National Nuclear Security Administration

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Office of Research, Development, Test, and Evaluation (RDT&E)

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CALENDAR

10/13-17
2019 Fall Meeting of the American Physical Society (APS) Division of Nuclear Physics, Arlington, Virginia

10/21-25
61st Annual Meeting of the APS Division of Plasma Physics, Ft. Lauderdale, Florida

11/17-22
SC19: The International Conference for High Performance Computing, Networking, Storage, and Analysis, Denver, Colorado

INSIDE

*Contractor Support

As the Acting Assistant Deputy Administrator for Research, Development, Test, and Evaluation (RDT&E), it is my pleasure to welcome you to the latest issue of *Stewardship Science Today* (SST). Over the last several months, our office has been able to recruit top talent to join the team, and in this issue we welcome our newest staff members and Fellows to RDT&E. We also feature the top talent that was awarded the prestigious 2019-2020 Stewardship Science Graduate Fellowships and Laboratory Residency Graduate Fellowships and highlight the research of this esteemed group of young researchers.

Other highlights of this issue include research into turbulence features critical to stockpile performance and to ignition work conducted at the National Ignition Facility. This work seeks to better understand the Richtmeyer-Meshkov instability through experiments conducted using vertical shock tubes at the University of Arizona's Fluid Instability Laboratory. We also feature research that seeks to better understand the impacts of additive manufacturing (AM) on materials, especially materials used in the stockpile. AM is an innovative approach to producing complex parts, but the impact of the manufacturing process on the microstructure of the materials produced still is relatively unexplored. Work conducted by Carnegie Mellon University using the experimental capabilities at the Advanced Photon Source at Argonne National Laboratory is working to close the gap on the unknowns associated with phase transformations, thermal effects, and microstructure evolution in AM materials. Last but not least, we are pleased to celebrate 10 years of operations and 2,700 experiments at the National Ignition Facility in Livermore, California. We wish the world-class facility many more years of success and technological breakthroughs.

We are dedicated to featuring the extraordinary talent and innovative research of the stockpile stewardship community. We hope that you enjoy this issue!

Dr. Mark Anderson
Acting Assistant Deputy Administrator
for Research, Development Test, and Administration

New Faces at the Office of Research, Development, Test, and Evaluation

We have the pleasure of welcoming two federal program managers and three Fellows from the National Nuclear Security Administration (NNSA) Graduate Fellowship Program to the Office of Research, Development, Test, and Evaluation (RDT&E).

Dr. Tod Caldwell comes to us from the NNSA Office of Nuclear Export Control. He has a PhD in condensed matter physics and will work for the Office of Experimental Sciences (OES). Caldwell will manage the Primary Assessment Technologies program and serve as the point of contact for the JASON study on plutonium aging.

Dr. Samantha Calkins comes to us from the Department of Energy Energy Information Administration, with previous experience at the Homeland Security Studies and Analysis Institute and as a postdoctoral Fellow at the Defense Threat Reduction Agency. She has a PhD in nuclear physics and will work for the OES. Calkins will manage the Advanced Radiography program and serve as the technical program manager for the radiochemistry and low energy nuclear science areas of the Stewardship Science Academic Alliances program.

Our Fellows this year each will work with an RDT&E office. We are pleased to welcome:

Office of Experimental Sciences

Bryant Vande Kolk
PhD candidate, Nuclear Physics, University of Notre Dame

Office of Advanced Simulation and Computing and Institutional Programs

Zachary Matheson
Dual PhD, Nuclear Physics and Computational Math, Science, and Engineering, Michigan State University, 2019. Stewardship Science Academic Alliances, 2015-2019.

