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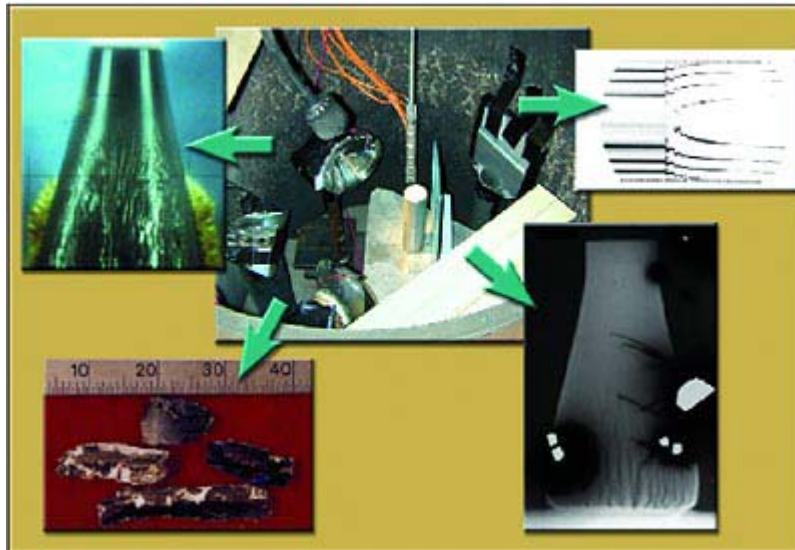
American Academy of Mechanics
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SELECTION OF THE EDITOR

Understanding Metal-Failure Dynamics

*Richard Becker, Dan Kalantar, Jim Belak, Geoff Campbell, Ted Orzechowski and Omar Hurricane,
Lawrence Livermore National Laboratory, Livermore, Calif.*

Lab experiments point the way to a new generation of computer codes for predicting metal failure. The development of a robust, flexible model that can simulate different metals under a wide range of extreme pressures and strain rates will provide increased confidence in the nation's nuclear stockpile.



Experiments using high explosives to study the dynamics of fragmenting cylinders are examined using diagnostic instruments including high-speed optical imaging, metallography, radiography, and Fabry-Perot interferometry.

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. Lawrence Livermore National Laboratory's (LLNL) defense-related activities require a better 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) 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 a particular metal's internal structure.

LLNL's ability to predict dynamic material failure is inadequate and, in some cases, primitive. Computational models need to reflect in detail how cracks form, evolve and lead to the failure of a part, and a code-development team that supports NNSA's Advanced Simulation and Computing (ASCI) program is using results from experiments conducted at LLNL and elsewhere to construct advanced computer models of how metals crack and ultimately fail. The new models will help to ensure nuclear weapon safety and reliability and advance nonnuclear military applications used to design equipment such as shaped charges and armor-defeating projectiles. They also likely will benefit a number of industrial processes, such as explosive welding and shock processing, which use high explosives.

The original architect of the combined modeling and experimental effort on dynamic failure is physicist Elaine Chandler, an associate division leader in the lab's Defense and Nuclear Technologies Directorate. The goal 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).

Experimental work



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.

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

Experimental results are being incorporated into advanced computational models. Traditional codes provide only simple characterizations of the dynamic fracture behavior of ductile metals and often prescribe just the minimum pressure at which the metal fails. What is required is the capability to more accurately capture the complex underlying processes to better account for the influence of microstructure, strain rate and pressure on the failure of ductile metals. It also is necessary to simulate the orientation of cracks and the recompression of material that is possible following severe cracking.

A significant drawback to current models is that they do not take into account a metal's microstructure (consisting of grains of different orientation and possibly contaminants), which controls its mechanical properties. 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 strength, ductility and resistance to cracking.

In addition, shocked ductile metals develop cracks by nucleation (formation), growth and linking up of microscopic voids. Microstructure also affects void nucleation and growth. For example, impurities and inclusions often serve as void nucleation sites. Microstructures of metals being studied in this work are being characterized before and after being subjected to different strain rates and pressures.

