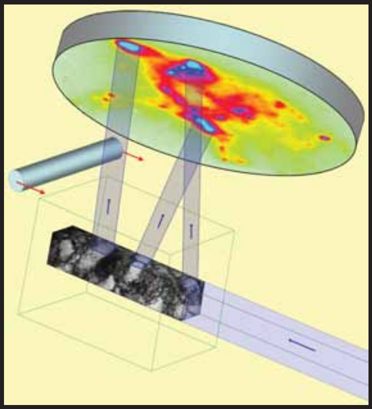
Fundamentals of Deformation

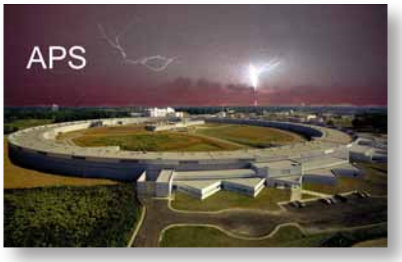
Objective



This project provides new measurement methods, property data and simulations for areas critical to US manufacturing, describing the mechanisms responsible for mechanical behavior. The mechanical behavior of virtually all materials (from nanostructures to bulk structural steels) depends upon processes active at the nanoscale; we provide critical evaluations of the sensitivity of nanomechanics test methods to uncontrolled experimental conditions and develop new measurement methods for probing elastic strains, defect structures and crystallographic orientations at the nanoscale within nanostructured materials and devices.

METALS

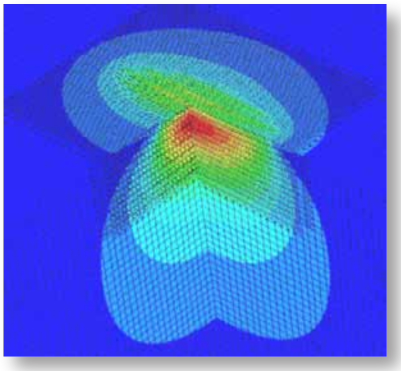
Impact and Customers



- We have provided users from industry, academia and national laboratories a completely new class of X-ray imaging techniques for materials studies (ultra-small-angle X-ray scattering imaging, or "USAXS imaging"), which we developed from basic concept to DOE-supported operations at the Advanced Photon Source (APS).
- A new, robust measurement capability has been developed for measuring elastic strains, defects and crystallographic orientations from buried nanoscale sample volumes within nanostructured materials and devices, and is now installed at the APS.
- NIST is working to provide researchers and engineers with a nano-Newton (nN)-level force standard. Quantum level simulations of gold nanowire deformation have confirmed that this system is suitable for an intrinsic force standard.
- We are providing the nanoindentation community with critical, quantitative evaluations of the indentation's sensitivity to unavoidable variations in indenter tip shapes and sample roughness.

Approach

The mechanical behavior of materials during device processing, assembly, and lifetime is a critical factor for nearly all industrial products. This behavior is generally determined by complex nanoscale processes such as the evolution of local stress concentrations, defect propagation, local slip, and delamination. Targeted quantitative measurement and modeling techniques are critical for making new products affordable and reliable. Topic areas include: 1) quantitative, experimentally validated computer simulations to evaluate nanoindentation and nanowire failure, and 2) new spatially resolved synchrotron X-ray diffraction and small-angle scattering measurement techniques for probing elastic strains, defect structures, crystallographic orientations and densities at the nanoscale, within nanostructured materials and devices.

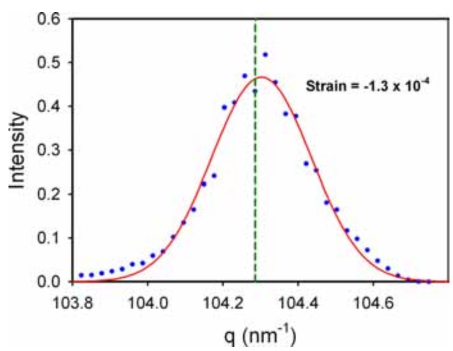


For example, USAXS imaging is now being used at the APS for research as diverse as the self-assembly of conductive nanowire networks and the distribution of second phase particles in artificial rubber materials.

