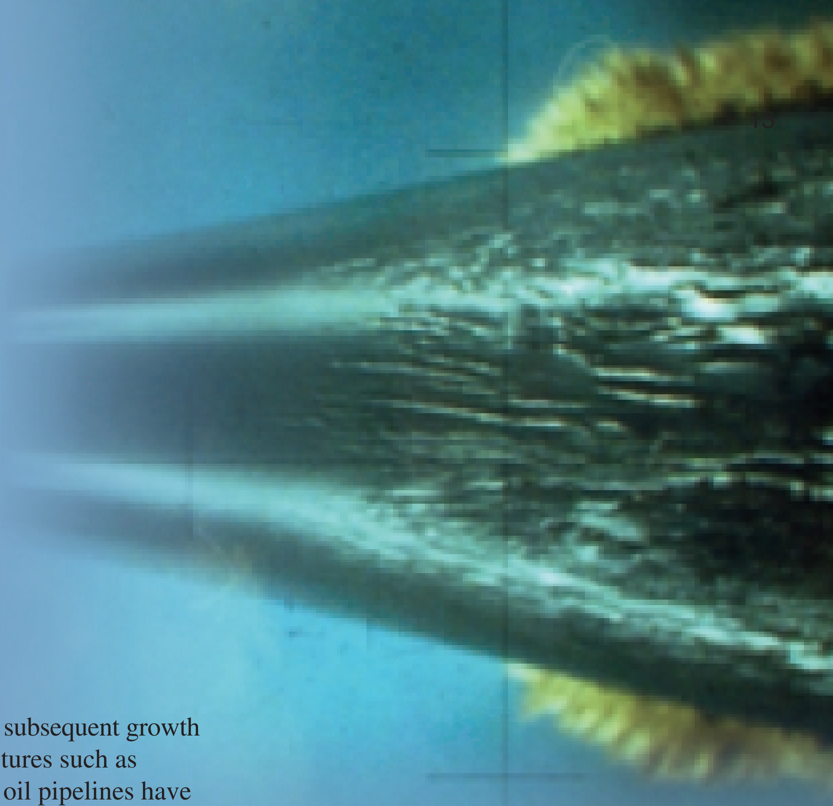
How Metals Fail

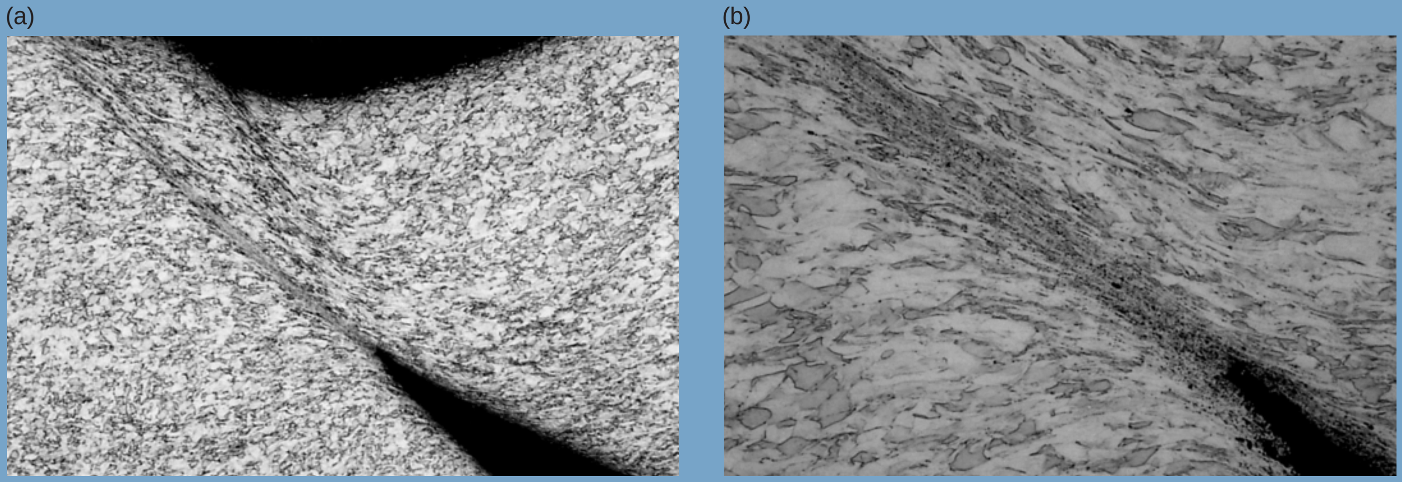


Laboratory experiments point the way to a new generation of computer codes for predicting metal failure.

