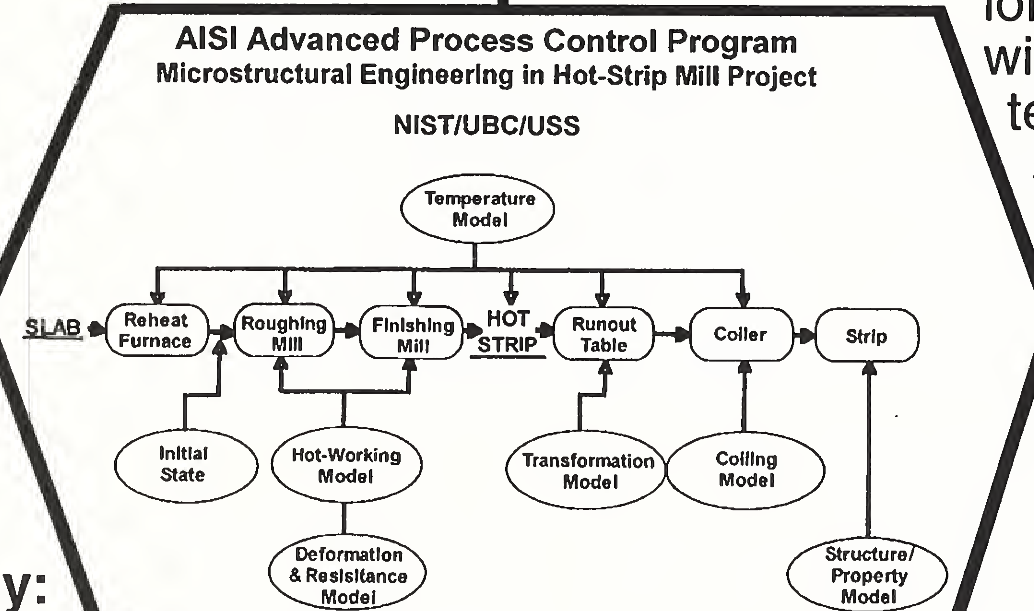
Constitutive Equations for Steels at High Temperatures

Problem:

Computer simulation models and data that relate the properties of steel to processing conditions are needed to develop new, high-performance microalloyed steels.

Technical Description:

Performed research on high temperature, high strain rate mechanical behavior. Provided data for models of the stress-strain behavior of steel for wide ranges of temperature, strain rate, and microstructure.



Need was determined by:

- An MSEL hosted workshop (NISTIR 89-4024) identified this as a critical problem of the steel industry
- Collaborative assessment with AISI and member companies

Impact:

MSEL data for computer simulation of hot rolling has allowed the steel industry to evaluate improved math models to reduce the cost of introducing new alloys.

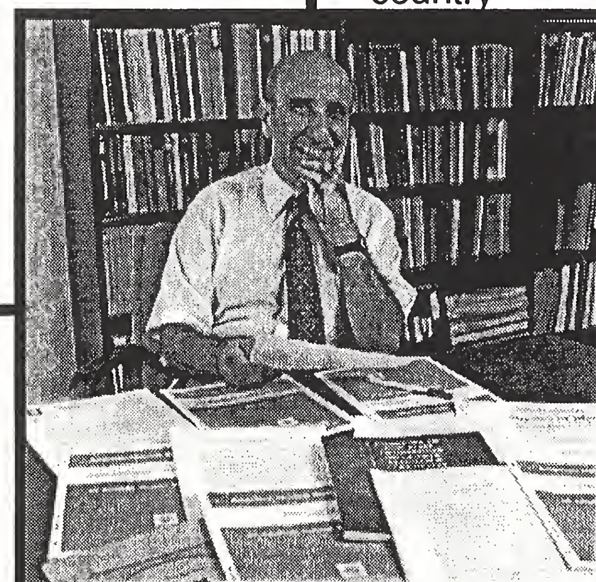
National User Facility
Tawfik Raby Receives ANS Standards Service Award

Problem:

To ensure the public safety, all nuclear reactors require well defined procedures and specifications (e.g. quality assurance, maintenance, limiting conditions for operation).