Shocking samples using lasers

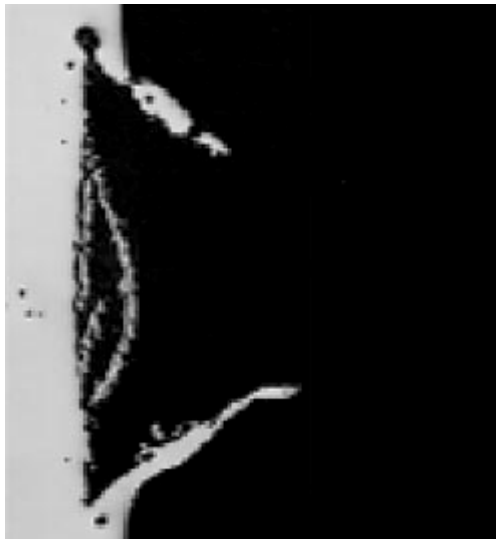
The connection between shear (displacement across a narrow band of material) and fracture in shocked metals is being investigated by LLNL materials scientist Geoff Campbell. When metals fail at high rates, their behavior often is associated with shear that is confined within narrow bands, which typically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

The mechanical properties of shocked metals are measured to gain a fundamental understanding of shear localization and fracture. The shocked microstructure is created using laser-shock processing, a method that is considerably easier and less expensive than using high explosives-driven methods. The solid-state, high-energy (50-J), 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.

The laser pulses the metal sample several times to achieve conditions similar to explosively shocked material. Each laser shot lasts only 20 to 50 ns compared with a high-explosive detonation that typically lasts about 1 ms. Copper, tantalum and a tantalum-tungsten alloy are being characterized.

Following laser shocking, mechanical properties including material strength as it is being deformed and the strain energy release required to propagate a crack are determined, as well as the degree to which the metals are susceptible to crack propagation and ultimate failure. This information is critical to the development and calibration of computational models. The same tests are performed on unshocked samples as controls.

Gas guns create spall



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.

Because a detailed model of spall fracture is lacking, the microstructural origins of dynamic fracture in ductile metals are being studied by physicist Jim Belak to obtain a better understanding of beginning damage from spallation, the scab that forms near the metal surface during high-explosive detonations. 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 the

understanding of spall requires correlating the observed incipient damage with the well-characterized microstructure.

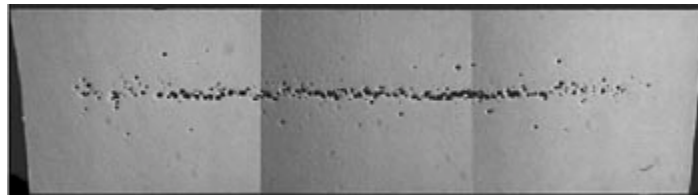
Belak and colleague James Cazamias use the gas-gun facility to create spall in samples of aluminum, copper, titanium and vanadium, metals having crystal structures of interest and that are well characterized. Other treated metals are samples containing engineered contaminants (that is, engineered grain-boundary and inclusion microstructures).

The gas gun shoots a metal flyer at velocities ranging from 150 to 210 m/s (335 to 470 mph). Though higher velocities are possible, the slower velocity is used to create incipient damage. The flyer hits a 25-mm 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-mm diameter center of the target flies into a catch tank, where it is recovered with minimal additional deformation.

Belak and physicist John Kinney obtain three-dimensional (3D) x-ray tomographs in 700 orientations of target pieces containing incipient spall using the Stanford Synchrotron Radiation Laboratory. The 5- μ m resolution images 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 tomographic data are taken, the samples are sectioned to make detailed comparisons with traditional two-dimensional microscopy. The synchrotron imagery is considered a breakthrough. Data are obtained of the 3D void distribution just from the images without having to take thin slices of the material and count the number of voids in each slice.

Three-dimensional simulations at the atomic level that track how voids grow and link are being performed by Belak and physicists Robert Rudd and Eira Sepp. The simulations feature 1-10 million atoms representing the crystal structure of aluminum and 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.

Closing up voids



Photomicrograph of a copper disk used in a gas-gun experiment showing the formation of voids in the spall layer

In some cases, layers of a spalled material can collide as the pressure from the high explosive continues to drive one of the surfaces, resulting in 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.

