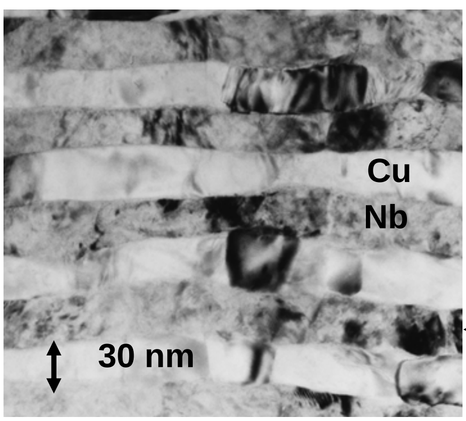
Materials Science & Technology Division

Structure/Property Relations Group

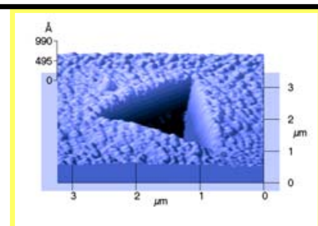
MST-8

Anna K. Zurek, Group Leader
Mark A. M. Bourke, Deputy Group Leader
Dorothy Lucero, Business Manager

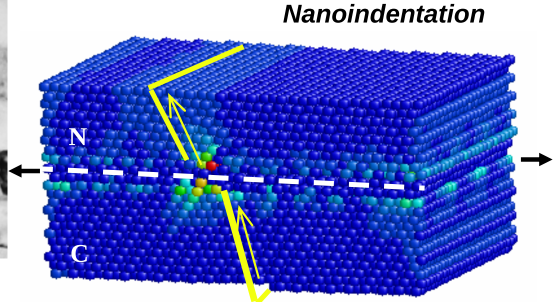
[LAUR 05-0996]



Deformed CuNb after 55% rolling reduction. Initial layer thickness 40nm.



Nanoindentation



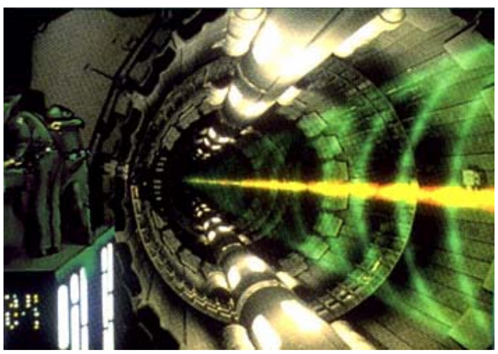
Theory and atomistic modelling

MST-8 Structure/Property Relations

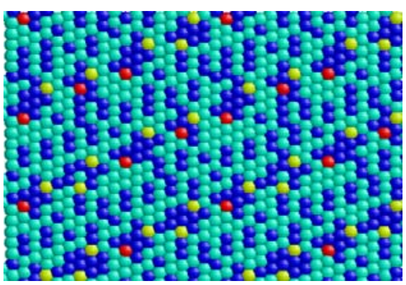
- Experimental Mechanics
- Dynamic Materials Properties
- Ion solid interactions
- Radiation Damage effects
- Optical materials
- Nuclear fuel materials
- Nanoscaled Materials
- Multiscale modeling
- Atomistic & mesoscale simulation
- Materials/Process Simulation
- Neutron & Synchrotron X -ray Scattering
- Scanning Probe microscopy
- Electron Microscopy
- Ion Implantation and analysis
- Single Crystal Synthesis

Anna Zurek, Group Leader

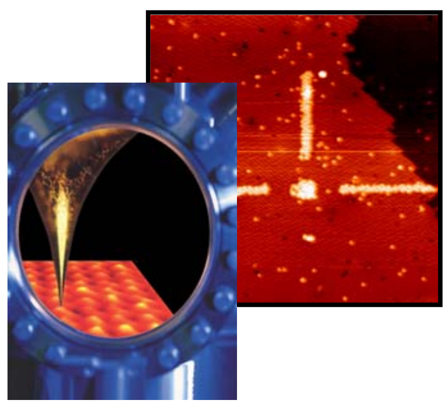
Gas guns: High strain-rate testing



3MV Tandem accelerator



Atomistic simulations



UHV scanning-/tunneling-microscopy lithography

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CONTENTS

MISSION

The mandate of the Structure/Property Relations Group, MST-8 (a group within the Materials Science and Technology Division at Los Alamos National Laboratory) is evaluation and prediction of the relationships between property and structure for length scales ranging from atomistic through microstructural to macroscopic. The group hosts a broad suite of state-of-the-art experimental methods which are complemented by a comparable modeling effort. Including approximately 110 members, the group encompasses six teams and two user facilities. The teams are Dynamic Materials Properties, Materials and Process Simulation, Ion/solid Interactions and Interface Engineering, Mechanical Performance (Prediction and Measurement), Alloy Theory, and Science of Defects. The two facilities are Scanning Probe Microscopy and the Ion Beam Materials Laboratory (which will be home to a new $2M ion implanter in 2006).

Focus areas include computational science, radiation tolerant ceramics, single crystal synthesis, multilayers, high-temperature structural materials, optically functional materials, and metastable and amorphous materials. Most areas of interest transcend the team structure, for example, the study of near-surface phenomena and thin films of materials ranges from ion-modified films (for tribological enhancement) to multilayered, nanostructured materials (that possess high strengths). Studies of the role of defects in materials, pursued using an ion implanter, allow inferences to be made about the radiation resistance of classes of ceramic materials. Several teams avail themselves of synchrotron x-ray and neutron scattering for characterization; indeed, MST-8 is responsible for operating one of the spectrometers at LANSCE.