Office of Engineering and Technology Maturation

Hannah Gardiner
PhD, Nuclear Engineering, University of Florida, 2019

Turbulence Measurements in Richtmeyer-Meshkov Instability Shock Tube Experiments

by E.G. Sewell, K.J. Ferguson, and J.W. Jacobs (University of Arizona)

The Richtmeyer-Meshkov instability (RMI) occurs when the interface between two fluids of different density is impulsively accelerated. This acceleration results in the growth of perturbations at the interface that can evolve into a turbulently mixed zone. The RMI appears in many natural phenomena, such as the mixing of stellar gases due to supernova explosion and in scramjet (supersonic combustion ramjet) engines where it is responsible for the mixing of air with fuel for combustion. It is one of the major obstacles in attaining positive net-yield inertial confinement fusion (ICF) at the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory. Accurate modeling of RMIs is a critical component of NIF experiments and stockpile stewardship research.

The University of Arizona Fluid Instability Laboratory studies the RMI using vertical shock tubes. A vertical shock tube is a long, narrow tube where pressurized gas, initially confined in the top end (the driver), is released suddenly by the bursting of a diaphragm. The release of pressure results in the formation of a shock wave that travels down the length of the tube through the first gas towards the interface that exists with the second gas at the other end. Figure 1 shows the interface formation method.

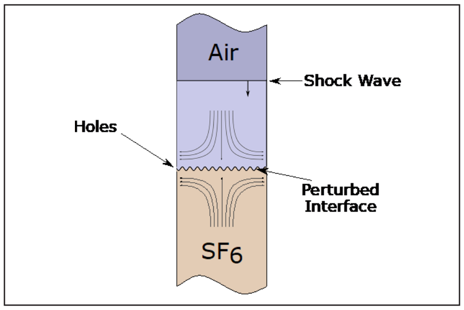

Figure 1. Gases flow from opposite ends of the shock tube meeting in the test section where small holes allow the gases to exit to form the interface. Faraday waves are excited on the interface by vertically oscillating the gas column to produce the perturbation. The downward travelling shock wave then impacts the perturbed interface resulting in the RMI.

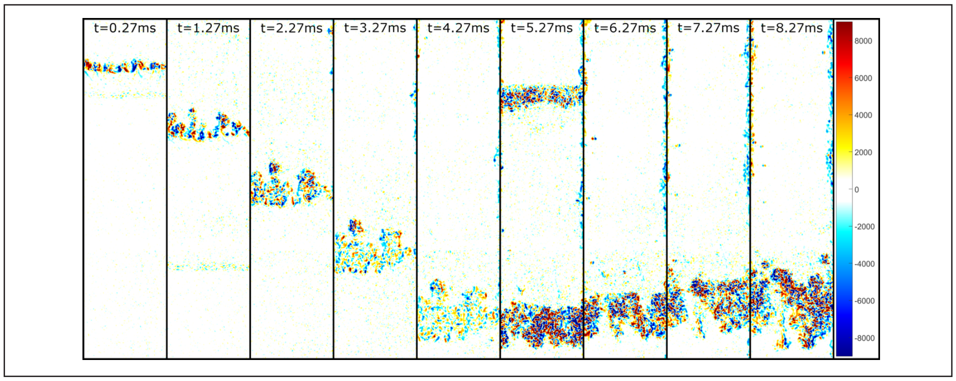

Figure 2. Velocity fields from a typical experiment with reshock rendered in pseudocolor of vorticity. The incident shock wave impulsively accelerates the interface at t = 0, after which RMI develops as the interface is pushed down the shock tube by the flow imposed by the shock wave. The interface is accelerated a second time at t ≈ 4.5 ms by the reflected shock wave producing reshock and resulting in significantly increased turbulent mixing.

This action accelerates both gases and produces the instability. A set of high-speed lasers and cameras are used to image the growth of the RMI in the shock tube, both in the "incident" regime after the shock wave first arrives at the interface and in the "reshock" regime when a second shock wave "reflects" off the bottom of the tube and interacts with the interface. These images then can be processed to extract meaningful data, such as a map of fluid velocity using high-speed particle image velocimetry as shown in Figure 2, or gas concentration fields within the tube using high-speed Mie scattering, or planar laser induced fluorescence. These measurements can be analyzed through various methods to extract useful properties describing the RMI, such as its growth rate, kinetic energy, and energy loss through dissipation.