THE initiation and subsequent growth of cracks in structures such as bridges, aircraft, and oil pipelines have been studied and modeled for years. In contrast, cracks and failures of parts driven by high-explosive detonations are less well understood and poorly modeled. Much more complete information is needed in these cases because the Laboratory's defense-related mission requires an understanding of how metals respond to the sudden shock waves and subsequent high-strain-rate deformations caused by high explosives.

In particular, one of the challenges facing the National Nuclear Security Administration's (NNSA's) Stockpile Stewardship Program is using computational models to predict dynamic material failure relevant to nuclear weapon safety and reliability. Changes in material properties caused by aging nuclear warheads must be represented in computer simulations that accurately reflect the particular metal's internal structure.

"Our ability to account predictively for dynamic material failure is inadequate and, in some cases, primitive," says Livermore engineer Richard Becker. "We want our computational models to reflect in detail how cracks form, evolve, and



(a) This micrograph of a tantalum–tungsten alloy cylinder driven by a gas gun shows that the material breaks along shear bands (darker diagonal line). (b) The crack tip at a higher magnification. (Micrograph produced by Anne Sunwoo.)

lead to the failure of a part," he says. Becker is a member of Livermore's code development team that supports NNSA's Advanced Simulation and Computing (ASCI) program. He is using results from experiments conducted at Livermore and elsewhere to construct advanced computer models of how metals crack and ultimately fail.

The new models will help to assure nuclear weapon safety and reliability as well as to advance nonnuclear military applications used to design equipment such as shaped charges and armor-defeating projectiles. The new models will also likely benefit a number of industrial processes, such as explosive welding and shock processing, which use high explosives.

Physicist Elaine Chandler, an associate division leader in the Laboratory's Defense and Nuclear Technologies Directorate, was the original architect of the combined modeling and experimental effort on dynamic failure, which now spans several Livermore directorates. The goal, she says, is to couple theory, simulation, and experiments to yield a much better predictive capability for the behavior of ductile metals—metals such as copper and aluminum that bend before breaking—under extreme conditions of high pressures and high strain rates (deformation). "We need real physics underpinnings for models of how materials fail," she says.

The experimental effort consists of several multidisciplinary projects, some supported by Laboratory Directed Research and Development funds, that investigate different aspects of dynamic failure.

The experiments use well-characterized ductile metals, experimental tools such as gas guns and scanning and transmission electron microscopes, and advanced facilities such as the Laboratory's Janus laser and High Explosives Applications Facility, the University of Rochester's Omega laser, and the Stanford Synchrotron Radiation Laboratory. Together, the experiments cover a wide range of strain rates and pressures. An important focus of the experimental effort is the development of novel diagnostics to illuminate the microsecond-by-microsecond details of material fracture and failure.

The experimental results are being incorporated into Becker's advanced computational models. Becker says that traditional codes provide only simple characterizations of the dynamic fracture behavior of ductile metals. Often, they prescribe just the minimum pressure at which the metal fails. "We need to more accurately capture the complex underlying processes so that we can better account for the influence of microstructure, strain rate, and pressure on the failure of ductile metals. We also need to simulate the orientation of cracks and the recompression of material that is possible following severe cracking."

Becker sees a significant drawback to current models in that they do not take into account a metal's microstructure, which is known to control its mechanical properties. Metals are composed of microscopic grains that have different orientations and, inevitably, contaminants. Some aspects of the subgrain microstructure change dramatically when subjected to a strong shock from a high-explosive detonation. In particular, a strong shock induces numerous dislocations within a metal's crystalline lattice, which changes the metal's mechanical properties such as its strength, ductility, and resistance to cracking.

In addition, shocked ductile metals are known to develop cracks by nucleation (formation), growth, and linking up of microscopic voids, and a metal's microstructure also affects void nucleation and growth. For example, impurities and inclusions often act as void nucleation sites. What makes the current suite of Livermore experiments so important, says Becker, is that the metals under investigation have their microstructure characterized both before and after being subjected to different strain rates and pressures.

Shocking Samples with Lasers

Materials scientist Geoff Campbell is looking at the connection between shear (displacement across a narrow band of material) and fracture in shocked metals. He notes that when metals fail at high rates, the behavior is often associated with shear that is confined within narrow bands. These shear bands are typically precursors to the formation of cracks. The metal deforming within the shear bands becomes hot and softens, which makes it susceptible to failure.