Why NIST and NCNR:

- The NIST Research Reactor is one of the largest in the country, with an outstanding record of safe cost effective operation, providing a national benchmark.
- Raby was and is recognized as the foremost authority on research reactor operation in this country
- Standards are an integral part of the NIST mission, and the NCNR, as the premier neutron research center in the country, has the responsibility to lead in this area



Solution:

- The American Nuclear Society, working with ANSI, developed a series of standards for all aspects of nuclear reactor operation, including Safety Analysis Reports, Technical Specifications and others
- Raby chaired many of the relevant committees and subcommittees that developed the necessary standards

Impact:

- The standards were adopted by national and international regulatory bodies as necessary and sufficient bases for safe and effective operation
- The adoption of these standards by the many small research reactors around the country resulted in substantially improved operating performance, thus increasing safety margins
- The voluntary nature of the standards, along with the agreement by regulators that they were sufficient, led to increased compliance, with strong peer pressure to conform

TECHNOLOGY TRANSFER

SUMMARY OF CRADA ACTIVITIES

FY 1997

Active Agreements	FY1997
NIST	366
MSEL	86 (23%)*
Industry	72
University	14
Government	0
New Agreements	24
Total Agreements (since 1988)	221

MSEL PARTNERS

Partners	FY1997
Bilateral Agreements	75
NIST-Led Consortia	6
TOTAL	**81**

Multiple Agreement Partners**(since 1988)

AlliedSignal, Inc. (2)
Aluminum Association, Inc. (2)
American Society for Testing and Materials (3)
American Superconducting Corp. (2)
Aristech Chemical Corp. (2)
Armstrong World Industries, Inc (2)
BDM, Inc. (2)
Cercom, Inc. (2)
Crucible Metals Corp. (2)
Dentsply International, Inc. (2)
Dow Chemical Co. (5)
E.I. du Pont de Nemours & Co. (9)
Eaton Corp. (2)
Exxon Research & Engr. Co. (2)
General Electric Co. (6)
General Motors Corp. (10)
Goodyear Tire & Rubber Co. (2)
Grumman Aerospace Corp. (2)
Materials Innovation, Inc. (2)
Michigan Molecular Institute (2)
Minnesota Mining & Manuf. Co. (3M) (3)
National Assn. of Corrosion Engineers (4)
National Center for Manuf. Sciences (2)
Norton Co. (3)
Norton Industrial Ceramics Co. (2)
Pennsylvania State University (2)
Raychem Corp. (2)
Rohm and Haas Co. (3)
Sonoscan, Inc (2)
United Technologies Corp., Pratt & Whitney Division (3)
University of Connecticut (3)
University of Delaware (2)

* MSEL percentage of all active NIST agreements

** Partners with more than one signed agreement. Number in parenthesis indicates total number of agreements since 1988

COOPERATIVE RESEARCH AND DEVELOPMENT AGREEMENTS

FY 1997
Active

ADVANCED MATERIALS

*B = Bilateral CRADA   C = NIST-Led Consortium

PROGRAM	SUBJECT	PARTNER	TYPE*	CONTACT
Ceramic Coatings	Conductivity of Ceramic Thermal Barrier Coatings	Pratt & Whitney	B	Andrew Slifka 303-497-3744
Dental and Medical Materials	Research in Dental and Medical Materials	American Dental Association Health Foundation	B	William Marjenhoff 301-975-6809
Dental and Medical Materials	Orthopedic Accelerated Wear Resistance Consortium	Biomet, Inc. Johnson & Johnson Professional, Inc Osteonics, Inc. Smith & Nephew Richards, Inc Wright Medical Technologies, Inc. Zimmer, Inc.	C	John Tesk 301-975-6799
Electronic Packaging and Interconnects	Solder Jet Science and Technology	MicroFab Technologies	B	Carol Handwerker 301-975-6158
Electronic Packaging and Interconnects	Materials Issues in Precision Optoelectronics Assembly	Boeing Information, Space and Defense Systems	B	James Warren 301-975-5708
Electronic Packaging and Interconnects	Acoustic Measurement of Stress in Microelectric Packaging	Sonix, Inc.	B	E. Drescher-Krasicka 301-975-6141