It is important to emphasize that, whereas many of the applications motivating the study of RMI involve high energy density (HED) physics and employ materials other than ideal fluids, one of the ultimate defining complexities most important to these applications is turbulent mixing, which is more effectively studied in lower energy gas flows such as in shock tube experiments. Shock tube experiments have much greater diagnostic capability than HED experiments making them the preferred experimental method for the study of turbulence in applications such as ICF.

The University of Arizona laboratory has two shock tube designs currently being used to study the RMI. The first is a "traditional" shock tube, which has a single pressurized driver section at the top of the tube and where the reshock is initiated by the reflected shock wave from the bottom of the tube. A second "dual shock" design also has been developed which has two pressurized driver sections, one located at the top of the tube and the other located at the bottom. The dual shock design enables greater flexibility over the arrival times of the incident and second shock waves, providing an improved ability to study the effect of reshock on the RMI. A second benefit of this design is that it eliminates additional reflected waves from the bottom of the tube allowing the instability following reshock to be studied at much later times than is possible using a traditional design.

The University of Arizona works closely with scientists at Lawrence Livermore National Laboratory to generate data which is then used in verification and validation studies of the hydrodynamic simulations where these instabilities also arise. The collaborative nature of this work is crucial to developing an advanced understanding of the many research problems that face the Department of Energy/National Nuclear Security Administration and stockpile stewardship programs.

This work is supported by the Department of Energy/National Nuclear Security Administration under Award Numbers DE-NA0002929 and DE-NA0003903. ◆

High-Speed Dynamic X-ray Diffraction Analysis of Additive Manufacturing

by Seunghee Oh[a], Joseph Pauza[a], Joseph Aroh[a], Sidi Feng[a], Rachel Lim[a], Christopher Kantzos[a], Andrew Chuang[b], Niranjan Parab[b], Cang Zhao[b], Tao Sun[b], Robert M. Suter[a], and Anthony D. Rollett[a]

Recent developments in additive manufacturing (AM) allow extremely complex parts to be produced that are not attainable with traditional techniques. Computer-based modeling, fine powder size, and a small laser spot size make it possible to manufacture metal parts that are highly accurate in their structure and geometry.[1,2] However, there are many scientifically unexplored issues that impact AM and the mission of stewardship science such as unusual microstructures and non-equilibrium phase transitions.[3] Moreover, because the extreme heating and cooling rates[4] (over 106 K/s), the characterization is complicated and challenging. There is no doubt that the characterization of the rapidly-evolving phases during melting and solidification is crucial for understanding the complexity of AM processes.

Our group from Carnegie Mellon University has been working on the high-speed characterization of AM in cooperation with the Advanced Photon Source (APS) at Argonne National Laboratory. Using a setup similar to that used to observe particle dynamics during laser melting, an *in situ,* high-speed, synchrotron X-ray dynamic diffraction and imaging technique[5] at the APS allows us to monitor high-speed events. This technique allows us to quantify transient behaviors including phase transformations, thermal effects, and microstructure evolution during melting and re-solidification. *In situ* measurements have been successfully conducted at beamline 1-ID with the help of APS beamline scientists. A 500 W laser coupled with a scan head, found in commercial three-dimensional (3D) printers, was utilized. A high-energy (55.6 keV), monochromatic X-ray beam allowed dynamic behavior in the melt pool to be measured in transmission. A Pilatus 2D detector with 2.5 million pixels and 250 Hz readout speed (4 ms frame interval) was used. Figure 1 illustrates the apparatus inside the X-ray hutch.