To gain a fundamental understanding of shear localization and fracture, Campbell conducts experiments in which he determines the mechanical properties of shocked metals. He creates the shocked microstructure with laser-shock processing, a method that is considerably easier and less expensive than high-explosives-driven methods. The solid-state, high-energy (50-joule), neodymium-doped glass laser was developed at Livermore as part of a method, now commercialized, to improve the fatigue performance of metals by imparting intense shocks. (See *S&TR*, March 2001, pp. 26–28.)

In Campbell's experiments, the laser pulses the metal sample several times to achieve conditions similar to explosively shocked material. Each laser shot lasts only 20 to 50 nanoseconds, compared to a high-explosive detonation that typically lasts about 1 microsecond.

Campbell's focus is on three metals: copper, tantalum, and a tantalum–tungsten alloy. "These are popular, well-understood materials at the Laboratory, and they allow different experimental teams to compare results," he says.

Following laser shocking, Campbell determines traditional mechanical properties and the degree to which the metals are susceptible to crack propagation and ultimate failure, information that is critical to the development and calibration of Becker's computational models. The information is obtained with tests that measure the material's strength as it is being deformed and the strain energy release required to propagate a crack. The same tests are also performed on unshocked samples as controls.

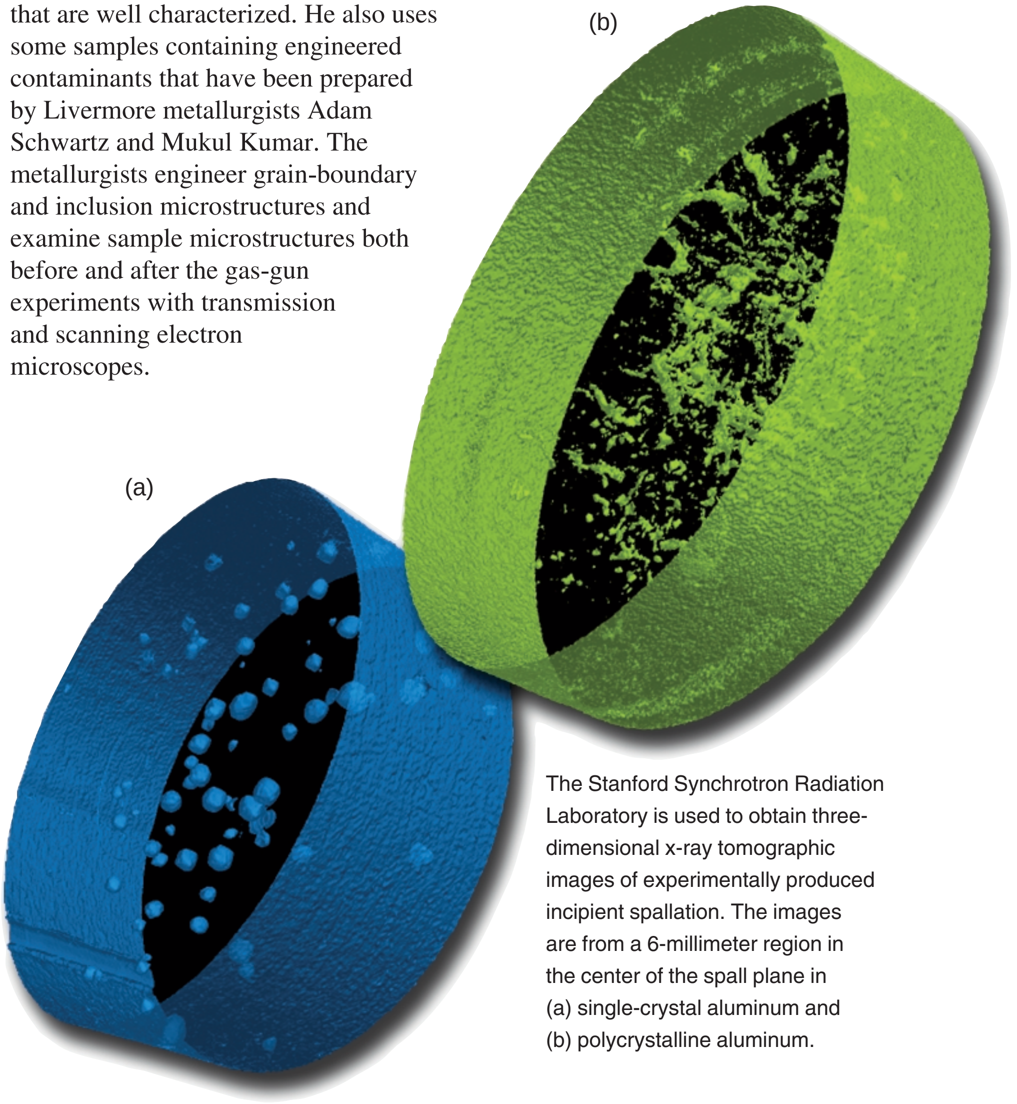
Campbell notes that understanding the real response of materials has always been important to national security as well as industry. During World War II, Liberty Ships were manufactured using welds for the first time instead of rivets. It was not appreciated at the time that the welds could become brittle below a certain temperature, and several ships broke in two. Some sank right after launch, while others were lost suddenly at sea.

