# Structure/Property Relations Group (MST-8)

## Mission

The activities of the Structure/Property Relations Group (MST-8) provide a focus on the evaluation and prediction of the relationships between property and structure for length scales ranging from atomistic through microstructural to macroscopic.

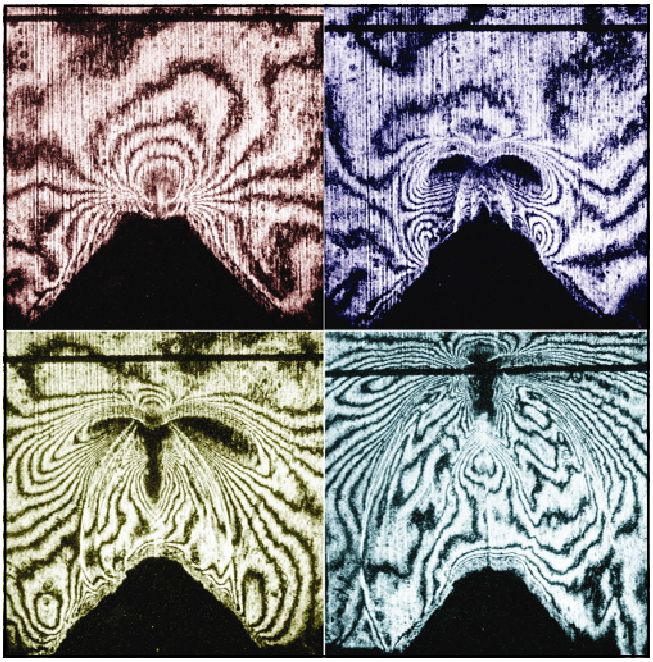
The group hosts a broad suite of state-of-the-art experimental methods which are complemented by a comparable modeling effort. The approximately 80-member group includes seven teams. MST-8 hosts two facilities—the Scanning Probe Microscopy and the Ion Beam Materials Laboratory, which will be home to a new $2M ion implanter in 2006.

## Strategic directions

MST-8's strategic directions include computational science, radiation tolerant ceramics, single crystal synthesis, multilayers, high-temp structural materials, optically functional materials, and metastable and amorphous materials.

Several 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 to multilayered, nanostructured materials. 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 material characterizations.

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 $10^{5}$ $s^{-1}$ and at temperatures from -200 to 1900°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) defense programs, as well as other governmental defense and civilian customers.



**Sequence of images of the dynamic inelastic behavior in a carbon fiber epoxy matrix composite employing the optical coherent gradient sensor technique.**

## Fast facts

The Materials Science and Technology Division's Structure/Property Relations Group features unique capabilities that address:

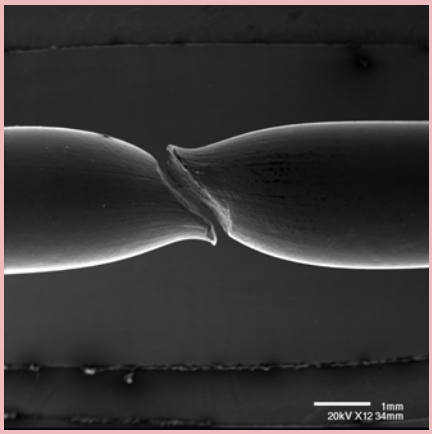
- **Multiscale modeling of structure property relations**
- **Dynamic testing**
- **Radiation damage (3.2 MV ion accelerator)**
- **Surface characterization ion implantation (5-800 KeV)**
- **Thermophysical property characterization**
- **Crystal growth**
- **Atomistic force microscopy**

**For more information on MST-8,** see our website, www.int.lanl.gov/orgs/mst/mst8/, or contact Mark Bourke (bourke@lanl.gov) or Marius Stan (mastan@lanl.gov).

**Principal customers:** Department of Energy (DOE) defense programs, Office of Basic Energy Sciences (OBES), Department of Defense (DoD), and Laboratory Directed Research and Development (LDRD).