Another scientific focal area is predictive capability for the constitutive performance, over a range of strain rates and temperatures, of polycrystalline materials. Experimental capabilities in this arena include the ability to perform stress-strain tests at strain rates from 10^{-3} to 10^{6} and at temperatures from -200 to 1900^{o}C. The commensurate evaluation of macroscopic flow under various conditions benchmarks polycrystalline constitutive performance codes. Collection of mechanical property data is performed for the US Department of Energy (DOE) weapons program, as well as for other governmental defense and civilian customers.

Principle MST-8 customers include DOE defense programs, Office of Basic Energy Science (OBES), Department of Defense (DoD) and Laboratory Directed Research and Development (LDRD). Major sponsors include the Advanced Strategic Computing Initiative (ASCI), Advanced Fuel Cycle Initiative (AFCI), and Enhanced Surveillance (EH). The MST-8 operating budget in fiscal year 2004 was approximately $25.4 M. MST-8 is the landlord for the Materials Science Laboratory building (Technical Area 3, Building 1698) and provides administrative services for its community.

STAFF

Group Leadership

Anna Zurek
Group Leader

Anna received a PhD in materials science from The University of Texas at Austin in 1981. Anna was a staff member at Rockwell Science Center from 1981 to 1985 and an MST staff member from 1985 to 2002. She joined the MST-8 group leadership team in March 2002. Anna's technical interests include physical metallurgy, high-strain deformation, fracture characterization and modeling. She is author or co-author of over 115 publications and over 60 invited presentations.

Mark Bourke
Deputy Group Leader

Mark received a PhD in mechanical engineering and bachelor's degree in physics both from Imperial College, London University in the United Kingdom. Before coming to LANL, he worked for the atomic energy research establishment (Harwell) for 5 years. He began his career at LANL in 1990 as a postdoctoral fellow working at LANSCE. Prior to becoming deputy group leader in MST-8 he was a team leader of the mechanical performance team. In the late 90s he was principal investigator (PI) on a project designing and constructing the new $4.5M Spectrometer for MAterials Research at Temperature and Stress (SMARTS) for characterization of structural engineering materials at LANSCE. Mark's research interests include measurement and prediction of residual stress, metallurgy and processing effects, constitutive performance prediction, x-ray, and neutron scattering. He is author or co-author of more than 150 papers.

Team Leadership

John Bingert
Team Leader
Dynamic Properties

John is team leader for the dynamic properties team. He received an MS in metallurgical engineering from Colorado School of Mines in 1990. John's research has included deformation processing, high-temperature superconducting fabrication, ferrous metallurgy, hydrostatic extrusion, and powder metallurgy processing. Current interests include texture characterization, plastic anisotropy, and microstructure quantification. John completed a two-year external change-of-station to the Naval Research Laboratory in 2003 during which he focused on image-based modeling and friction-stir welding research, and remains active in DoD programmatic work. He is the coauthor of over 40 peer-reviewed publications and the recipient of six patents related to advanced materials processing.

Marilyn E. Hawley
Team Leader
Scanning Probe Microscopy

Marilyn received her Ph.D. in 1986 from The Johns Hopkins University and Argonne National Laboratory. She is founder and team leader for the Scanning Probe Microscopy Laboratory. She built one of first low-temperature electron vacuum tunneling devices to measure energy gaps superconductors and successfully measured the gap in Beta-(ET)2AuI2, an organic superconductor, and was one of the first to measure the gap in LaSrCuO3 and Yba2Cu3O7 (YBCO) high temperature superconductors. Using

Scanning Tunneling Microscopy (STM), she was the first to image the spiral growth and pinning mechanism in YBCO films. Those results appeared on the cover of SCIENCE (ranked in top 10 physics citations 4/93 and has been cited over 340 times). Her scanning probe work includes studies that cover a broad spectrum of materials that includes metals, semiconductors, superconductors, complex oxides, and polymers. She has over 100 publications including 2 book chapters. She presently leads a LDRD-DR solid-state quantum computer project, which includes fabricating atomic-scale spin arrays using ultra-high vacuum STM lithogaphic techniques and developing a unique 0.4K photoluminescence spectrometer with 7T magnet, NMR and ESR spin manipulation capabilities, and optical access. Marilyn is also a member of the Quantum Institute steering committee at Los Alamos National Laboratory.

George Kaschner

Team Leader *(acting)*

Mechanical Performance: Prediction and Measurement

After completing a six-year tour in the U.S. Navy including duty as an instructor at the nuclear power prototype (A1W) and as a nuclear-qualified electrical operator on the submarine USS Shark (SSN591), George worked as a quality control engineer at Tekna, a world leader in innovative SCUBA equipment. Returning to academic pursuits at the University of California at Davis, he received his BS in applied physics, then an MS and PhD both in materials science and engineering. George's research activities have included superplastic deformation, cyclic fatigue, and biomedical materials. Current interests include twinning in low-symmetry metals, mechanical properties of plutonium alloys, and knowledge capture of plutonium technology.