Gas Guns Create Spall

Physicist Jim Belak is looking at the microstructural origins of dynamic fracture in ductile metals to obtain a better understanding of beginning damage from spallation, the scab that forms near the metal surface during high-explosive detonations. "We lack a detailed model of spall fracture," says Belak. He explains that spall fractures occur when a shock wave reflects from a surface and produces extreme tension inside the solid. When this tension exceeds the material's internal rupture strength, the solid fails by rapidly nucleating voids, which quickly link to form fractures. The origin of the voids is tied to the solid's microstructure, especially weak points such as inclusions and boundaries between metal grains. Improving our understanding of spall requires correlating the observed incipient damage with the well-characterized microstructure.

Belak and colleague James Cazamias use the Livermore gas-gun facility to create spall in samples of aluminum, copper, titanium, and vanadium, metals with crystal structures of interest and that are well characterized. He also uses some samples containing engineered contaminants that have been prepared by Livermore metallurgists Adam Schwartz and Mukul Kumar. The metallurgists engineer grain-boundary and inclusion microstructures and examine sample microstructures both before and after the gas-gun experiments with transmission and scanning electron microscopes.

The gas gun shoots a metal flyer at velocities ranging from 150 to 210 meters per second. Though higher velocities are possible, the slower velocity is used to create incipient damage. The flyer hits a 25-millimeter-diameter thin metal target of the same material. The target has outside rings that reduce unwanted effects associated with the specimen's edges. At impact, the rings break off, and the 16-millimeter-diameter center of the target flies into a catch tank, where it is recovered with minimal additional deformation.

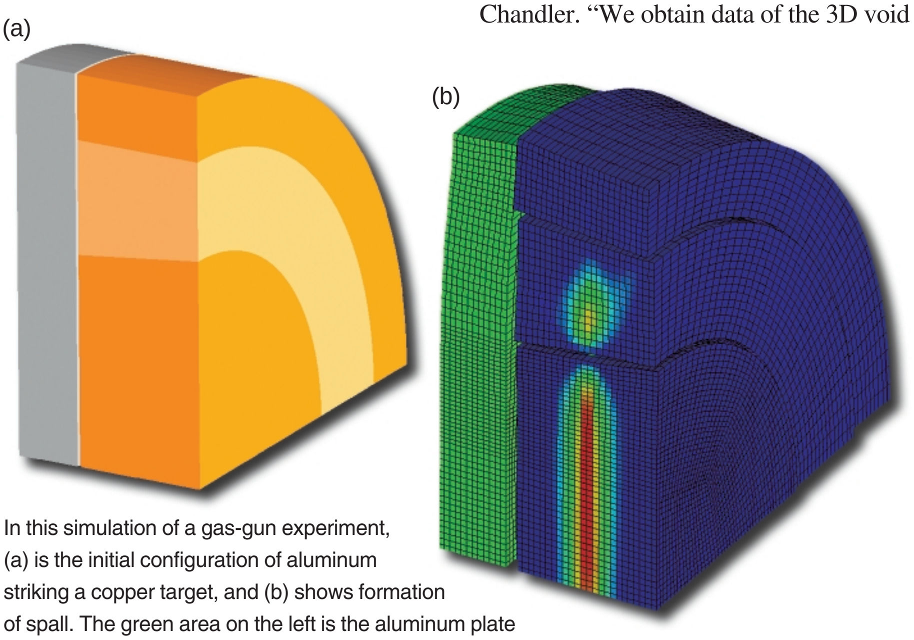


The Stanford Synchrotron Radiation Laboratory is used to obtain three-dimensional x-ray tomographic images of experimentally produced incipient spallation. The images are from a 6-millimeter region in the center of the spall plane in (a) single-crystal aluminum and (b) polycrystalline aluminum.