Simulations currently do not include experimentally based models of recompression behavior. Including such models is necessary for accurate stockpile stewardship calculations. The objective is 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 the ASCI code. Recompression experiments are being performed on recovered metal disks that contain well-characterized spall damage using a gas gun and copper targets the same size and shape as those used in the experiments to create spall.

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 compressed at various rates to close the voids. Microstructural evolution and the manner in which the damage is being closed are characterized in sections of the targets.

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

Probing with x rays

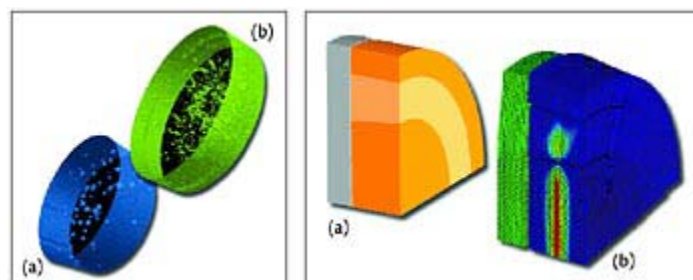


Fig. 1: The Stanford Synchrotron Radiation Laboratory is used to obtain three-dimensional x-ray tomographic images of experimentally produced incipient spallation. The images are from a 6-mm region in the center of the spall plane in single-crystal aluminum (a) and polycrystalline aluminum (b). Fig. 2: Simulation of a gas-gun experiment; initial configuration of aluminum striking a copper target (a), and formation of spall (b). The green area on the left is the aluminum plate that strikes a 5-mm 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.

LLNL physicist Dan Kalantar demonstrated the recovery of 500-um thick shocked single-crystal copper samples using lasers. The experimental results are helping to refine the development of models of void growth and spall formation. The laser experiments provide pressures greater (in some cases exceeding 100 GPa) than those produced in experiments using high explosives. The laser pulse lasts 2 to 5 ns 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 aimed at developing a technique called time-resolved, dynamic x-ray diffraction, which 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.

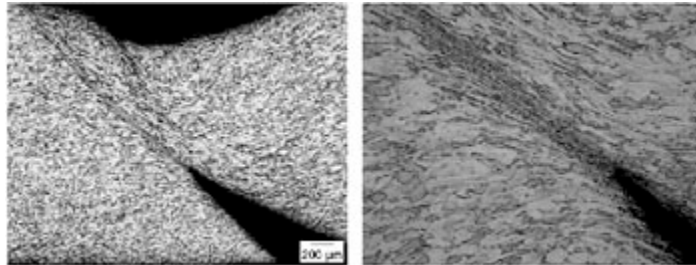
The diagnostic x rays provide a means to record the response of the metal's lattice as the shock from the laser pulse passes through. The x-rays are diffracted simultaneously from multiple planes within the metal's crystalline lattice. Kalantar developed a large-angle film detector that records the diffracted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

The recovery of 500-um thick shocked single-crystal copper samples also was demonstrated using an Omega laser. Direct laser irradiation generates a high-pressure shock that causes the formation and coalescence of voids, which, in turn, creates spall. The final structure is characterized by examining thin

slices of the targets, and the effect of the dislocation microstructure on the x-ray diffraction pattern is compared with the dynamic x-ray diffraction pattern.

Further work is aimed at extending the dynamic diffraction experiments using the two beams of the Janus laser. In addition, two-beam experiments are being designed to shock materials, create voids and incipient spall with one beam, and then recompact them with the second beam.

Exploding metal cylinders solve part of the puzzle



Micrograph of a tantalum-tungsten alloy cylinder driven by a gas gun shows that the material breaks along shear bands (darker diagonal line), left; crack tip at a higher magnification, right. Micrograph courtesy of Anne Sunwoo.

Physicists Ted Orzechowski, Omar Hurricane and colleagues are exploding cylindrical samples of metals and monitoring how they fracture and then fly apart. The failure of the metal cylinders is analyzed via high-speed images. Hurricane, in collaboration with a group of scientists led by Lalit Chhalabildas at Sandia National Laboratories (Albuquerque, N.M.), is looking at the failure of metals at high strain rates caused by 2.5-cm long Lexan(tm) flyers fired from a gas gun and traveling at about 2 k/s. The flyer slams into another piece of Lexan inside a 5-cm long metal cylinder 1, 3 or 5 mm thick having a 1.2 cm inside diameter. Cylinders are made of AISI 1045 carbon steel, Nitinol (Ni-Ti alloy) and tantalum-tungsten alloy. Upon impact, the Lexan behaves a bit like a working fluid, driving the cylinder radially outward.