Mike Nastasi

Team Leader

Nanoscale Materials and Ion-Solid Interactions

Mike received a PhD in materials science and engineering from Cornell University in 1986. Appointed a LANL Fellow in 2000, he received the LANL Fellows Prize in 1995, and an R&D 100 Award in 1997. He was appointed an executive officer of The Bohmische Physical Society in 1997, was a member of the editorial board of Nuclear Instruments and Methods in Physics Research, Section B *from 1997-2004,* principal editor for J. of Materials Research *from 1997 to 2000, and chair of the* MRS Bull *publications subcommittee from 1994 to 1999. Mike has been a member of International Meeting Committee on Ion Beam Modification of Materials since 1995, and was chair of the editorial board of* MRS Bull *from 1996 to 1999. Mike is an adjunct professor for the University of Colorado, Arizona State University, and the University of Maryland.*

Ricardo Schwarz

Team Leader

Alloy Theory

Ricardo received a PhD in physics from the University of Virginia at Charlottesville and an associate degree in materials science from the California Institute of Technology, Pasadena, California. Ricardo is a LANL Fellow, ASM International Fellow, a invited lecturer of the Morrison Memorial Lectures (McMasters University, 1995). His current research interests include bulk metallic glasses, crystal plasticity, ultrasonic characterization of solids and thin films, hydrogen storage in alloys, and pressure-induced phase transformations.

Kurt Sickafus

Team Leader

Science of Defects in Materials

Kurt's areas of specialization are materials science, ceramic science, solid state chemistry, electron microscopy, and radiation damage in materials. Kurt's research at LANL has been funded primarily by OBES Division of Materials Sciences & Engineering. He has served as long-time project leader for an OBES program concerning radiation damage effects in ceramics. In recognition for his research on this project and specifically for his co-discovery of a large class of oxide ceramic materials highly resistant to radiation damage, Kurt was awarded the

LANL Fellows Prize in 2001. In further recognition of Kurt's contributions to the science of radiation effects, Kurt was recently invited to membership on the advisory editorial board of the Journal of Nuclear Materials. *Kurt is an adjunct professor at New Mexico Tech and an Instructor at the University of New Mexico, Los Alamos.*

Yong Wang
Team Leader
Ion beam materials Laboratory
Yong received a PhD in nuclear physics and technology from Lanzhou University in China in 1992. He came to LANL in 2003 after managing the ion beam analysis facility at the University of Minnesota for nearly six years. Yong's primary research interest is in materials analysis, modification, irradiation, and synthesis using energetic ion beams. He is currently a co-principal investigator on two Center for Integrated Nanotechnologies Jump Start Projects. He is the author/coauthor of more than 50 peer-reviewed publications, three book chapters, and one US patent, and he has organized two technical sessions for International Conference Series on Application of Accelerators in Research and Industry on ion beam analysis.

Alek Zubelewicz
Team Leader
Materials and Process Simulation
Alek received a PhD in applied mechanics from the Technical University of Warsaw, Poland. He is a former senior engineer with Motorola, and with IBM, where his focus was in reliability engineering. Alek was an adjunct professor at the State University of New York, a research scientist in the Departments of Civil Engineering and Materials Science at Northwestern University, and an assistant professor at the Polish Academy of Science.

MST-8 Organization Chart (as of January 2005)

MST-8
Structure/Property Relations

Anna K. Zurek, Group Leader
Mark Bourke, Dep. Group Leader
Dorothy Lucero, Business Manager

Christina Martinez
Michael Naranjo
James Gurule

Teams

Alloy Theory
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- Jose Archuleta
- Steve Conradson
- Rafael Howell
- Douglas Safarik
- Tong-De Shen

Dynamic Materials Properties
John Bingert

- Mike Bange
- Tom Bell
- Bill Blumenthal
- Carl Cady
- Ellen Cerreta
- Reynaldo Chavez
- Shuh-Rong Chen
- George Gray (Fellow)
- Benjamin Henrie
- Benito Jacquez
- Richard Korzewka
- Veronica Livescu
- Mike Lopez
- Thomas Mason
- Phillip Rae
- Hakan Sencer
- Pei-Ling Sun
- Carl Trujillo
- Qing Xue
- Clarissa Yablinsky

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- Michael Baskes
- Petrica Cristea
- Chaitanya Deo
- Juan Carlos Ramirez
- Srini Srivilliputher
- Marius Stan
- Steve Valone

Mechanical Performance: Prediction & Measurement
George Kaschner (Acting)

- Don Brown
- Ron Ellis
- Fred Kocks (ret. Fellow)
- Ricardo Lebensohn
- Saiyi Li
- Cheng Liu
- Manuel Lovato
- Sivasambu Mahesh
- Tarik Saleh
- Thomas Sisneros
- Mike Stout
- Carlos Tomé

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Mike Nastasi

- Ivan Afansyev
- Caleb Evans
- Richard Hoagland
- Tobias Hoechbauer
- Luiz Jacobsohn
- Jung-Kun Lee
- Amit Misra
- Lin Shao
- Greg Swadener
- Eric Vandersen
- Yun-Che Wang
- Xinghang Zhang

Science of Defects in Materials
Kurt Sickafus

- Bryan Bennett
- Darrin Byler
- Wayne Cooke
- Gerald Egeland
- Gene Gosnell
- Stuart Maloy
- Ken McClellan
- Ross Muenchausen
- Chris Stanek
- Ming Tang (Affiliate)
- James Valdez
- Blas Uberuaga
- Chris Wetteland

Facilities

Ion Beam Materials Laboratory
Yongqiang Wang

- Gene Gonsnell
- Mark Hollander
- Carl Maggiore (Assoc.)
- Joe Tesmer (Assoc.)