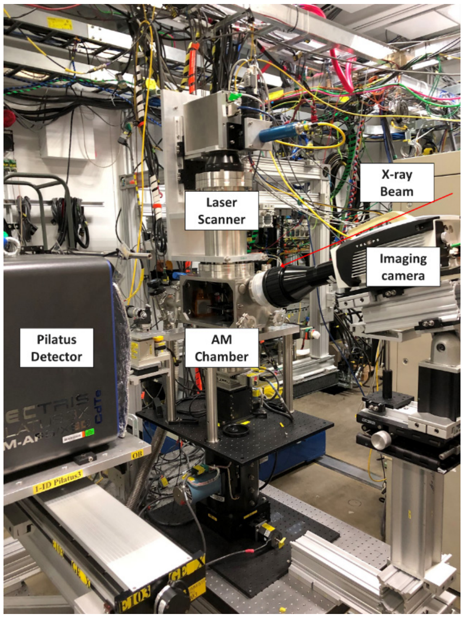

Figure 1. In-situ high-speed synchrotron X-ray diffraction and imaging system. X-rays, incident from the right, are diffracted at AM samples inside the stainless steel chamber below the laser scanner. Diffracted beams are collected by the Pilatus detector. A separate imaging detector (not shown), in-line with the incident beam, allows for imaging of laser-powder interactions via absorption contrast.

Each output image (frame) exhibits well-resolved Bragg rings from each phase (see Figure 2a). Bragg rings are the angles for coherent and incoherent scattering angles from a lattice. The time-resolved image sequences reveal the structural evolution happening within less than a second. Right after the laser light heats the material, the Bragg rings are contracted and diffused out as melting proceeds. After the laser light turns off, the Bragg rings reappear and return to their original positions as the material cools. Whereas the image array sequence illustrates the qualitative behavior, converting data through several calibrations and calculations provides more fundamental and quantitative information about the material phase changes. Various time-resolved, structural information such as the temperature of specimens, the local strain of crystal phases, phase transformations, and the occurrence of precipitation is obtained and quantified.

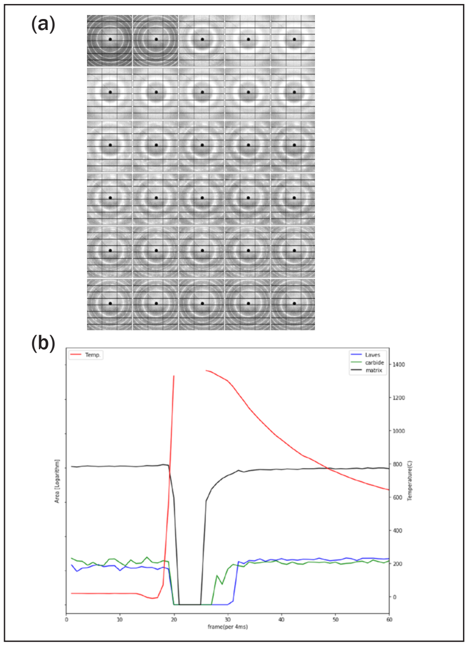

Figure 2. Time-resolved data by dynamic X-ray diffraction. (a) Expansion, vanishing, spatial distribution, and reformation of Bragg rings present qualitative information about melting, intermetallic compound formation, and solidification. (b) The quantitative analysis in peak area (shown in Log scales) demonstrates the transforming behavior of matrix, Laves and carbide phases over a time span around melting and solidification.

As an example, Figure 2b shows the integrated area of selected peaks in the diffraction patterns that measure the relative amount of each phase. The example is from an experiment conducted on Inconel 718, which is one of the few AM-qualified, nickel-based superalloys needed for high-temperature service. As shown, the quantities of each phase vary strongly over time, as the melting and solidification proceed. Moreover, the rapid re-precipitation of the Laves and carbide phases is surprising in comparison to standard information on time-temperature-transformation behavior in this alloy. The *in-situ* measurement, therefore, provides useful information for understanding the kinetics of phase formation which already reveals marked differences from the existing metallurgical literature on this alloy. Such results are critical for understanding the mechanical properties and quality of AM products.

