Office of Defense Science

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Chris Deeney, Director, Office of Defense Science

Welcome to the inaugural issue of the Office of Defense Science newsletter!

These newsletters will communicate two themes important to the Office of Defense Science (also know as the Science Campaign): the direct impact of the Science Campaign on the nuclear weapons program; and the quality of the science supported by our program. To achieve these goals, each quarterly newsletter will contain unclassified articles that discuss major progress within the Science Campaign and they will highlight recent high-impact journal papers and awards. We will also take the opportunity to demonstrate the strong ties that the Science Campaign has with the other parts of the Defense Program (in particular with Advanced Simulation and Computing, Inertial Confinement Fusion, Engineering, and Directed Stockpile Work) and the collaboration between the laboratories, the Nevada Test Site, and other DOE/NNSA organizations.

In this issue we will discuss THERMOS and DARHT. The THERMOS series at the Nevada Test Site has yielded high quality data on damage and failure in plutonium that will be critical to developing predictive physical models for these mechanisms in stockpile applications. In addition, these experiments were a terrific demonstration of cost-effective (always appealing to someone born in Scotland) use of a major NNSA asset. The second article discusses the progress with the DARHT 2nd axis which has demonstrated multi-pulse capability and achieved full energy and current operation from the refurbished accelerator. On the quality of science front, we have selected three excellent recently published papers on materials in extreme conditions, which is a subject garnering much attention just now, in part due to the recent outstanding workshop in the field conducted by Jeff Wadsworth under the auspices of DOE's Office of Basic Energy Sciences. This field offers a wonderful opportunity for collaboration between NNSA and the Office of Science, especially in predicting material performance based on processing, i.e. process-aware models.

On a personal note, I have been in my new position as Director of the Office of Defense Science for a year now, and I truly enjoying working here. The Science Campaign and Defense Programs are a great group of people and make an excellent team. I am very proud of the accomplishments of the Science Campaign, the university programs and our international collaborations. This Office is committed to excellence in getting the job done, and I am delighted that a science goal that integrates the Office of Defense Science, the Office of Advanced Simulation and Computing, the Office of Stockpile Assessments and Certification, and the Office of Inertial Confinement Fusion and the National Ignition Facility Project activities has made it to Tom D'Agostino's "Getting the Job Done" list for FY2008.

The next fiscal year will be a busy year for the Office of Defense Science: completing two "Getting the Job Done" goals (DARHT and Energy Balance); restarting a defense science program on ZR; and working with the rest of NA-11 to complete the Predictive Capability Framework (PCF) Roadmap. As a part of the PCF, we will also begin the implementation of the Boost Initiative. The National Integrated Project Team has been working hard over the summer to plan the program and create the defining strategy document. This is an exciting endeavor since it will create a significant advance in the Stockpile Stewardship program plus it will be an integrating theme for our key scientific pillars (materials, hydrodynamics, nuclear physics, and high energy density plasmas). This initiative will also be another opportunity to show how integrated experimental, theoretical and computational science impacts NNSA's overall program, just as the energy-balance goal will in 2008.

Thank you all for your dedication and your interest in stockpile science, and now for the cool technical work.....

THERMOS – A Small-Scale Experimental and Computational Study of Plutonium Deformation/Damage/Failure Physics by Curt Bronkhorst, LANL

During the months of February, March, and April of this year, a series of twelve small-scale explosively driven plutonium experiments were successfully conducted underground at a test complex at the Nevada Test Site. The purpose of these experiments was to explore the physical processes involved in the deformation, damage, and failure process under such loading conditions as well as provide a comprehensive data set for equation of state and material model development and validation. These experiments represent the experimental component of a combined theoretical/computational/ experimental collaborative effort being conducted in order to further advance our ability to predict weapons performance within the stockpile stewardship program. These experiments were conducted by scientists at Los Alamos National Laboratory with strong collaboration with the Joint Nevada Project Office, National Security Technologies, and Sandia National Laboratory. The experimental work is being funded collaboratively through the Science Campaign and Pit Lifetime. Modeling and theoretical work is being funded by the Advanced Simulation and Computing (ASC) program.