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 GPa. Although there is a shock, it is the rapid radial expansion that causes the material to fracture.

The experiments are heavily monitored using diagnostics that record the strain rate at different positions on the cylinder. Optical cameras allow watching 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. The soft-captured fragments (fragments captured with light materials to prevent further damage) are sectioned and examined using 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 using high explosives to study the dynamics of fragmenting cylinders measuring about 5 cm OD by 20 cm long. The "pipe-bomb" experiments involve

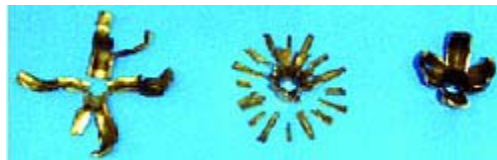
pressures up to 10 times greater (about 20 GPa) than those generated in the gas-gun experiments, but the different pressure regimes complement each other. The experiments provide the data required to develop, improve and validate material failure models for different kinds of weapons. The goal is to improve the understanding of failure and fragmentation of metals and alloys subjected to explosive force. 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 Office of Munitions.

Preliminary experiments were conducted by John Molitoris at Livermore's High Explosives Applications Facility, and physicist Peter Bedrossian is continuing the experiments at the lab's remote Site 300. The cylinders, made of 1045 carbon steel, Cartech's AerMet 100 steel and a uranium alloy, are detonated from one end. The high-explosive detonation front sweeps along the axis, with the shock lasting for several microseconds. The metal fragments that are violently produced are soft captured using glass wool or other light materials.

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 Los Alamos National Laboratory Neutron Science Center by LLNL physicists Bedrossian and Hye-Sook Park. Proton radiography provides sequential radiographs that show the details of cracks evolving and the cylinder disintegrating into many fragments. The cylinder material is characterized before the experiment and fragments are examined to determine their mode of failure.

As in the gas-gun experiments, shear bands are present where the cylinder rips apart. Test results show that material microstructure may affect its performance. For example, experiments reveal differences between steel cylinders that are heat-treated to increase hardness and those that are untreated.

Putting It All Together



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.

Results from the various LLNL experimenters are incorporated into the evolving computational models of how materials fracture and fail under extreme conditions. Data on material characterization, metallurgical analysis and dynamic experiments are helping to constrain and guide the 3D-code development. In particular, the code development is being aided by insights gained from examining different material microstructures both before and after experiments. Initial simulations using the advanced models are encouraging, but more research is necessary.

The modeling effort is aided by simulation advancements made by other Laboratory researchers. For example, geophysicists 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. Also, glass, a highly brittle material, is vitally important to scientists preparing to operate the National Ignition Facility, now under construction at LLNL to serve the stockpile stewardship mission.

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ANNOUNCEMENTS

AAM Fellow awarded 2005 A. C. Eringen medal

Cornelius (Niall) O. Horgan, University of Virginia, has been awarded the 2005 A. C. Eringen medal by the Society of Engineering Science (SES). The prize is awarded by the SES in recognition of “sustained outstanding achievements in Engineering Science”. The award certificate cites Horgan’s “seminal contributions to applied mathematics and the theory of elasticity”. The Eringen medal was first awarded in 1976 and previous recipients have been selected from a diverse group of outstanding engineers and scientists including three Nobel laureates. The medal was presented to Professor Horgan at the joint SES/ASME/ASCE Meeting on Mechanics and Materials, Baton Rouge, LA, June, 2005 on which occasion he presented the SES Annual Engineering Science Plenary Lecture entitled “ Continuum mechanics based hyperelastic strain-stiffening constitutive models for rubber-like materials”. This lecture described recent research of Professor Horgan and colleagues on the mathematical and continuum mechanical modeling of rubber-like and biological materials. This work has numerous applications in engineering ranging from rubber vibration isolators for structures to modeling of soft biological tissues.