The employment of this novel measurement is expected to present

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[a] Carnegie Mellon University

[b] Advanced Photon Source, Argonne National Laboratory

new information that will contribute to ongoing improvements in AM processing. The precise data obtained from high-speed, zero background, and high dynamic range images from the Pilatus detector enable us to observe even minor changes during the high- speed AM melting process. In addition to the AM field, this analysis also will give the stewardship science community ways to explore other phase change phenomena not accessible with conventional tools. For example, the development of residual stress from the rapid temperature drop evidently influences properties and the formation, e.g., thermal cracking. This *in situ* high-speed X-ray dynamic diffraction analysis will expand our capability from static to transient vision for better understanding of physical behaviors.

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2019 DOE/NNSA Stewardship Science Graduate Fellowship and Laboratory Residency Graduate Fellowship Annual Program Review

To support a pipeline of the next generation of world class scientists and engineers to the NNSA national laboratories, the Office of Research, Development, Test, and Evaluation (RDT&E) sponsors the Stewardship Science Graduate Fellowship (SSGF) and Laboratory Residency Graduate Fellowship Programs (LRGF). The SSGF and LRGF Annual Program Review was held in Washington, D.C. June 25-27 and attended by more than 67 NNSA and national laboratory professionals, graduate students, and members of the scientific community. Some photos from the review follow. (a) Dr. William Bookless, NNSA Principal Deputy Administrator, welcomed attendees. (b) Dr. Njema Frazier, Director, NNSA Office of Experimental Sciences, gave the keynote address on Science, Stewards, and the Nuclear Deterrent. (c) Dr. Sarah Nelson Wilk, Deputy Director, NNSA Office of Experimental Sciences, kicked off the Fellows' Poster Session with a welcome. For more information about these fellowship programs, visit: https://www.krellinst.org/ssgf/.

2019 DOE/NNSA Computation Science Graduate Fellowship Annual Program Review

The 2019 Computational Science Graduate Fellowship (CSGF) Annual Program Review, held in Arlington, Virginia, July 14-18, hosted nearly 200 attendees this year. Jointly sponsored by DOE's Office of Science and NNSA's RDT&E, CSGF helps ensure a supply of scientists and engineers trained to meet workforce needs in computational science. Pictured on the right: Dr. Charles P. Verdon, NNSA Deputy Administrator for Defense Programs welcomes attendees on behalf of DOE/ NNSA.

2019 Presidential Early Career Award for Scientists and Engineers (PECASE)

Two of this year's PECASE winners are alumni of the Stewardship Science Graduate Fellowship program. **Dr. Matthew Gomez** works in Radiation and Fusion Sciences at Sandia National Laboratories. **Dr. Richard Kraus**, a research scientist at Lawrence Livermore National Laboratory, studies materials at high pressures. The PECASE is the highest honor bestowed by the U.S. Government to outstanding scientists and engineers who are beginning their independent research careers and who show exceptional promise for leadership in science and technology.

2019-2020 Stewardship Science Graduate Fellowship and Laboratory Residency Graduate Fellowship Classes

by The Krell Institute

Five students will join the Department of Energy/National Nuclear Security Administration (DOE/NNSA) Stewardship Science Graduate Fellowship (SSGF) this fall, and a cohort of four joins the DOE/NNSA Laboratory Residency Graduate Fellowship (LRGF) in its second year. The SSGF program requires fellows to serve a 12-week practicum at an NNSA lab. The LRGF extends that to at least two practicums and encourages fellows to pursue their thesis research in collaboration with lab scientists. Fellows in both programs receive tuition, a stipend, and other benefits. The following accounts summarize research statements each fellow submitted.