Belak and physicist John Kinney take the target pieces containing incipient spall to the Stanford Synchrotron Radiation Laboratory to obtain three-dimensional (3D) x-ray tomographs in 700 orientations. The images, which have a resolution of about 5 micrometers, are combined to compute the 3D size and space distribution of the voids that have been created during spallation fracture. The data are essential input to spallation models. After the tomographic data are taken, the samples are sectioned to make detailed comparisons with traditional two-dimensional microscopy.

"The synchrotron imagery that Jim is obtaining is quite a breakthrough," says Chandler. "We obtain data of the 3D void distribution just from the images and without having to take thin slices of the material and count the number of voids in each slice."

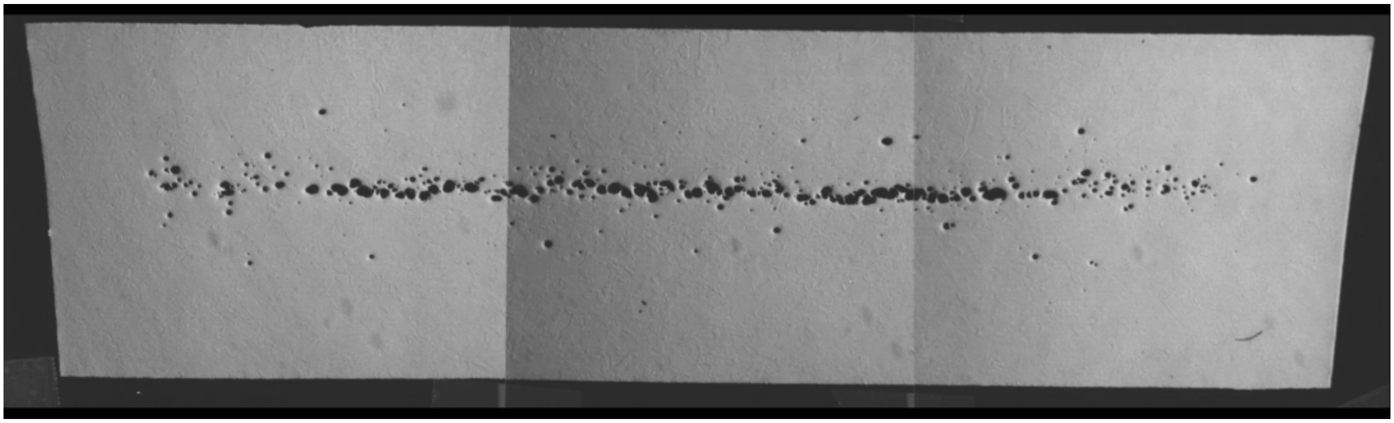
Belak and physicists Robert Rudd and Eira Seppälä are also performing 3D simulations at the atomic level that track how voids grow and link. The simulations feature 1 to 10 million atoms representing the crystal structure of aluminum or copper. When tensile forces are applied in different directions, the simulations reveal the dislocation mechanism by which microscopic voids grow. The spall recovery experiments using single-crystal copper and aluminum will enable direct validation of these dislocation mechanisms.



In this simulation of a gas-gun experiment, (a) is the initial configuration of aluminum striking a copper target, and (b) shows formation of spall. The green area on the left is the aluminum plate that strikes a 5-millimeter-thick cylindrical disk target. The target's two spall rings can be seen on the disk. The formation of voids (red) is seen in the center of the disk.

Closing Up Voids

In some cases, layers of a spalled material can collide as the pressure from the high explosive continues to drive one of the surfaces. The result can be recompression of the spalled material, which closes the voids created by the original shock. Under these conditions, the damaged material could jet out from pores, continue deforming, have localized heating, and even melt.



This photomicrograph of a copper disk used in a gas-gun experiment shows the formation of voids in the spall layer.

Currently, simulations do not include experimentally based models of recompression behavior. Including such models is necessary for accurate stockpile stewardship calculations, says Becker. "We want to determine the material response as these two pieces meet, obtain estimates for the strength of the recompressed region, and insert a recompression model in our ASCI code."

Becker and his colleagues are performing recompression experiments on recovered metal disks that contain well-characterized spall damage. They use a gas gun and copper targets the same size and shape as those used in Belak's experiments.