Scanning Probe Microscopy
Marilyn Hawley

- Kiran Chitanvis
- Geoff Brown
- Holger Grube
- Robert Houlton

- Jim Smith
- Terry Mitchell (ret. Fellow)

Staff
Post Docs
Techs
Students
Office Support

[Jan-2005]

TEAMS

Alloy Theory Team

The alloy theory team works mainly in the area of synthesis. Historically the focus of this work has been on amorphous and metastable systems. Currently the focus includes nanocrystalline materials. The work is complemented by a wide variety of characterization tools, including x-ray diffraction, density measurements, differential scanning calorimetry, thermogravimetric analysis, magnetic moment, coercivity, losses under AC excitation, resonant ultrasound spectroscopy (to measure elastic constants), thermal expansion, mechanical properties, physical vapor deposition of thin films, and elastic properties of thin films by Rayleigh wave-propagation. Areas of excellence for the team include mechanical alloying through ball milling and elastic constant measurement from scanning resonant waves. (*For recent literature see p17)*

Dynamic Materials Properties

The dynamic materials team encompasses a spectrum of experimental and modeling programs that systematically quantify the influence of variables such as strain rate, temperature, stress state, processing microstructure, and alloy content on the constitutive behavior, damage evolution, fracture, and fragmentation of materials that include polymers, metals, and alloys. The team is actively involved in developing and validating constitutive models describing the mechanical behavior of weapons materials including beryllium, uranium, and plutonium (part of the ASCI program). The majority of materials under study are of interest to the DoD and DOE. Experimental tools include gas guns, Taylor anvil facilities, and a Hopkinson bar as well as orientation imaging microscopy.

Recent activities include quantification of the influence of interstitial content and niobium alloy content on mechanical behavior of wrought uranium and uranium-niobium alloys**, c**haracterization and modeling of the influence of manufacturing on constitutive response, and support of the hydro test program through constitutive data and models**;** investigation of the constitutive response of uranium-alloy as a function of stress state; and quantification of the influence of shock pre-straining on post-shock mechanical behavior, damage evolution, and propensity to strain localization / fragmentation. A new avenue of research has been on quantification of the influence of temperature and strain rate on the constitutive response of structural polymers and binders in energetics. (*For recent literature see p18)*

Materials and Process Simulation

The materials and process simulation team provides expertise in modeling and simulations for LANL strategic materials across length scales that comprise atomistic, nano, meso, and the continuum. Customers include enhanced surveillance, BES, and the AFCI programs. Research areas include; shock dependent kinetics models for polymers and porous materials, phase stability in alloys and ceramics, kinetics of chemical reactions under shock loading, heat and mass transfer modeling and simulations, fracture mechanisms in ductile materials, and a new theory of non-local plasticity in application to static and dynamic loading conditions. One focus has been on aging and phase stability of plutonium alloys. This has lead to the development of plutonium/gallium/helium potentials and the first plutonium-gallium phase stability diagram obtained from first principles. Typically tools include molecular dynamics, the CALPHAD, SOLGASMIX method, and Truchas (casting simulation software).

A considerable BES-funded effort is focused on atomistic simulations and the development of interatomic potentials for atomic level calculations of bulk properties, surfaces, dislocations, grain boundaries and solid/solid or solid/liquid phase transformations. From these calculations estimates of properties for longer length and time scales can be made. This work complements experimental research for the advanced fuel cycle initiative (AFCI) on nuclear fuels most notably in the development of iron/hydrogen/helium potentials pertaining to models of reactor radiation damage. (*For recent literature see p21)*

Mechanical Performance: Prediction and Measurement

Activities in the mechanical behavior team include fundamental studies of slip, twinning, creep, grain refinement, and grain rotation. Experimental work is typically complemented by elastoplastic and viscoplastic self consistent models. The fundamental goal is a description of how microstructures and deformation processes evolve collectively. The scope includes length scales from atomistic, thru nano, and micro, to macroscopic. Deliverables are typically validated, predictive capability of macroscale mechanical response in polycrystalline metals; although there has also been considerable work developing a constitutive model for PBX 9501 in which energetic crystals of PDX are embedded in a polymeric binder. Current models that predict constitutive performance are limited by the inherent granularity of the system and the grossly disparate mechanical behavior between the binder and the energetic crystals. However, a new two-phase composite model, incorporating but not limited to a correlation function, size distribution and volume fractions, has been developed which is being applied to constitutive performance prediction of explosive and binder over a range of thermo-mechanical conditions.

There is a close synergy with the dynamic materials team in the efforts to develop constitutive equations describing the mechanical response under a wide range of strain, temperature, and strain-rate regimes. This resulted in the Mechanical Threshold Strength model which is now widely used in Los Alamos and also in other research institutions worldwide. Recently this team incorporated experimental evidence about dislocation structures and their evolution into polycrystal models to predict the mechanical response associated with strain path changes.