PROGRAM	SUBJECT	PARTNER	TYPE	CONTACT
High Temperature Superconductivity	Microstructural Modes of Failure of Bi2223-based HTS Composites	American Superconductor Corp.	B	Stephen Freiman 301-975-6119
Magnetic Materials	Magnetic Nanocomposites Derived from Dendritic Hosts	Michigan Molecular Institute	B	Robert Shull 301-975-6035
Magnetic Materials	Development of Computer Software for Corrosion Control	NACE, International (2)	B	Richard Ricker 301-975-6023
Magnetic Materials	Small Angle Neutron Scattering from Complex Fluids	Texaco Research and Development	B	Charles Glinka 301-975-6242
Magnetic Materials	Surface Chemistry of the Contact Recording Head-Disk Interface	Censtor Corporation	B	Stephen Hsu 301-975-6120
Magnetic Materials	Tribology of Magnetic Recording	Digital Equipment Corporation	B	Stephen Hsu 301-975-6120
Mechanical Properties of Brittle Materials	Ceramics for Gas Turbines	General Electric Company	B	Edwin Fuller 301-975-5795
Mechanical Properties of Brittle Materials	Characterization of Dual Purpose Ceramic Membrane Material	BP Chemicals, Inc.	B	Edwin Fuller 301-975-5795

PROGRAM	SUBJECT	PARTNER	TYPE	CONTACT
Polymer Characterization	Viscoelastic Properties of Polymer Materials	Armstrong World Industries, Inc.	B	Edmund DiMarzio 301-975-6773
Synchrotron Radiation Characterization	Materials Characterization Using Synchrotron Radiation	Dow Chemical Co.	B	Daniel Fischer 301-975-5972
Thin Film Measurements and Standards	Characterization of and Process Diagnostics for Optical Memory Phospor Films	ETOM Technologies Corp.	B	John Hastie 301-975-5754
Ultrasonic Characterization of Materials	Stress Measurement in Steel Building Beams and Columns	SonicForce Company	B	Alfred Clark 303-497-3159
Ultrasonic Characterization of Materials	Innovative Ultrasonic Instrumentation and Testing Techniques	RITEC, Inc.	B	Chris Fortunko 303-497-3062
Ultrasonic Characterization of Materials	Gas-Coupled Ultrasonic Inspection Technology	Southwest Research Institute	B	Chris Fortunko 303-497-3062
Ultrasonic Characterization of Materials	Measurement of Texture and Grain Size in Copper, Copper Alloys and Stainless Steel Sheet	Olin Corporation	B	George Alers 303-497-7899

Ceramic Machining	Ceramic Machining Consortium	Cabot Corp. Ceradyne, Inc. Cercom, Inc Chand Associates, Inc.. Cincinnati Milacron, Inc. Eaton Corporation Ford Motor Co. General Electric Co. General Motors Corporation Georgia Tech Research Corporation Heraeus Amersil Inc. Kansas State University Landis Lehigh University Norton Company Stevens Institute of Technology Technology Assessment & Transfer Torrington Co. University of Delaware University of Maryland University of Massachusetts University of Rochester West Advanced Ceramics, Inc.	C	Said Jahanmir 301-975-3671

PROGRAM	SUBJECT	PARTNER	TYPE	CONTACT
Intelligent Processing of Materials	Non-Contact Temperature Measurement	Aluminum Association Inc.	B	George Alers 303-497-7899
Intelligent Processing of Materials	Consortium on Modeling of Casting of Aerospace Metal Alloys	American Foundrymen's Society Auburn University Case Western University General Electric Co. Howmet Corporation Mass. Institute of Technology PCC Airfoils, Inc. Pennsylvania State University Purdue University NASA UES, Inc. University of Alabama University of Arizona University of Illinois Worcester Polytechnic Institute	C	Robert Schaefer 301-975-5961