The targets are soft-recovered—that is, captured using soft materials that do not further damage them—and small specimens containing spall are excised from them. The samples are then compressed at various rates to close the voids. Becker monitors the microstructure evolution and the manner in which the damage is being closed. Then the targets are sectioned and micrographs taken of them to examine the recompressed microstructure and track the evolution of the voids.

The data obtained from these experiments will be used to construct a model describing the material behavior during recompression and the residual strength in the damaged samples. The recompression component of an overall model will provide a more accurate representation of material behavior for explosively loaded materials.

"This is a first-cut model based on limited data, but it is a major step along the way toward developing an accurate and robust simulation capability for recompressed damaged materials for stockpile stewardship," says Becker.

Probing with X Rays

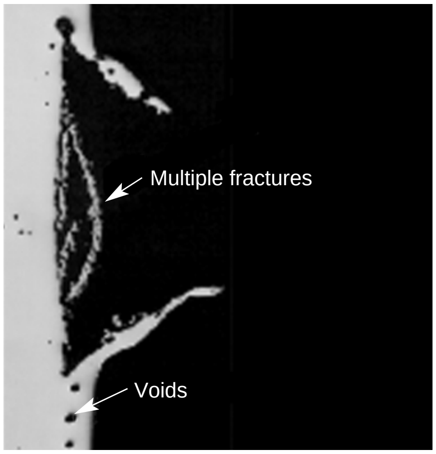
Using lasers, physicist Dan Kalantar has also demonstrated the recovery of shocked single-crystal copper samples about 500 micrometers thick. The experimental results are helping to refine the development of models of void growth and spall formation.

The laser experiments provide pressures—in some cases exceeding 100 gigapascals—greater than those produced by related laboratory experiments using high explosives. The laser pulse lasts 2 to 5 nanoseconds and exerts a maximum pressure at the driven side of the sample. The pressure wave decays as it propagates into the material, resulting in a range of pressures accessed in a single experiment.

One series of experiments is devoted to developing a technique called time-resolved, dynamic x-ray diffraction. This technique uses a high-intensity laser beam focused on a thin metal foil (such as vanadium or iron) to create a source of x rays. The x rays diffract from a single-crystal sample that is shocked by direct laser irradiation with a separate laser beam.

The diagnostic x rays provide a means for recording the response of the metal's lattice as the shock from the laser pulse passes through. The x rays are diffracted simultaneously from multiple planes within the metal's crystalline lattice. Kalantar has developed a large-angle film detector that records the diffracted x rays. In addition, optical and electron microscopes are used on recovered shocked targets to determine the metal's altered microstructure.

Kalantar has also demonstrated, with the Omega laser, the recovery of shocked single-crystal copper samples about 500 micrometers thick. Direct laser irradiation generates a high-pressure shock that causes the formation and coalescence of voids, and this void formation and coalescence in turn create spall. Optical and electron microscopy are used on thin slices of the targets to investigate the final structure. The effect of the dislocation microstructure on the x-ray diffraction pattern is compared with the dynamic x-ray diffraction pattern.



Example of void formation and spall fracture in a copper sample after the passage of a powerful shock wave from the Janus laser at Livermore. Direct laser irradiation generates a high-pressure shock that causes the formation and coalescence of voids, which in turn create spall.

Kalantar is working to extend the dynamic diffraction experiments using the two beams of the Janus laser. In addition, to expand the experiments that Becker is performing, he is designing two-beam experiments to shock materials, create voids and incipient spall with one beam, and then recompact them with the second beam.

Putting It All Together

As experimenters across the Laboratory acquire data, Becker incorporates them into his evolving models of how materials fracture and fail under extreme conditions. "The data from material characterization, metallurgical analysis, and dynamic experiments are helping to constrain and guide our 3D code development," says Becker. In particular, the code development effort is being aided by

Exploding Metal Cylinders Solve Part of the Puzzle

Physicists Ted Orzechowski, Omar Hurricane, and colleagues are exploding cylindrical samples of metals and monitoring how they fracture and then fly apart. The researchers analyze the failure of the metal cylinders through high-speed images and characterize the fragments that are explosively produced. “We’re missing a fundamental understanding of material failure. Just having a big computer, without the correct physics models, is not going to help,” says Hurricane.