Studies on “shape memory” super-elastic and thermo-elastic nickel-titanium and nickel titanium with titanium carbide reinforcement have shown for the first time the texture evolution of the stress-induced phase. This work has recently been complemented by new studies of the shape memory effect in uranium 7 wt% niobium. Model descriptions of twinning have been added to the visco-plastic self consistent models and shown to predict the constitutive performance of clock-rolled zirconium deformed under a variety of temperature and strain rate conditions. The phenomenology is being extended to other systems including magnesium and uranium 6 wt% niobium.

One unique element of the team’s activity is the use of SMARTS (Spectrometer for MAterials Research at Temperature and Stress) and HIPPO (High Intensity Pressure and Preferred Orientation), two state-of-the-art neutron diffractometers located at LANSCE. These unique instruments make non-destructive measurements of bulk averaged microstructural deformation and texture evolution. *In situ* deformation studies on composites such as titanium with silicon carbide, aluminum with titanium carbide (particulate), dispersion strengthened nickel aluminide with alumina particluate, nickel titanium with titanium carbide reinforcement, copper molybdenum, tungsten carbide cobalt, and gamma gamma prime nickel base superalloys have provided insights about co-deformation behavior and quantified the effects of residual stress on macroscopic performance. (*For recent literature see p22)*

Nanoscale Materials and Ion-Solid Interactions

The primary focus of the team is to explore the structure-property relations in nanoscale materials using a synergistic approach that integrates nanoscale synthesis via physical vapor deposition or ion implantation, characterization via nanomechanical testing, high-resolution TEM, ion-beam analysis, and atomistic modeling.

One focus area of this team has been to explore how to control and utilize the stresses which are developed from ion-solid interactions. Measurements of the intrinsic stress in thin films formed by ion-assisted deposition showed that it is strongly influenced by grain boundaries, vacancies, interstitials, and dislocations. An atomic interaction model has been developed to explain the effect. Moreover the stress generated by radiation defects produced during the ion implantation of hydrogen into silicon promotes the formation of hydrogen-planar defects. The stress and resultant strain facilitate the nucleation and growth of hydrogen platelets on planes normal to the ion-implantation direction. The platelets grow and lead to cleavage of the silicon. However, we have discovered that ion implantation increases the fracture toughness, which affects the location of the cleavage plane. This process can be applied to integrate a thin monocrystalline layer onto a secondary wafer without the restriction of lattice-matching between the transferred layer and the secondary wafer, which is an inherent problem in making heterostructures by traditional deposition techniques. Also, we are enhancing the functionalities to optical and magnetic materials using ion implantation, which takes advantage of the fact that virtually any element can be implanted into any substrate independent of thermodynamic factors, thus making it possible to incorporate active dopants into host materials well beyond the limits of equilibrium solid solubility, thereby allowing for the production of novel materials that cannot be synthesized by conventional means.

Another focus of this team are the anomalous mechanical properties that result in nanostructured materials from reductions in the characteristic length scales, Using a combination of microscopy and atomistic modeling, we are exploring dislocation motion and interactions and the role of interfaces in blocking, storing, and/or annihilating dislocations. Since nanostructured materials exhibit unusual, and, in some cases, unique deformation mechanisms, we are exploring their fatigue resistance under cyclic loading conditions and their ability to tolerate radiation damage without loss of structural integrity.

Finally, we are synthesizing and characterizing quantum dot structures, whose optical and magnetic properties are controlled by quantum confinement effects, allowing us to study optical-band tuning and magnetic anisotropy. We are also exploring the combination of conventional photonic crystal nanostructures with “active” materials and/or elements that exhibit nonlinear-optical, electro-optical, piezo-electrical, or electro-mechanical properties. Such structures can, in addition to the passive manipulation of light, provide “active” functions such as optical amplification, lasing, light switching and steering, optical logic, and chemical sensing. (*For recent literature see p24)*

Science of Defects in Materials

The science of defects team has three thrust areas: fundamental studies of radiation effects, optical materials studies and support for the advanced fuels cycle initiative. The common themes to these activities are the Crystallography and microstructure of materials particularly as they relate to radiation damage. In this context team capabilities include the synthesis and fabrication of complex oxide ceramics ion beam irradiation and characterization using a suite of tools including but not limited to TEM, x-ray diffraction, and ion-beam analysis.

The first major element is to develop an understanding of the radiation damage response of materials (ceramics and metals) exposed to neutrons or other energetic particles. The objectives are twofold: (1) to predict microstructural evolution in materials exposed to radiation; and (2) to identify the physical aspects of materials that are effective in promoting radiation resistance. Particle irradiation experiments are complemented by atomistic computer simulations. Recently, the team has combined density functional theory, molecular dynamics, and temperature-accelerated dynamics to demonstrate how irradiation-induced defects evolve over long timescales. Ultimately, the work is aimed at finding application to existing fission reactors, future fusion reactors or accelerator-based reactors, or as actinide-host ceramic fuelforms and wasteforms. Many of the compounds of interest have proven to be suitable hosts for actinide species (thallium, uranium, plutonium, etc.) as well as other radiotoxic nuclides, including fission products.

Finally the team has several initiatives relating to AFCI. These initiatives are underpinned by a new materials-characterization laboratory rated for handling depleted uranium. The capabilities it engenders have relevance to LANL initiatives in AFCI and space-fuel initiatives. The laboratory is certified for processing depleted uranium–containing oxides and nitrides and comprises a suite of state-of-the-art characterization tools. These tools include particle-size analysis, thermo-gravimetric analysis, thermo-mechanical analysis, and pycnometry. Two LECO chemical-analysis units provide carbon-sulfur and oxygen-nitrogen analyses. Controlled-atmosphere glove boxes and high-temperature furnaces enable synthesis and fabrication. The ability to handle depleted uranium has lead to a strong relationship between MST and the Nuclear Materials and Technology Division.