PROGRAM	SUBJECT	PARTNER	TYPE	CONTACT
Intelligent Processing of Materials	Gas Metal Arc Welding	General Motors Corporation Delco Division	B	Thomas Siewert 303-497-3523
Intelligent Processing of Materials	Application of Weld Sensing and Control to Manufacturing	A.O. Smith Corporation	B	Thomas Siewert 303-497-3523
Intelligent Processing of Materials	Investigation of the Application of Weld Sensing and Control to Automotive Seat Manufacturing	Johnson Controls, Inc.	B	Thomas Siewert 303-497-3523
Intelligent Processing of Materials	On-Line, Non-Destructive Mechanical Properties Measures and Microstructure Engineering in Hot Strip Mills	American Iron and Steel Institute	B	Lydon Swartzendruber 301-975-6034
Metals Data and Characterization	Modeling of the Noise Characteristics of Magnetic Recording Heads	George Washington University	B	Robert McMichael 301-975-5121
Metals Data and Characterization	Corrosion Fatigue of Duplex Stainless Steels	Sandusky International Inc.	B	Mark Stoudt 301-975-6025

PROGRAM	SUBJECT	PARTNER	TYPE	CONTACT
Metals Processing	Nitrogen Additions to Corrosion Resistant Metals	Crucible Materials Corporation Crucible Compaction Metals Div.	B	Frank Biancaniello 301-975-6177
Metals Processing	Optimization of Atomization Head Assembly	Carpenter Technology Corp.	B	Frank Biancaniello 301-975-6177
Metals Processing	Compressibility Measurement and Modeling	IAP Research Inc.	B	Roger Clough 301-975-6143
Metals Processing	Eta-Phase Precipitation and Low Cycle Fatigue in Alloy 706	Wyman-Gordon Co.	B	Richard Fields 301-975-5712
Polymer Blends and Processing	Characterization of PAMAM Dendrimers and Complexes with Biomolecules by Neutron Scatteirng Studies	Michigan Molecular Institute	B	Eric Amis 301-975-6681
Polymer Blends and Processing	Measurements of the Dielectric Properties of Polymer Blends During Extrusion Processing	Chemical ElectroPhysics Corp.	B	Anthony Bur 301-975-6748
Polymer Blends and Processing	Small Angle Neutron Scattering	Eastman Kodak Co.	B	Charles Han 301-975-6772
Polymer Blends and Processing	Phase Behavior of Polyolefin Blends	Exxon Research and Engineering Co.	B	Charles Han 301-975-6772

PROGRAM	SUBJECT	PARTNER	TYPE	CONTACT
Polymer Blends and Processing	Small Angle Neutron Scattering Characterization of Silicon Polymer/Filler Blends	Dow Corning Corporation	B	Alan Nakatani 301-975-6782
Polymer Composites	Testing of Process Simulation Model for Resin Transfer Molding	Grumman Aerospace Corporation	B	Richard Parnas 301-975-5805
Polymer Composites	Composite Civil Structure Consortium Process Simulation Method	Production Products Manufacturing and Sales	B	Fred Phelan 301-975-6761

Numbers in parenthesis indicate the number of same subject agreements

PATENTS

FY 1997

GRANTED

STRATEGIC THRUST	PROGRAM	SUBJECT
Advanced Materials	Dental and Dental Materials	Non-Destructive Method for Determining the Extent of Cure of a Polymerizing Material and the Solidification of a Thermoplastic Polymer Based on Wavelength Shift of Fluorescence F. Wang, K. Lin, R. Lowry (Polymers) Patent No. 5,598,005
Advanced Materials	Metals Processing	Electrochemical Fluidized Bed Coating of Powders C. Johnson, D. Kelly (Metallurgy), two others (non-NIST) Patent No. 5,603,815
Advanced Materials	Metals Processing	Methods and Electrolyte Composition for Electrodepositing Metal-Carbon Alloys C. Johnson (Metallurgy), two others (non-NIST) Patent No. 5,672,262
Advanced Materials	Other	Friction and Wear Resistant Coating for Titanium and its Alloys S. Hsu (Ceramics) Patent No. 5,633,212
Advanced Processing	Intelligent Processing of Materials	Wall Thickness and Flaw Detection Apparatus and Method for Gas Pipelines C. Fortunko (Materials Reliability) Patent No. 5,587,534