Hurricane, in collaboration with Lalit Chhalabildas and his group at Sandia National Laboratories, is looking at the failure of metals at high strain rates caused by 2.5-centimeter-long, Lexan™ flyers fired from a gas gun and traveling at about 2 kilometers per second. The flyer slams into another piece of Lexan inside a metal cylinder about 5 centimeters long, with an inner diameter of 1.2 centimeters, and 1, 3, or 5 millimeters thick. The cylinder materials are 1045 steel (a common steel formulation), nitinol (nickel–titanium alloy), and tantalum–tungsten alloy. “Upon impact, the Lexan behaves a bit like a ‘working fluid,’ driving the cylinder radially outward,” says Hurricane.

The gas-gun experiments are more controlled and compact than high-explosives experiments, and researchers do not have to contend with smoke obscuring the high-speed cameras. The shock wave from the Lexan–Lexan impact sweeps through the surrounding metal cylinder with a pressure of about 2.4 gigapascals. “Although there is a shock, it is the rapid radial expansion that causes the material to fracture,” says Hurricane.

The experiments are heavily monitored with diagnostics that record the strain rate at different positions on the cylinder. Optical cameras allow Hurricane to watch stop-action movies as cracks form, spread, and quickly tear apart the cylinder. In the case of the tantalum–tungsten alloy, the cracks are associated with shear bands, which tend to form at 45-degree angles from one another.

In what Hurricane likens to a forensic examination, metallurgist Anne Sunwoo cuts up the soft-captured fragments (that is, fragments captured with light materials to prevent further damage) and examines them with a transmission electron microscope to study the metal’s altered microstructure.

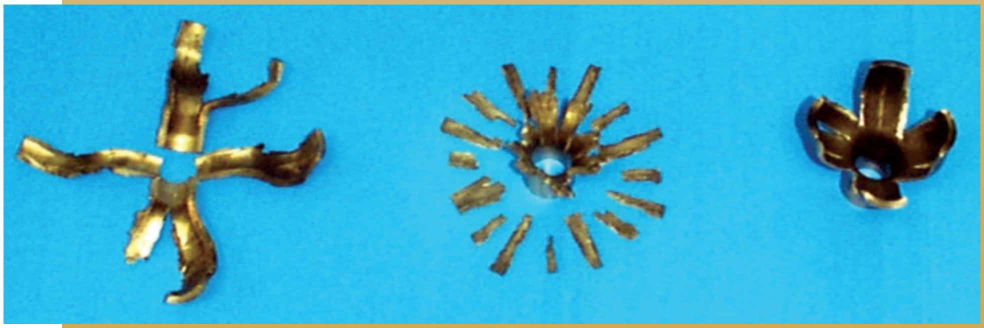
The gas-gun cylinder experiments provide a direct way to document differences in failure according to the changing microstructure of the metal cylinder. Although identical Lexan projectiles are used, there are obvious differences in cracks, fragment size and number, and microstructure of the failed pieces, depending on the metal.

High Explosives Increase the Pressure

Orzechowski and colleagues are conducting experiments similar to Hurricane’s, but they are using high explosives to study the dynamics of fragmenting cylinders. These “pipe bomb” experiments involve pressures some 10 times greater (about 20 gigapascals) than those generated in the gas-gun experiments, but the different pressure regimes complement each other, Orzechowski says.

The experiments are providing the data required to develop, improve, and validate material failure models for different kinds of weapons. “We want to improve the understanding of failure and fragmentation of metals and alloys subjected to explosive force,” Orzechowski says. In addition to stockpile stewardship applications, the research is relevant to understanding material failure in conventional weapons. The research is funded by Laboratory programs and a Memorandum of Understanding with the Department of Defense’s Office of Munitions.

The cylinders measure about 5 centimeters in outside diameter and 20 centimeters long. Preliminary experiments were conducted by John Molitoris at Livermore’s High Explosives Applications Facility. Physicist Peter Bedrossian is continuing the experiments at the Laboratory’s remote Site 300. The cylinders, made from 1045 steel, Aermat 100 steel, or a uranium alloy, are detonated from one end. The high-explosive



Gas-gun cylinder experiments provide a direct way to quantify differences in material failure. Even under identical drives, differences in cracking and failure are obvious.

detonation front sweeps along the axis, with the shock lasting for several microseconds. The metal fragments that are violently produced are soft-captured with glass wool or other light materials.

A wealth of information is provided by diagnostics, including Fabry–Perot interferometry (which provides time-dependent surface velocity measurements), high-speed optical imaging, and conventional radiography. In addition, a series of proton radiograph experiments, using smaller scale pipes, was conducted at the Los Alamos National Laboratory Neutron Science Center by Livermore physicists Bedrossian and Hye-Sook Park. The proton radiography provides sequential radiographs that show the details of cracks evolving and the cylinder disintegrating into many fragments. (See *S&TR,* November 2000, pp. 12–18.) Metallurgist Sunwoo also characterizes the cylinder metal before the experiment and examines the recovered fragments to help determine their mode of failure.