**Major sponsors:** Advanced Strategic Computing Initiative (ASCI), Advanced Fuel Cycle Initiative (AFCI), Enhanced Surveillance (EH), and DOE Basic Energy Sciences (BES).

**Operating budget in FY 2006:** $25.4M.




**Scanning electron microscopy of fracture deformation localization in ultrafine-grained aluminum.**

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The **Alloy Theory Team,** led by Ricardo Schwarz *(rxzs@lanl.gov),* works in the area of synthesis, with a focus that includes nanocrystalline materials. The work is complemented by 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 include mechanical alloying through ball milling and elastic constant measurement from scanning resonant waves.

The **Characterization and Modeling of Mechanical Properties Team**, led by William Blumenthal *(blumenthal@lanl.gov),* provides expertise in modeling and simulations for Los Alamos National Laboratory strategic materials at multiple scales that include atomistic, nano, meso, and the continuum. 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 nonlocal plasticity in application to static and dynamic loading conditions. One focus has been aging and phase stability of plutonium alloys.

The **Science of Defects in Materials Team**, led by Kurt Sickafus *(kurt@lanl.gov),* studies radiation effects and optical materials and supports the advanced fuels cycle initiative. Common themes include crystallography and microstructure, particularly as they relate to radiation damage. Capabilities include the synthesis and fabrication of complex oxide ceramics; ion beam irradiation and characterization using transmission electron microscopy, X-ray diffraction, and ion-beam analysis. Recently, the team has combined density functional theory, molecular dynamics, and temperature-accelerated dynamics to demonstrate how irradiation-induced defects evolve over long timescales.

Fracture plane morphology of a carbon fiber epoxy matrix composite material illustrating prevalent fiber pull-out.

The **Dynamic Materials Properties Team**, led by John Bingert *(bingert@lanl.gov)*, systematically quantifies the influence of variables such as strain rate, temperature, stress state, microstructure, and alloy content on the constitutive behavior, damage evolution, fracture, and fragmentation of metals, ceramics, energetic materials, and polymers. The team develops and validates constitutive models describing the mechanical behavior of nuclear and conventional weapons materials. The team utilizes experimental tools that include gas guns, Taylor guns, and Hopkinson bars, as well as advanced characterization capabilities such as orientation imaging microscopy and three-dimensional reconstruction.

The **Thermodynamics and Kinetics of Materials Team**, led by Marius Stan *(mastan@lanl.gov),* models properties of materials for nuclear fuels design and processing, as well as designing fabrication processes for transmutation applications. Its work in support of the advanced fuel cycle initiative program has led to a new atomistic model of thermal conductivity. The team has designed and implemented new components that improved the heat transfer simulations and solidification models of casting simulation software. Studies of plutonium aging and radiation damage support the Enhanced Surveillance

The **Scanning Probe Microscopy Team,** led by Marilyn Hawley, (*hawley@lanl.gov),* hosts scanning tunneling microscopy (STM) and atomic force microscopy (AFM). Projects include a scaleable silicon-based nuclear spin quantum computer for which STM fabrication and characterization techniques are used to create a solid-state quantum computer and atomic-level engineering of nanostructures and devices in which STM-based lithography helps 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 used to support modeling efforts.

The **Ion Beam Laboratory Team**, led by Yongqiang Wang (*yqwang@lanl.gov)*, conducts cutting-edge research in ion-solid interactions, ion beam analysis, ion implantation, and radiation damage effects. It provides ion beam instrumentation for materials modification and characterization which is maintained and upgraded by experts. In addition to the existing high energy tandem ion accelerator, the new high current ion implanter can produce virtually any ions in the periodic table. Projects include in-situ surface characterizations, gas radiolysis, and gas-solid reactions induced by alpha beam irradiations. The team has achieved novel materials synthesis through ion implantation and studies radiation tolerance in various materials related to nuclear reactors, nuclear waste management, and nuclear weapons.

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