STRATEGIC THRUST	PROGRAM	SUBJECT
Advanced Processing	Intelligent Processing of Materials	Apparatus and Method for Monitoring Casting Process T. Siewert, W. Dube, D. Fitting (Materials Reliability) Patent No. 5,589,690
Advanced Processing	Intelligent Processing of Materials	Steel Hardness Measurement System and Method of Using Same G. Kohn, G. Hicho, L. Swartzendruber (Metallurgy) Patent No. 5,619,135
Advanced Processing	Polymer Blends	Method and Apparatus for Measuring the Temperature of a Liquid Medium A. Bur, K. Migler (Polymers) Awarded 08/662,030

PATENTS
FY 1997

PENDING

STRATEGIC THRUST	PROGRAM	SUBJECT
Advanced Materials	Dental and Medical Materials	Improved Monomers for Double Ring-Opening Polymerization with Expansion J. Stansbury (Polymers) Application No. NIST 90-030D (11/2/90) PTO 08/273,753 (7/12/94)
Advanced Materials	Dental and Medical Materials	Pre-Ceramic Polymers in Fabrication of Ceramic Composites J. Antonucci (Polymers), one other (non-NIST) Application No. NIST 95-006 (10/26/94) PTO 08/487,557 (6/7/95)
Advanced Materials	Dental and Medical Materials	Ultra-Low Temperature Neck Bonding Process J. Antonucci (Polymers), one other (non-NIST) Application No. NIST 96-031 PTO 08/660,000 (6/7/96)
Advanced Materials	Dental and Medical Materials	Photoinitiators for Free-Radical and Cationic Polymerization J. Antonucci, J. Stansbury (Polymers), one other (non-NIST) Application No. NIST 95-015 PTO 08/611,786 (3/6/96)

STRATEGIC THRUST	PROGRAM	SUBJECT
Advanced Materials	Dental and Medical Materials	Acid Assisted Cold Welding and Intermetallic Formation and Dental Applications Thereof C. Johnson (Metallurgy), five others (non-NIST) Application No. NIST 95-037D
Advanced Materials	Thin Film Measurements and Standards	The Synthesis of Fine Powder Polycrystalline Bi-Se-Te-, Bi-Sb-Te, and Bi-Sb-Se-Te Alloys for Thermoelectric Applications J. Ritter (Ceramics), one other (non-NIST) Application No. NIST 96-016PA
Advanced Materials	Other	Methods for Welding Cryogenic Alloys T. Siewert, C. McCowan (Materials Reliability) Application No. NIST 95-048D (7/31/95)
Advanced Materials	Other	Friction and Wear Resistant Coating for Titanium and its Alloys S. Hsu (Ceramics), one other (non-NIST) Application No. NIST 94-031 (5/3/94) PTO 08/455,212 (5/31/95)
Advanced Processing	Ceramic Machining	A Chemically Assisted Diamond Machining Process Using Alcohols R. Gates, S. Hsu (Ceramics), three others (non-NIST) Application No. NIST 96-022PA
Advanced Processing	Intelligent Processing of Materials	Acoustic Resonator for Measuring Force G. Alers, W. Johnson (Materials Reliability), one other (non-NIST) Application No. NIST 95-017
Advanced Processing	Intelligent Processing of Materials	Methods for Welding Cryogenic Alloys C. McGowan, A. Clark (Materials Reliability), one other (non-NIST) PTO 08/531,254

STRATEGIC THRUST	PROGRAM	SUBJECT
Advanced Processing	Intelligent Processing of Materials	Texture Measurements Using Reverse Geometry X-Ray Diffraction W. Dube, D. Fitting, T. Siewert (Materials Reliability) NIST 97-026
Advanced Processing	Intelligent Processing of Materials	Prevention of Contact Melting in Arc Welding T. Siewert, R. Madigan, T. Quinn (Materials Reliability) Application No. NIST 93-057 PTO 08/226,040
Advanced Processing	Intelligent Processing of Materials	Sensing of Constant Voltage Gas Metal Arc Welding Process Characteristics to Welding Process Control T. Quinn, B. Madigan (Materials Reliabiltiy) Application No. NIST 95-044PA
Advanced Processing	Intelligent Processing of Materials	Methods for Welding Cryogenic Alloys C. McGowan, A. Clark (Materials Reliability), one other (non-NIST) PTO 08/531,254
Advanced Processing	Polymer Composites	Non-Destructive Method for Determining the Extent of Cure of a Polymerizing Material and the Solidification of a Thermoplastic Polymer Based on Wavelength Shift of Fluorescence F. Wang, R. Lowry, C. Lin (Polymers) Application No. NIST 95-011 (1/9/95) PTO 08/389,823 (2/15/95)