The team also addresses optical materials with a focus on developing novel materials with characteristics suitable for a wide variety of detectors. This subset of the team, headed by Wayne Cooke, uses a wide suite of capabilities to explore optical properties. Research and development of optical materials requires fundamental understanding of the underlying mechanisms responsible for absorption and emission of light. Current research is focused on fabrication and characterization of inorganic nanomaterials, especially rare-earth doped oxyorthosilicates. In macroscopic form these phosphors exhibit excellent quantum efficiency, favorable absorption and emission characteristics, and good lifetime. By reducing the size of the material to nanoscale dimensions, we expect to improve on each of these properties and to gain insight into the effects of reduced dimensionality on optical processes. Characterization employs absorption, diffuse and specular reflectance, photoluminescence, radioluminescence, thermally stimulated luminescence, excitation spectra, and lifetime. A state-of-the-art, lifetime flourimeter is a recent addition to this suite of experimental tools. A recent addition to the suite of characterization tools is an X-band electron spin resonance spectrometer. This can be used to detect and identify unpaired spins providing atomic-level information on electronic processes that are associated with optical excitation and emission in materials. Primary research includes development and characterization of bulk phosphors, nanophosphors, porous silicon, hydrogen-loaded erbium films, and role of free radicals in polymer aging. (*For recent literature see p28)*

FACILITIES

In addition to the primary teams, MST-8 also hosts several small scale user facilities.

Ion Beam Materials Laboratory

The Ion Beam Materials Laboratory (IBML) is devoted to the characterization and modification of surfaces through the use of ion beams. The core of the laboratory consists of a 3.2-MV tandem ion accelerator and a 200-kV ion implanter together with several beam lines. Attached to each beam line is a series of experimental stations that support various programs.

An *in situ* dual ion-beam facility provides ion-beam irradiation and *in situ* ion-beam characterization. In this facility, an analytical beam line from the 3.2-MV tandem accelerator and an irradiation beam line from the 200-kV ion implanter are connected to a common surface modification chamber. Rutherford backscattering-spectrometry (RBS) and nuclear-reaction analysis (NRA) are available in conjunction with ion-channeling techniques to monitor *in situ* changes of composition and crystallinity of materials being irradiated at temperatures from -100 to 500ºC.

The general-purpose, experimental IBML station is a highly versatile, easy-to-use chamber for materials analysis using beam-induced x rays, gamma rays, NRA, RBS, and elastic recoil detection techniques, as well as for high-energy implantation. The chamber is equipped with a five-axis, computer-controlled goniometer for sample changing and channeling measurements.

The dedicated tritium analysis chamber is specifically designed to accurately measure hydrogen isotopes (prodium, deuterium, and tritium) to metal ratios in metal hydrides. It is also used to measure oxygen depth profiles in the metal hydride targets.

The high-energy alpha-beam irradiation chamber is available to study alpha-induced radiolysis in gases, liquid, and plastics. The in-situ residual gas analyzer and infrared spectrometer (being installed) are available to measure gas emission and formation during the irradiation.

The nuclear microprobe beam line provides highly focused proton or alpha beam (a few microns in diameter) that is used to do ion-beam microanalysis as well as microfabrication through high-energy proton-beam writing lithography.

The 200 kV ion implanter is capable of producing many ion species from gases, transition metals, and rare earth metals with a beam current ranging from microamperes to hundreds microamperes. Different target temperatures ranging from liquid nitrogen to 1000ºC can be used during the implantation.

In 2006 a new state-of-the-art ion implanter will be added to the IBML suite. It will be the first of its kind in North America and will have a high current source that can operate either in gas/vapor or sputter configuration. Typical operation will be from 5 to 200 kV but it could offer up to 800-KeV implants. A high current chamber with target heating and cooling capability will allow high dose fluences such that 10^{19} to 10^{20} atoms/cm^2 implants could be achieved in less than an hour. Because ion implantation is a non-equilibrium process in which energetic ions are forced to mix with target species, it is expected to form new phases or structures not formed by conventional physical or chemical processes. Applications include the synthesis of nanostructured materials and metastable phases of otherwise immiscible solids, studies of radiation damage, doping of semiconductors or optoelectronic materials, and modification of polymers and metal/polymer interfaces for new sensing elements. (*For recent literature see p30*)

Scanning Probe Microscopy

Under the direction of Marilyn Hawley, MST-8 hosts a suite of scanning probe microscopes which map surface properties by rastering a solid state probe very near to a surface. Scanning tunneling microscopy (STM) and atomic force microscopy (AFM) are the most well known techniques. In contrast with electron microscopy these techniques do not use electron optics or high energy focusing. Current capabilities include the following:

Variable Temperature Ultrahigh Vacuum System (Omicron VakuumPhysik, Ultrahigh vacuum system: base pressure 2 x 10^{-11} Torr, Scanning Tunneling Microscopy, Atomic Force Microscopy (optical detection system), Scanning from 40K to 1400K, gas phase dosing, separate preparation chamber for epitaxial growth, Reflection High Energy Electron Diffraction (RHEED), Low Energy Electron Diffraction (LEED), Auger Electron Spectroscopy
Digital Instruments Nanoscope IIIA Scanning Probe Microscopes with:
Dimensions 3000 & 3100 Atomic Force Microscope Probes; Atomic Force Microscopy; Magnetic Force Microscopy; Electric Force Microscopy; Tunneling Atomic Force Microscopy; Samples up to 6 inches diameter and ~0.5 inch thick; Controlled atmosphere; Kelvin Probe Force Microscopy, Piezo Response Force Microscopy, Contact Mode AFM in liquids, Tunneling Atomic Force Microscopy (TUNA), Low Temperature Magnetic Imaging System, Magnetic field mapping at 77 K (immersed in liquid nitrogen)

Current projects titles include “A Scaleable Silicon-Based Nuclear Spin Quantum Computer,” for which STM fabrication and characterization techniques are being use to create a solid-state quantum computer and “Atomic-Level Engineering of Nanostructures and Devices,” in which STM-based lithography is helping to fabricate and characterize nanoelectronic devices. In other work, systematic AFM and mechanical properties studies of the relationship between filler content and cross-linking in polydimethylsiloxane formulations are being used to support modeling efforts. For enhanced surveillance, STM is being used to characterize the structure and electrical properties of oxide coatings and hydride-generated defects in depleted uranium. (*For recent literature see p30)*

Single Crystal Growth Laboratory

Ken McClellan is responsible for the single crystal growth laboratory which consists of five dedicated crystal growth units and ancillary support equipment. Floating-zone, Czochralski, and Bridgman growth methods are employed. There are two float-zone units, two RF-heated Czochralski units, a Czochralski-type tri-arc unit, and three 3-zone furnaces for Bridgman growth. Support equipment includes a cold isostatic press, an arc melter, and various controlled atmosphere furnaces and ovens for materials preparation.

Fundamental understanding of advanced materials often requires access to research-size “custom” single crystals. This is a critical capability for research on advanced high temperature, radiation resistant, detector/sensor, and electronic materials where synthesis of new materials and subsequent doping studies within an identified system are essential. This state-of-the-art bulk crystal growth user facility permits growth of single crystals of advanced materials, such as refractory metals, intermetallics, complex oxides, and non-oxides, some that melt at temperatures greater than 3000ºC.

Recent activity includes the production of cerium-activated, rare-earth oxyorthosilicate-scintillator single crystals for the second axis detector of the Dual-Axis Radiographic Hydrodynamic Test (DARHT); scintillator development for DARHT, Pegasus, and the Advanced Hydrotest Facility; the development of new, fast, bright, and dense scintillator materials; and production process–development for oxyorthosilicate scintillator crystals. These materials are used in radiographic cameras for hydrotest imaging applications. Typically, they have high melting points and require controlled cerium doping.

Appendix I Capabilities

Characterization technique	Equipment	Scientific insight	MST-8 PI	E-mail
Calorimetry	Perkin Elmer DSC-7	Specific heat ; thermodynamic heat of transition	Ricardo Schwarz	rxzs@lanl.gov
Diffraction, neutron – polyxtal	SMARTS @ LANSCE	Residual stress, / atomic structure	Don Brown	dbrown@lanl.gov
Diffraction, neutron – polyxtal	SMARTS @ LANSCE	Constitutive performance (microstructural)	Don Brown	dbrown@lanl.gov
Diffraction, neutron – polyxtal	HIPPO @ LANSCE	Texture - bulk	Don Brown	dbrown@lanl.gov
Diffraction, neutron – small angle	LQD @ LANSCE	Porosity 10nm -1000nm	Don Brown	dbrown@lanl.gov
Diffraction, X-ray – LAUE	SX - LAUE	Atomic structure single crystal	Ricardo Schwarz	rxzs@lanl.gov
Diffraction, X-ray – polyxtal	Powder , HiTemp	Atomic structure	Ricardo Schwarz	rxzs@lanl.gov
Electron spin resonance	Bruker X-band ESR	Atomic level defects	Wayne Cooke	cooke@lanl.gov
Ion beam, general purpose spectroscopy	3MV Tandem accelerator		Yong Wang	yqwang@lanl.gov
Ion beam, microprobe	3MV Tandem accelerator		Yong Wang	yqwang@lanl.gov
Ion beam, tritium and plutonium analysis	3MV Tandem accelerator		Yong Wang	yqwang@lanl.gov
Indenter	Buehler (micro, macro tips)	Hardness	Mike Lopez	mflopez@lanl.gov
Luminescence	Photoluminescence, Radioluminescence, Thermally Stimulated Luminescence	Defect characterization	Wayne Cooke	cooke@lanl.gov
Magnetometry	KHH	Magnetic BH hysterois curve coercivity & moment	Ricardo Schwarz	rxzs@lanl.gov
Microscopy, electron – high resolution transmission	FEI CM30 300KV, FEI Tecnai 300KV, Jeol 3000F 300KV	Nanoscale microstucture	Rob Dickerson	dickerson@lanl.gov

Appendix I Capabilities (continued)