Most metallic materials are polycrystalline in nature which means that they are an aggregate composite of metallic single crystals. As the polycrystal is deformed the single crystals interact with each other so that the internal stress within the polycrystal is highly non-uniform. Simulations predict a factor of two or so difference between the minimum and maximum stress within the aggregate. If these materials are deformed a great deal, they begin to develop damaged regions and failure zones. The location of these damaged and failed regions is highly dependent upon microstructural characteristics (e.g. grain size distribution, impurity content, grain boundary strength) and the nature of the loading (e.g. time rate of loading, total strain, maximum stress). Figure 1 shows an image of tantalum deformed by plate impact loading. The individual single crystals are displayed as different colored regions while the damaged and failed regions are black. This image displays a snapshot of a material which has failed by the process of pore nucleation, growth and coalescence (a ductile process). Note that the failed regions are spread out and indicate that the physical processes involved are stochastic in nature.

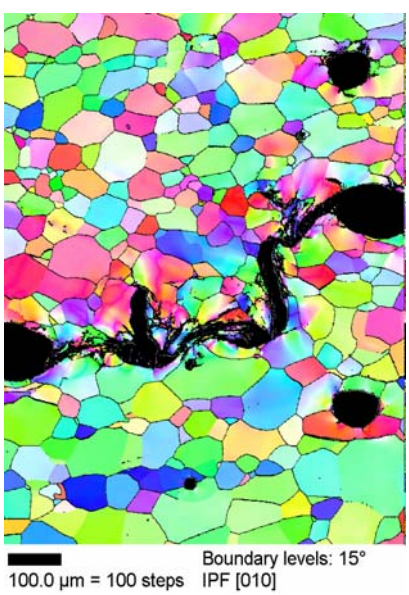

Figure 1. Orientation Image Map of a deformed tantalum plate impact sample

The THERMOS series of experiments was designed to explore the physical processes involved in the deformation, damage, and failure behavior for plutonium. The sample was a wafer of plutonium with dimensions 2 mm thick and 8 mm diameter. The sample was loaded by a wafer of explosive material of the same diameter and three different thicknesses to vary the loading rate and maximum pressure achieved. Two different detonation positions were also used as well as two different perimeter boundary conditions. These three variables comprised the twelve shots in the series of experiments.

The complex has the capability to take transmission radiographic images of the sample as it is in the process of being deformed. This was done for these experiments. In addition, the time history of the free surface velocity of the sample at six different positions was measured through the use of laser based photon doppler and visar velocimetry techniques. Finally, the experiment was conducted in a small canister (Figure 2) which was specially designed to arrest the sample and preserve its integrity so that the deformed sample could be extracted and examined metallographically. The metallographic analysis of the deformed sample is crucial to our gaining the understanding necessary to developing adequate physically based constitutive models to represent this complex physical process in materials of strategic importance.

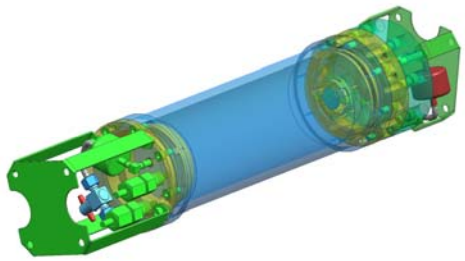

Figure 2. A scaled drawing of the THERMOS canister, which has an outer diameter of 105mm

In conclusion, the THERMOS series of experiments were highly successful and represent the results of a highly collaborative experimental/theoretical effort. These results will teach us much over the next several months and years as we put the pieces of experimental data together with theoretical results to advance our predictive capability and continue the success of the Science Campaign, ASC, and the Stockpile Stewardship Program.

Dual Axis Radiographic Hydrodynamics Test (DARHT) 2nd Axis Achieves Full Accelerator Configuration by Shahzaman Jaghoory, NNSA

Figure 1. DARHT Facility, Technical Area 15 at the Los Alamos National Laboratory

When underground nuclear testing was abandoned in 1992, the highest risk in the stockpile was the potential for an aged, remanufactured, or redesigned primary system to fail to provide the desired yield. A key method for diagnosing primary performance is radiography, which is why DOE identified and supported DARHT as one of its highest priority construction projects.

The DARHT facility is located within Technical Area-15 and is a reinforced concrete structure (see Figure 1). The facility was constructed in two phases as two separate line-item projects to support the primary assessment mission of NNSA. The first phase constructed the first axis, which was completed in FY 1999, was commissioned, and began operations as the Nation's foremost x-ray radiography hydrotest facility. The first axis has been producing high-quality radiographs of weapon systems that were previously not amenable to radiographic methods.