Figure 1. 2019-2020 LRGF and SSGF Classes. Left to right: Eldred Lee, LRGF; Dane Sterbentz, LRGF; Ryan Childers, LRGF; Lauren Smith, SSGF; Patrick Adrian, SSGF; David Chin, SSGF; Sylvia Hanna, SSGF; and Justin Cheng, SSGF. Not pictured: William Brooks, LRGF.

Stewardship Science Graduate Fellowship

Massachusetts Institute of Technology student **Patrick Adrian** is designing OMEGA laser experiments to diagnose the magnitude of electron heat conduction for plasma conditions in spherical, shock-driven implosions. With advisor Johan Frenje, he'll stage low-density implosions and track the electron temperature at their cores where they are sensitive to the balance between energy gains by pdV work and losses due to heat conduction. Adrian will compare measurements gathered with the particle X-ray temporal diagnostic (PXTD) against simulations, aiming to constrain different electron heat conduction theories in high energy density plasmas. He will work on improving the PXTD instrument. "I plan to contribute both to the basic science of high-density plasmas and to their application" in inertial confinement fusion, he wrote.

At the University of Minnesota, **Justin Cheng** and advisor Nathan Mara will probe the properties of nanolayered bimetallic composites. These materials have outstanding strength and deformation resistance while tolerating radiation damage thanks to their high bimetal interface content where interfaces with specific atomic arrangements mitigate damage accumulation by atomic-scale defects. Their research will link synthesis parameters to interfacial structure before and after exposure to high temperatures and ion irradiation. Cheng will focus on deformation physics, radiation-induced defects and their interactions with interfaces, and microstructural stability. The team will quantify microstructure with scanning and transmission electron microscopy and perform *in-situ* testing to image and characterize deformation processes.

David Chin will tap compression techniques at the Laboratory for Laser Energetics at his home institution, the University of Rochester, to explore the extreme high energy density matter at planetary interiors through the study of iron oxide. His goal is to characterize complex phase transitions the materials undergo in extreme environments. Such experiments are key to understanding the nature of Earth and Earth-like planets, Chin writes. With advisor Gilbert Collins, he'll use X-ray absorption fine structure (XAFS) spectroscopy to characterize these compressed metal oxides *in situ*, providing simultaneous data on their local structure, density, and temperature. He plans to develop new diagnostic tools to improve the XAFS platform.

Metal-organic frameworks (MOFs), crystalline materials with such desirable properties as large internal surface areas, high porosity, and uniform channels, are the subject of **Sylvia Hanna's** research with Omar Farha at Northwestern University. MOFs of Zr_6O_8 have demonstrated stability and promise for capturing toxic radioactive compounds but could lose their structural integrity under extreme radiation. To gauge these effects, Hanna will expose Zr_6O_8 MOFs of varying topologies, porosities, and defect densities to extreme radiation. She'll explore how long-term radiation alters the materials' composition, arrangement, and aging. Hanna will collaborate with Sandia National Laboratories' Tina Nenoff to bombard the MOFs with extreme radiation and use instruments at Northwestern and at Argonne National Laboratory to characterize them before and after exposure.

Fellow **Lauren Smith** at the University of California, Santa Barbara, will use an open-source code from Los Alamos National Laboratory to model the effects of high strain rates on metals at the mesoscale. The Phase Field Dislocation Dynamics (PFDD) code will examine deformation dynamics at a range that will bridge atomic-scale and continuum-scale models. But PFDD was designed to treat dislocations, the primary metal deformation mechanism, in quasi-static loading conditions. To simulate strain rate, it must include accurate dislocation mobilities. Smith, working with Irene Beyerlein, will adapt the code to incorporate rate dependence. They will use this new model to study multi-principle element alloys, promising materials for use under extreme conditions.