STRATEGIC THRUST	PROGRAM	SUBJECT
Advanced Processing	Ultrasonic Characterization of Materials	Electromagnetic Acoustic Transducer and Methods of Determining Physical Properties of Cylindrical bodies Using an Electromagnetic Acoustic Transducer W. Johnson, G. Alers (Materials Reliability), one other (non-NIST) Application No. NIST 94-004 (10/13/93) PTO 08/285,018 (8/2/94)
Advanced Processing	Ultrasonic Characterization of Materials	Apparatus and Method for Monitoring Casting Process T. Siewert, W. Dube, D. Fitting (Materials Reliability) PTO 08/407,699
Advanced Processing	Ultrasonic Characterization of Materials	Wall Thickness and Flaw Detection Apparatus and Method for Gas Pipelines W. Dube, C. Fortunko (Materials Reliabiltiy) three others (non-NIST) PTO 08/330,592
Advanced Processing	Ultrasonic Characterization of Materials	Non-Contact Method and Apparatus for Inspection of Inertia Welds S. Schaps, A. Clark (Materials Reliability), one other (non-NIST) PTO 08/651,254
Advanced Processing	Other	Alcohols Used for Diamond Machining of Materials S. Hsu (Ceramics)

FY 1997 SRM's IN PRODUCTION*

STRATEGIC THRUST	PROGRAM	SRM#	TITLE
Advanced Materials	Ceramic Processing	1900	Specific Surface Area Si3N4
Advanced Materials	Mechanical Properties of Brittle Materials	2831	Ceramics Hardness
Advanced Materials	Neutron Characterization	2450/2451/2452	Zeolite
Advanced Materials	Polymer Characterization	1482	Polyethylene Molecular Weight Standard
Advanced Materials	Other	1878A	X-Ray Alpha Quartz
Advanced Materials	Other	1879A	X-Ray Cristobalite
Advanced Materials	Other	1990	Ruby Lattice Parameter
Advanced Materials	Other	2092/2094/2096	Charpy V-Notch
Advanced Processing	Metals Data and Characterization	2810	Rockwell C Scale Hardness - Low Range
Advanced Processing	Metals Data and Characterization	2811	Rockwell C Scale Hardness - Mid Range
Advanced Processing	Metals Data and Characterization	2812	Rockwell C Scale Hardness - High Range
Advanced Processing	Metals Processing	1358	Cu and Cr Coating on Steel
Advanced Processing	Metals Processing	1359	Cu and Cr Coating on Steel
Advanced Processing	Metals Processing	1362A	Cu and Cr Coating on Steel
Advanced Processing	Metals Processing	1363A	Cu and Cr Coating on Steel
Advanced Processing	Metals Processing	1364A	Cu and Cr Coating on Steel
Advanced Processing	Other	711A	Glass Viscosity

*During FY97 MSEL had 118 active SRMs for sale. The total number of units sold in FY97 is 4,363 at a cost of $1,550,720.