The second phase covered the construction of the 2nd Axis and received Critical Decision 4 in December 2002. The buildings housing the two axes are oriented orthogonal to each other, which enables a dual-axis time-resolved capability (Figure 2). Data from the 2nd axis is especially critical to reducing the uncertainties in predicted performance of a primary system.

DARHT 2nd Axis is made up of the injector vacuum vessel, 6 injector cells, 68 accelerator cells and associated controls and data acquisition system. The design-voltage for each of the injector and accelerator cells was 175 kV and 193 kV, respectively (Figure 3). While attempting to raise the accelerator cells operating voltage to the required levels, the cells started experiencing high voltage breakdowns at voltages well below their design levels. As a result, NNSA decided to establish a research and development (R&D) program to understand the causes of the problems and to identify potential design fixes.

The R&D program for the cell redesign was initiated in early FY04. The R&D program was merged with a new initiative, entitled "DARHT 2nd Axis Refurbishment and Commissioning Project", which was funded as an Expense Funded Congressionally approved project. The baseline total project cost was and still is $89.8M and was funded over a five-year period starting in FY 2004. The scope consisted of identifying the problem areas that led to the high-voltage breakdown, reengineering the cells using the information from the R&D Program, verifying the redesign by subjecting a specific number of cells to a pre-established acceptance tests, installing the cells and commissioning the 2nd axis to provide four radiographic pulses.

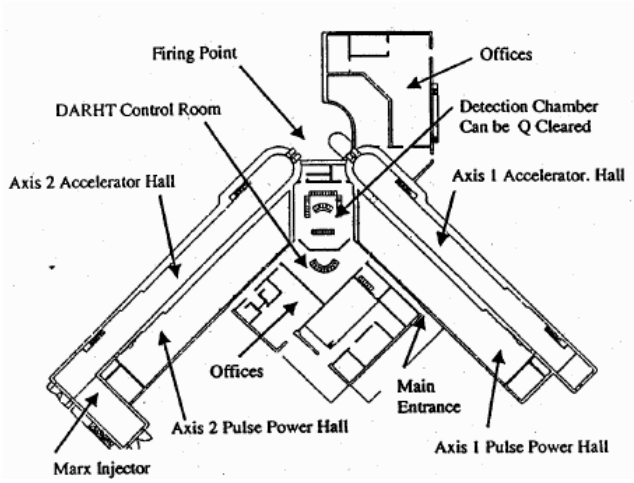

Figure 2. DARHT Facility Schematic Layout

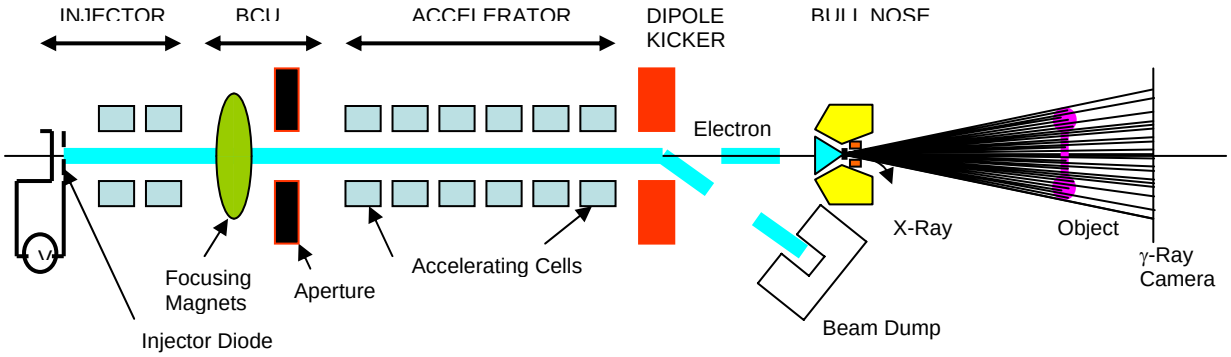

Figure 3. DARHT 2nd Axis Schematic

As part of the R&D Program, cells were studied experimentally and through modeling to develop a redesigned solution that will operate reliably at 200 kV per cell. Operating the cells at higher voltage of 200 kV, than the original goal, also helped reduce the total number of cells from 78 to 74 (68 accelerator and 6 injector cells) and allowed creation of some needed space between cell groupings to facilitate maintenance.