Laboratory Residency Graduate Fellowship

Texas Tech University student **William Brooks** will head to Sandia's New Mexico campus to investigate detection of electron multiplication onset in vacuum and the consequent breakdown and flashover in pulsed-power devices. For example, a resonant condition of secondary emission with a radio frequency field can occur in waveguides carrying microwave radiation. The electrons moving in synch with the microwaves can strike component walls, desorbing gas molecules, generating heat, and leading to plasma generation and electric breakdown. With advisor Andreas Neuber, Brooks will detect electron number increases and track plasma development. He plans to test plasma/chemical vapor deposition surfaces for breakdown onset and increase electric field levels and diagnose developing electron numbers to validate experiments. He hopes to recommend materials and treatments to mitigate electron multiplication and plasma development.

Ryan Childers of the University of Nevada, Reno, also will go to Albuquerque to model X-ray spectroscopy from the Z machine, aiming to determine the primary mechanism behind Kα fluorescent emission in high energy density plasmas. Both hot, non-thermal electron excitation and photon excitation/ionization drive this emission, but it's unknown which, and under what conditions one dominates. With advisor Alla Safronova, Childers will use theoretical spectral modeling of Kα emission data and advanced diagnostic energy-flux data from Z machine experiments to seek spectroscopic-energy signatures associated with excitation mechanisms. They'll compare theoretical analysis of Z machine nested wire array data with X-pinch data from the University of Nevada's Zebra pulsed-power generator, seeking similar and/or different characteristics alluding to excitation modes.

At Los Alamos, **Eldred Lee** of Dartmouth College will target X-ray imaging detectors. Advisor Jifeng Liu's lab previously tested tin-based, metal-oxide silicon (MOS) structures to absorb hard X-rays and transport UV-excited hot electrons to the silicon conduction band. They've tested detectors with a copper layer over a thin-film CdTe detector. To develop efficient methods to detect hard X-rays (40 to 100 keV photon energies) with ultra-fast imaging, Lee will use MOS structures by generating hot electrons in an effective X-ray absorber and transferring them to a semiconductor, integrating the method into CMOS image sensors. He will investigate materials combinations for metal buildup layer-thin-film semiconductor X-ray detectors and determine scaling feasibility. Integrating findings from the approaches may lead to more efficient hard X-ray detection.

With advisor Jean-Pierre Delplanque, **Dane Sterbentz** of the University of California, Davis, will devise a theoretical framework to address the lack of time to reach true equilibrium in high energy density equation-of-state experiments. This can cause a lag in time needed for a transition to become observable. With his models, users could deconvolve the transition kinetics found in dynamic-compression experiments to determine materials' true equilibrium behavior. At Lawrence Livermore National Laboratory, he has created a standalone solver for the Zel'dovich-Frenkel equation for the evolution of phase transitions. His code appears to produce the observed lag but without a need for empirical scaling to account for kinetic transience. Using the transition of water to ice VII, Sterbentz plans to couple this model with a continuum multiphysics code that Jonathan Belof and other Livermore researchers developed. He'll validate the code with comparisons to experiments. ◆

The National Ignition Facility Celebrates 10 Years of Operations

The National Ignition Facility (NIF) at Lawrence Livermore National Laboratory (LLNL) recently celebrated 10 years of operations and more than 2,700 experiments. Several distinguished guests/speakers attended the anniversary celebration on August 13, including (from left) Bill Goldstein, director of LLNL; John Marchand, mayor of the City of Livermore; Representative Jerry McNerney; Mark Herrmann, director of the National Ignition Facility; Lisa E. Gordon-Hagerty, Department of Energy Under Secretary for Nuclear Security and Administrator of the National Nuclear Security Administration (NNSA); Mark Anderson, NNSA's Acting Assistant Deputy Administrator for Research, Development, Test, and Evaluation; Pete Rodrik, manager of the Livermore Field Office; Jeff Wisoff, principal associate director of NIF and Photon Science; Representative Zoe Lofgren; Kim Budil, principal associate director of Weapons and Complex Integration; and Representative Bill Foster.