FY 1997 SRM PROJECTS UNDER DEVELOPMENT

STRATEGIC THRUST	MSEL PROGRAM	SRM TITLE
Advanced Materials	Ceramic Coatings	1984 Tungsten Th. Spray Powder
Advanced Materials	Ceramic Coatings	High Temperature Thermal Conductivity
Advanced Materials	Ceramic Processing	1983 C,N,O in Si3N4
Advanced Materials	Ceramic Processing	8010 Particle Size Sand
Advanced Materials	Mechanical Property of Brittle Materials	2100 Ceramic Fracture Toughness
Advanced Materials	Polymer Characterization	New Polytheylene Standards
Advanced Materials	Polymer Characterization	Nonlinear Fluid for Rheological Measurements
Advanced Materials	Other	640C Silicon X-Ray
Advanced Materials	Other	660A Lab6 X-Ray
Advanced Processing	Ceramic Processing	1004B Particle Size Glass Beads
Advanced Processing	Ceramic Processing	1979 Crystallite Size
Advanced Processing	Intelligent Processing of Materials	Ferrite in Stainless Welds
Advanced Processing	Metals Data and Characterization	Rockwell Diamond Indenter
Advanced Processing	Metals Data and Characterization	Rockwell B Scale Hardness - Low Range
Advanced Processing	Metals Data and Characterization	Rockwell B Scale Hardness - Mid Range
Advanced Processing	Metals Data and Characterization	Rockwell B Scale Hardness - High Range

STRATEGIC THRUST	MSEL PROGRAM	SRM TITLE
Advanced Processing	Metals Processing	Zn on Steel
Advanced Processing	Metals Processing	Gold Microhardness Standard
Advanced Processing	Metals Processing	White Case Iron
Advanced Processing	Metals Processing	Stainless Steel, AISI 446
Advanced Processing	Metals Processing	Inconel 625

STANDARD REFERENCE DATABASES

MSEL developed 8 databases that contain information about materials properties. Seven of these databases are available through the NIST Standard Reference Data Program. A list of databases currently available through this venue and a brief summary of their contents are provided below. A polymer composite database was recently completed and will be available during FY98. More detailed information about the content of these databases and how to acquire them is provided through the at the following e-mail address: http://www.nist.gov/srd/srd.htm#nsrds.htm.

- **NIST/Sandia/ICDD Electron Diffraction Database**
  Designed for phase characterization obtained by electron diffraction methods, this database and associated software permit highly selective identification procedures for microscopic and macroscopic crystalline materials.

- **NIST/NRIM High Temperature Superconductors Database: Version 2.0**
  The database of materials properties provides evaluated property data for high temperature superconductors. The range of materials covers the many series of compounds derived from the Y-Ba-Cu-O, Bi-Sr-Ca-Cu-O, Tl-Sr-Ca-Cu-O and La-Cu-O chemical families, along with numerous other variants of the cuprate and bismuthate, and borocarbide materials that are known to have superconducting phases.

- **Phase Equilibria Diagrams Database: Version 2.1**
  The software permits searches for diagrams by chemical system, author, or year of publication. The database includes all diagrams from Volumes 1-10, annual volumes for 1991-93, and Phase Equilibria Diagrams (PED) for High-Tc Superconductors in the PED series.

- **NIST Structural Ceramics Database Version 2.0**
  Version 2.0 contains thermal, mechanical, and corrosion properties of silicon carbides and silicon nitrides in a self-contained database system that operates on DOS-based personal computers. This database contains state-of-the-art materials property data for both research and commercial grades of silicon carbides and silicon nitrides.

- **NACE/NIST Corrosion Performance Databases and Expert Systems**
  Corrosion databases and expert systems developed under the NACE-NIST Corrosion Data Program give users reference data for general guidance on the performance of engineering materials in corrosive environments.

    - **COR·SUR®** 1 includes data for 25 common metals for exposures in over 1,000 corrosive environments at various temperatures and concentrations.

    - **COR·SUR®2** provides similar data for 36 nonmetallic materials (elastomers, polymers, composites, thermoplastics, etc.) in over 850 environments.

- **NIST Crystal Data**
  NIST Crystal Data contains chemical, physical, and crystallographic information useful to characterize more than 210,403 inorganic and organic crystalline materials. The data include the standard cell parameters, cell volume, space group number and symbol, the calculated density, and classification by chemical type, chemical formula, and chemical name. Each entry has an associated literature reference.