After the selection and acceptance testing of a final cell re-design, the physics testing and commissioning was planned in 3 steps: 1) performing the Beam Stability experiments; 2) performing the Scaled Accelerator Validation tests; and 3) the full energy commissioning tests. The steps are explained below.

1) Beam Stability tests: These tests were designed to address the long pulse (>1.5 μsec) beam transport stability issues which were observed during the original commissioning of 2nd Axis; specifically Beam Break-Up and Ion Hose instabilities. These tests used 50 of the existing, un-refurbished accelerator cells and 6 un-refurbished injector cells. These cells were operated at 100 kV in order to minimize the risk of further damage to the cells. These tests were successfully completed in October 2005.

2) Scaled Accelerator Validation tests: These tests used 26 of the refurbished accelerator cells and were operated at the design voltage of 200 kV per cell. The cells were aligned to final specifications and operated in the final configuration. After beam transport commissioning through the 26 cells was completed, the Down Stream Transport (DST) kicker, dump and target were tested. Although these components have been tested at the Lawrence Livermore National Laboratory, this was the first full test of the multi-pulse kicker and multi-pulse target over a full time duration of > 1.5 μsec to produce the four pulses. It also served as the initial test of the accelerator as a system.

The Scaled Accelerator tests were successfully completed at the end of March 2007 and all of physics issues associated with the beam transport, beam quality, centroid motion, kicker performance and target performance were resolved, albeit at a lower energy of 8.0 MeV.

3) Full Energy Commissioning Tests: During these tests (which started in June 2007), all refurbished components will be in place and full beam energy and performance will be attempted for the first time. This series of tests will end with the measurement of the beam x-ray dose and spot size for each of the four output pulses. At the completion of the full energy commissioning tests, presently scheduled for the second quarter of FY 2008, the second axis will be ready for integration into the DARHT facility to support the hydro-testing program. Initial results have been obtained at 18 MV and 2 kA.

The 2nd Axis Refurbishment and Commissioning Project is being performed in collaboration with three of our national laboratories. The Los Alamos National Laboratory is leading the project team, while the Lawrence Livermore National Laboratory and the Lawrence Berkeley National Laboratory teams are supporting the design and testing of the key components.

During the course of redesign and refurbishments, a number of technical reviews were conducted by external experts and all concluded that the redesign and refurbishment will achieve the desired objectives. The most prominent outside team to review the 2nd Axis progress was the JASON team, which reviewed the project progress over a three day schedule of talks in June 2006. Results of the review were published in a report and sent to Congress to comply with the Congressional direction contained in the Fiscal Year 2006 appropriation.

In November 2006, the 2nd Axis achieved the objective of creating the four pulses. This is something which had never been achieved on any accelerators of similar capability and which the JASON report had indicated would be difficult to achieve. Results of the four pulses are shown on Figure 4.

When the second axis is completed, DARHT will represent a substantial leap forward in linear induction accelerator technology, and the DARHT facility will be the only facility in the world that will provide orthogonal multi-pulse x-radiography capability, which is essential to ensuring the continued safety and reliability of the stockpile under a "zero-yield" test ban.