Accomplishments

High impact and effective dissemination of NIST measurement capabilities can be achieved by directly incorporating these experimental techniques into national user facilities such as the DOE-operated APS. One such measurement method is USAXS imaging, which was conceived by NIST scientists in 2000. Since that time, the required instrumentation, experimental techniques and underlying theory have been developed and implemented. USAXS imaging is extremely sensitive to density changes in materials, and provides quantitative measurement of the sizes, shapes and spatial arrangements of their underlying microstructural features. In 2005, DOE added USAXS imaging to the APS ten year tactical plan, with the highest possible priority. It has now been incorporated into a new imaging beamline and the first DOE-supported user experiments (with no NIST involvement) were conducted in November 2007. Continued development of USAXS imaging is supported through a Partner User Agreement between NIST and DOE.

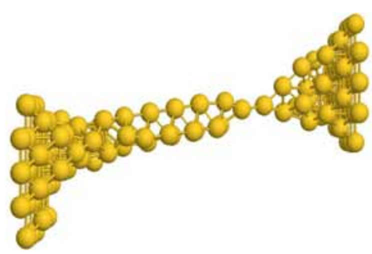
In a similar vein, NIST staff are collaborating with researchers from Oak Ridge and Argonne National Laboratories to develop a robust measurement capability for measuring elastic strains, defect densities and crystallographic orientations from buried sample volumes smaller than 0.004 μm^3. This technique was first utilized in 2006 to measure elastic strains within individual dislocation cell interiors in plastically deformed Cu, with a 3D spatial resolution of 0.5 μm. Full diffraction line profiles can now be obtained from contiguous buried sample volumes. For example, in a recent experiment, diffracted intensity from a 0.07 μm^3 sample volume, buried 11 μm deep in a deformed Cu sample, was isolated and analyzed. This sample volume contained a single dislocation wall, separating two low dislocation density regions. Independent line profiles were extracted from all three sub-volumes, allowing quantitative determination of local elastic strain, dislocation density and angular misorientation. The figure below shows the diffraction line profile from the dislocation wall. The location of the peak gives the average elastic strain, while the width of the peak is determined by the dislocation density.



Line profile from individual dislocation wall

On another topic, current methods for measuring local mechanical properties at the nanoscale are sensitive to nanoscale variations in the probe geometry, but the magnitude of this sensitivity is largely unknown. NIST researchers used atomic force microscopy to characterize the 3D shape of a new nanoindenter tip which was subsequently used to indent single crystal tungsten. Stress estimates obtained from the resulting experimental data, using conventional approaches (Hertizian approximation for a spherical tip), were over 30 % larger than those determined from a detailed finite element model of this experiment.

Finally, plastic deformation of gold nanowires has received considerable attention recently, due to their ability to form single atom chains which result in quantized conductance. NIST has identified the breaking of such nanowires as a likely candidate for a much needed intrinsic force standard for very small loads, and accurate quantum mechanics simulations have been used to explore the deformation behavior over a wide range of deformation conditions. It was found that single atom chains are easily formed, and that the breaking force of these chains is extremely consistent, (1.53 ± 0.02) nN, confirming that this system is suitable for an intrinsic force standard.



Deformed gold nanowire

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Publications

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Zhang F, Long GG, Levine LE, Ilavsky J and Jemian PR *Quantitative Characterization of the Contrast Mechanisms of Ultra-Small-Angle X-ray Scattering Imaging* Journal of Applied Crystallography, 41: 416 (2008)

Levine LE, Long GG, Gerhardt RA, Ou R, Ilavsky J and Parker CA *Self-assembly of a Nanoscale Three Dimensional Conductive Network Within a Polymer Matrix* Applied Physics Letters, 90: 014101 (2007)

Levine LE, Larson BC, Yang W, Kassner ME, Tischler JZ, Delos-Reyes MA, Fields RJ and Liu W *X-ray Microbeam Measurements of Individual Dislocation Cell Elastic Strains in Deformed Single Crystal Copper* Nature Materials, 5: 619 (2006)