Horgan is the Wills Johnson Professor of Applied Mathematics and Mechanics in the Department of Civil Engineering, School of Engineering and Applied Science, University of Virginia. He was educated at the National University of Ireland (B.Sc. 1964, M.Sc. 1965, Mathematical Science) and at the California Institute of Technology (Ph.D. 1970, Applied Mechanics). He has held positions at the University of Michigan, The University of East Anglia, Norwich, England, the University of Houston and Michigan State University. He has held visiting summer appointments at Caltech (1979, 1981) and Cornell University (1982), and visiting professorships at Northwestern University (1977-1978), Caltech (1984-1985), Universita di Pisa, Italy (1996, 1997), Universita di Ferrara, Italy (2001, 2003), Universita di Lecce, Italy (2001, 2003) and Universidad Politecnica de Catalunya, Barcelona, Spain (1999, 2003). His research interests are in applied mechanics (mechanics of solids and materials) and applied mathematics, in which fields he has authored or co-authored nine invited book chapters, over 150 publications in refereed archival journals and numerous Conference Proceedings papers. Dr. Horgan is a member of the American Society of Mechanical Engineers (founding chairman of the Elasticity Committee, AMD, 1981-1986), the American Academy of Mechanics, the Society for Natural Philosophy, the American Mathematical Society, the Society for Industrial and Applied Mathematics, the Society of Engineering Science (Board of Directors 1993-1999) and the International Society for the Interaction of Mechanics and Mathematics (Executive Committee 2001-2005). He is one of the managing and founding editors of *Mathematics and Mechanics of Solids*, and serves on the Editorial Boards of the *J. of Elasticity* and the *International J. of Nonlinear Mechanics*. He was a member of the editorial board of the *SIAM J. on Applied Mathematics* from 1995-2004, an Associate Editor of the *Journal of Applied Mechanics* from 1988 – 1992, and an Associate Editor of *Applied Mechanics Reviews* from 1985-2000. In 1983 he was awarded the degree of Doctor of Science (D.Sc.) by the National University of Ireland, in 1985 was elected Fellow of the American Academy of Mechanics and was elected Fellow of ASME in 1992.

Faculty Position

UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN (UIUC).

The Department of Civil and Environmental Engineering (CEE) invites applications for a full-time structural engineering faculty position in **COMPUTATIONAL MECHANICS**. Qualified applicants at all levels will be considered. Successful candidates are expected to develop an internationally recognized research program and to contribute fully as a scholar through teaching of undergraduate and graduate courses and through service to the profession. Candidates should complement, strengthen, or open new directions pertinent to structural engineering and computational mechanics in CEE at UIUC. We are particularly interested in candidates pursuing research in multiscale, multiphysics computational methods, adaptive material and structural systems, and the merging of computations with experimental testing. The Department is home to the new George E. Brown Network for Earthquake Engineering Simulation (NEES) Multi-Axial Full-Scale Sub-Structures Testing and Simulation (MUST-SIM) facility, as well as to the NSF-sponsored Mid-America Earthquake (MAE) Center. In addition, significant opportunities exist with the National Center for Supercomputing Applications (NCSA), the Computational Science and Engineering (CSE) Program, the Materials Computation Center (MCC), and the Center for Advanced Studies (CAS). An earned doctoral degree is required, with background in civil engineering preferred. Salary is open and based on qualifications. Starting date is negotiable, but is preferred to be no later than January 16, 2006. To ensure full consideration, applications must be received by September 1, 2005. Interviews of promising candidates may be conducted before the closing date, but the final decision will not be made until after that date. All applications should be submitted electronically (paperless process) as a single PDF document to: cee-searches@uiuc.edu. Electronic applications should include a cover letter describing the principal expertise of the applicant, a statement of teaching and research interests and experiences, and a complete resume. Candidates at the Assistant Professor level should also provide addresses of at least three references. The cover letter should be addressed to Professor Robert H. Dodds, Head, Department of Civil and Environmental Engineering, 1114 Newmark Civil Engineering Laboratory, 205 North Mathews Avenue, Urbana, IL 61801. Telephone: 217-333-3814. Information about the department may be found at our website at <http://cee.uiuc.edu/>. The Department is committed to building a diverse environment; minorities, women, and other designated class members are encouraged to apply.

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