Like the gas-gun experiments, shear bands are found where the cylinder rips apart. As with the experiments conducted by other researchers, the tests show that a material's microstructure may affect its performance. For example, the experiments reveal differences between steel cylinders that are heat-treated to increase hardness and those that are untreated.

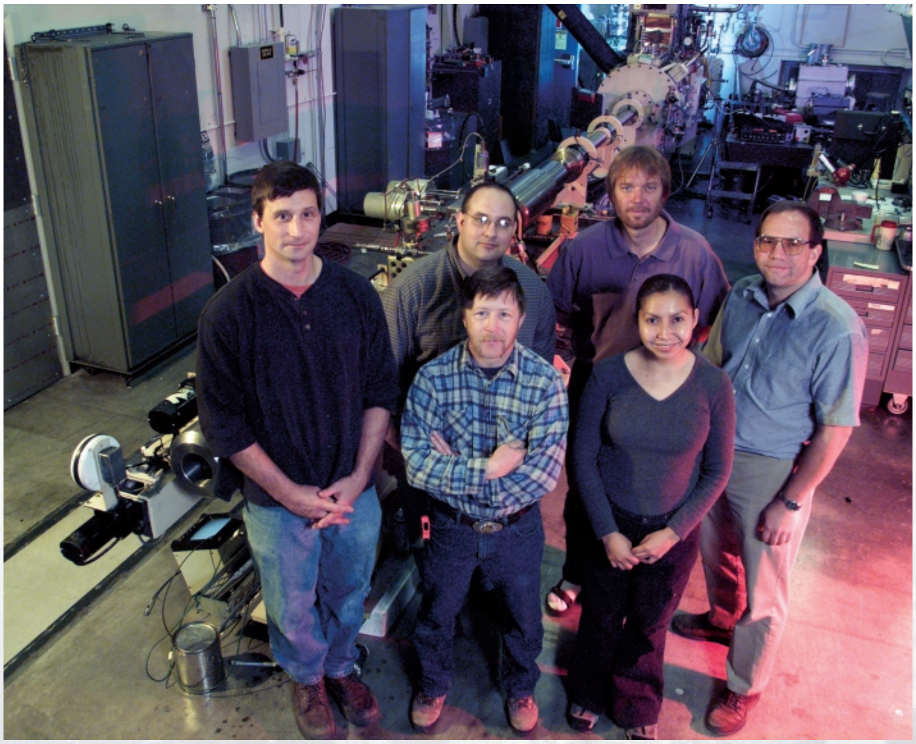
Experiments using high explosives to study the dynamics of fragmenting cylinders are well-diagnosed. Diagnostic instruments include high-speed optical imaging, metallography, radiography, and Fabry–Perot interferometry.

insights gained from examining different material microstructures both before and after experiments. Initial simulations employing the advanced models are encouraging, but much work remains to be done.

Becker notes that the modeling effort is aided by simulation advances made by other Laboratory researchers. Geophysicists such as Lew Glenn have long sought to accurately model the way rocks fracture. Because rocks are brittle, simulations of their fractures are not directly applicable to ductile metals, but methods to account for crack orientation and certain numerical techniques can be applied to modeling ductile metal fractures. Also, some metals important to stockpile stewardship, such as beryllium, are brittle. And glass, a highly brittle material, is vitally important to scientists preparing to operate the National Ignition Facility, now under construction at Livermore to serve the stockpile stewardship mission.

Becker is looking forward to offering scientists a robust, flexible model that can simulate different metals under a wide range of extreme pressures and strain rates. The payoff will be increased confidence in the nation's nuclear stockpile.

—Arnie Heller



Researchers at the gas-gun facility. In the front row, from left, Keith Lewis, Sam Weaver, and Erica Nakai. In the back are James Cazamias, Jim Belak, and Rich Becker.

Key Words: Advanced Simulation and Computing (ASCI), Fabry–Perot interferometry, gas gun, high explosives, High Explosives Applications Facility, Janus laser, Office of Munitions of the Department of Defense, Omega laser, proton radiography, Site 300, spall, Stanford Synchrotron Radiation Laboratory, stockpile stewardship, three-dimensional x-ray tomography.

For more information contact Richard Becker (925) 422-1302 (becker13@llnl.gov).