APPENDICES

HONORS AND AWARDS

FY1997

DEPARTMENT OF COMMERCE AWARDS

GOLD MEDAL (Exceptional Service)

Reactor Operations and Engineering Group (Single Organizational Award)	for cost effective operation and management of the NIST Research Reactor as a national resource for neutron based measurements in science

SILVER MEDAL (Meritorious Service)

Charles Glinka	for leadership in developing at NIST the foremost facilities in the United States for neutron small angle scattering measurement.

BRONZE MEDAL (Superior Service)

Sharon Glotzer **Andrew Roosen** **W. Craig Carter** **James Warren** **(Group Award)**	for their major contributions to the creation of the Center for Theoretical and Computational Materials Science.

SAMUEL WESLEY STRATTON AWARD (Outstanding Scientific or Engineering Achievement)

Wen-Li Wu	for pioneering research in the use of X-ray and neutron reflectivity to study the molecular-level structure of thin polymer films on solid substrates.

WILLIAM P. SLICHTER AWARD (Outstanding Achievements in Building or Strengthening Ties Between NIST and Industry)

Francis Wang **Kalman Migler** **Anthony Bur**	for their developing and transferring to industry measurement methods based on fluorescent probes to monitor properties of polymers critical to their effective processing

EXTERNAL AWARDS

Charles Bouldin	Japan Atomic Energy Research Institute "Senior Research Fellow" Award
A. Bur	Federal Laboratory Consortium Award for Excellence in Technology Transfer
John W. Cahn	Doctor Honoris Causis, Universite d'Evry, France
Ared Cezairliyan	ASME International (Heat Transfer Division) Yeram S. Touloukian Award (to recognize outstanding contributions to the field of thermophysical properties) for distinguished achievement in thermophysics especially through pioneering development of ultrahigh-speed dynamic techniques for thermophysical properties measurements
Stanley J. Dapkunas	1997 ASM International Fellow Award
Stephen W. Freiman	Induction into the Georgia Institute of Technology's Academy of Distinguished Engineering Alumni
Said Jahanmir	Society of Tribologists Lubrication Engineer (STLE) 1997 International Award
Christian E. Johnson	For outstanding scientific contributions that have advanced the theory and practice of electroplating, metal finishing and allied arts
Ralph Napolitano	Sigma Xi Doctoral Dissertation Award (Georgia Institute of Technology) for the best PhD thesis during the academic year 1996-1997
R.E. Schramm **A.V. Clark**	Outstanding Paper Award from ASNT for paper titled, "Ultrasonic Measurement of Residual Stress in Rims and Inductively Heated Railroad Wheels"
T.A. Siewert	Best Program Award given by the James F. Lincoln Arc Welding Foundation. Award received for design of a procedure to repair the precision support track for the hydrodynamic test carriage at the Naval Surface Warfare Center in Bethesda, Maryland
T.A. Siewert **C.N. McCowan**	First Place Award at the Annual Meeting of the American Welding Society for their poster on a new welding electrode composition for cryogenic applications

STANDARDS COMMITTEES MEMBERSHIP

FY 1997

MSEL Unit	Staff	Memberships
Laboratory Office	1	5
Office of Intelligent Processing of Materials	0	0
Ceramics	14	64
Materials Reliability	7	16
Polymers	10	33
Metallurgy	18	79
NIST Center for Neutron Research	2	2
	53*	207

*Includes 26 leadership positions

Representation

Organization
American Chemical Society (ACS)
American National Standards Institute (ANSI)
American Nuclear Society (ANS)
American Society for Testing and Materials (ASTM)
American Society for Testing and Materials/Society of Automotive Engineers (ASTM/SAE)
American Welding Society (AWS)
Compressed Gas Association (CGA)
Electronic Industries Association (EIA)
European Thermophysical Properties Committee (ETPC)
Initial Graphics Exchange Specification/Product Data Exchange Specification (IGES/PDES)
Institute of Electrical and Electronic Engineers (IEEE)
International Institute of Welding (IIW)
International Organization for Standardization (ISO)
National Association of Corrosion Engineers (NACE)
Safety Glazing Certification Council (SGCC)
Technical Association of the Pulp and Paper Industry (TAPPI)
Versailles Project on Advanced Materials and Standards (VAMAS)

National Institute of Standards and Technology

Organizational Chart