Characterization technique	Equipment	Scientific insight	MST-8 PI	E-mail
Microscopy, electron – orientation imaging	FEI XL30 OIM	Surface - texture	John Bingert	bingert@lanl.gov
Microscopy, electron – scanning	Jeol 6300	Surface - structure	Ellen Cerretta	ecerreta@lanl.gov
Microscopy, optical – metallography	Zeiss (digital) 10X thru 1000X , Leitz thru 500X	Metallography - microstructure grain structure	Mike Lopez	mflopez@lanl.gov
Microscopy, photoluminescence spectrometer	Low T	Spin state , exciton energy	Marilyn Hawley	hawley@lanl.gov
Microscopy, scanning probe	Magneto resistive head	Current distribution	Marilyn Hawley	hawley@lanl.gov
Microscopy, scanning probe – atomic force	Magnetic head	Magnetic domain structure - nanoscale	Marilyn Hawley	hawley@lanl.gov
Microscopy, scanning probe – atomic force	Piezoelectric head	Piezoelectric domain structure nano scale	Marilyn Hawley	hawley@lanl.gov
Microscopy, scanning probe – atomic force	Nano mechanical head	Stiffness nano scale	Marilyn Hawley	hawley@lanl.gov
Microscopy, scanning probe - atomic force	Potentiometric head	Resistance (kelvin probe) nano scale	Marilyn Hawley	hawley@lanl.gov
Microscopy, scanning probe – tunneling	Air based Veeco , UHV omicron	Density of states - atomic resolution	Marilyn Hawley	hawley@lanl.gov
Mechanical testing	Digital Image correlation	Full field deformation ; localized crack fields	Cheng Liu	cliu@lanl.gov
Mechanical testing, 25-mm gas gun	Custom built + Laser interferometry	Constitutive performance; Crack initiation, growth	Ron Ellis	rwe@lanl.gov
Mechanical testing, 7.62-mm gas gun ;-	Custom built / Taylor test cylinders	Constitutive performance; Time resolved dynamic plasticity	Rusty Gray	rusty@lanl.gov
Mechanical testing, 80-mm gas gun	Custom built	Constitutive performance; Shock recovery, spallation, Equation of state	Rusty Gray	rusty@lanl.gov

Appendix I Capabilities (continued)

Characterization technique	Equipment	Scientific insight	MST-8 PI	E-mail
Mechanical testing, dynamic spectroscopy	Perkin Elmer DMA-7	Real and imaginary modulus	Ricardo Schwarz	rxzs@lanl.gov
Mechanical testing, tension/compression quasistatic (77k to 1000C)	MTS 880, Instron 1125	Constitutive performance (modulus, yield, ductility) <xs-1	Manny Lovato	mllovato@lanl.gov
Mechanical testing, tension torsion	Tension-compression-torsion-internal pressure	Constitutive performance	Manny Lovato	mllovato@lanl.gov
Mechanical testing, tension torsion	Tension/compression - high rate w/ option of synchronized high speed video.	Constitutive performance	Ron Ellis	rwe@lanl.gov
Mechanical testing, tension/compression, Hopkinson bar	Custom built w induction heater	Constitutive performance; stress strain f strain rate , damage evolution	Carl Cady	cady@lanl.gov
Modelling, micromechanical analytical	Tanaka- Generalized self consistent	Constitutive performance - heterogeneous / composite systems	Cheng Liu	cliu@lanl.gov
Modelling, “MTS” and “PTW”	Thermally activated strength	Constitutive performance prediction; (Temp strain rate)	Shuh Rong Chen	srchen@lanl.gov
Modeling, finite element		Constitutive performance prediction (plasticity/texture)	John Bingert	bingert@lanl.gov
Modeling, self consistent	Elastoplastic model	Constitutive performance prediction (microstructural)	Carlos Tome	tome@lanl.gov
Modeling, self consistent	Viscoplastic model	Texture prediction	Carlos Tome	tome@lanl.gov
Modeling, self consistent	Modified viscoplastic model	Damage	Ricardo Lebensohn	rlebenso@lanl.gov
Nanoindentation	Nano II Nanoindenter	Mechanical properties in small volumes	Greg Swadener	swadener@lanl.gov

Appendix I Capabilities (continued)

Characterization technique	Equipment	Scientific insight	MST-8 PI	E-mail
Optical absorption	Cary 5E, Absolute specular refl., Variable angle refl., Diffuse reflectance, Integrating sphere	Defect energy levels	Wayne Cooke	cooke@lanl.gov
Optical fluoroscopy	PTI fluorimeter	Electronic energy levels; lifetime of excited states	Wayne Cooke	cooke@lanl.gov
Thermo-gravimetry	Perkin Elmer TGA	Oxidation/reduction kinetics	Ricardo Schwarz	rxzs@lanl.gov
Ultrasound, Rayleigh wave	Custom design in situ UHV	In situ Elastic moduli thin films	Ricardo Schwarz	rxzs@lanl.gov
Ultrasound, Resonant spectroscopy	Dynamic resonant systems	Elastic constants	Ricardo Schwarz	rxzs@lanl.gov
Fabrication tool	**Equipment**	**Function**	**MST-8 PI**	
Thin film deposition			MNRS	
Ion beam implanter	200KV Implanter		Mike Nastasi	nasty@lanl.gov
Single crystal growth				
Cold isostatic press			Ken Mclellan	kmcclellan@lanl.gov
Arc melter			Ken Mclellan	kmcclellan@lanl.gov
Furnaces			Men Mclellan	kmcclellan@lanl.gov

Appendix II Selected Literature

Alloy Theory

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