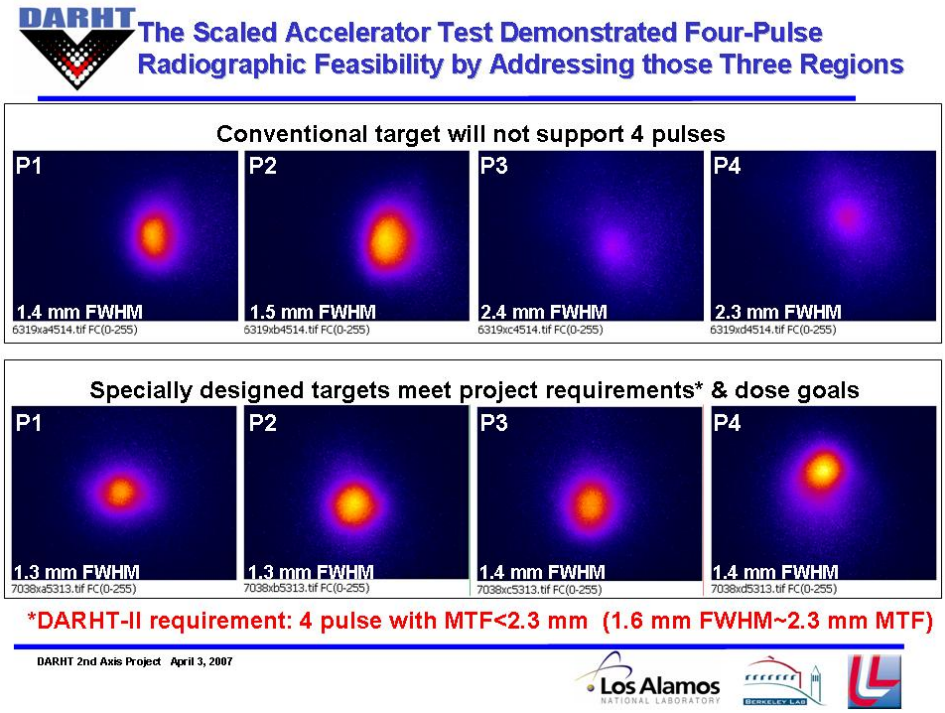

Figure 4

Science Campaigns Support High-Impact Basic Research by Cris Barnes, LANL

In this section we highlight recent publications in high-impact scientific journals of research supported by the NNSA Science Campaigns. This quarter we feature a set of fundamental research into dynamic materials properties, including one by our own new leader, Dr. Chris Deeney!

"Stiff Response of Aluminum under Ultrafast Shockless Compression to 110 GPA" by Raymond F. Smith, Jon H. Eggert, Alan Jankowski, Peter M. Celliers, M. John Edwards, Yogendra M. Gupta, James R. Asay, and Gilbert W. Collins (of Lawrence Livermore National Laboratory and Washington State University), PHYSICAL REVIEW LETTERS, FEB 9 2007, v.98, no.6, p.065701.

Understanding the stress-strain response of matter at extreme compressions is an important element of contemporary research in physics and materials science. Depending on the compression technique this data can be obtained along very different and individually limited thermodynamic paths. Quasihydrostatic compression in diamond-anvil-cell (DAC) experiments typically provides

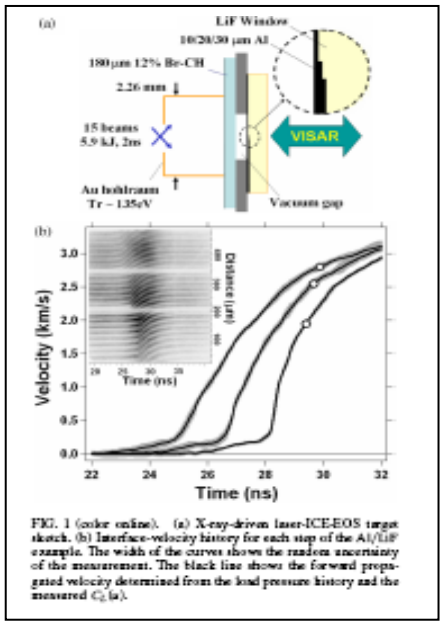

FIG. 1 (color online). (a) X-ray-driven laser-ICE-EOS target sketch. (b) Interface-velocity history for each step of the Al/LiF example. The width of the curves shows the random uncertainty of the measurement. The black line shows the forward propagated velocity determined from the load pressure history and the measured C_0 (a).

isothermal data up to a pressure range of 200 to 300 GPa, with experimental times ranging from seconds to days. Shock-wave experiments, which uniaxially load material with a step function in time, can provide a single longitudinal stress-density point along the shock adiabat to several TPa. Shock compression produces a significant temperature increase so that at high stresses (>100 GPa) they sample very different regions of thermodynamic space than DAC experiments. Recently developed ramp-wave-loading experiments (commonly referred to as quasi-isentropic compression experiments, or ICE) permit the sampling of thermodynamic space not accessible by shock-wave or static pressure methods, ensure a solid state even at very high pressures, and provide data intermediate between shockwave and static pressure results. This Letter presents the first accurate P_x–ρ data obtained on a laser-ICE platform. These are the fastest shockless compression $P_x(\rho)$ results reported to date, with compression times comparable to the intrinsic stress relaxation time.

"Shock Waves in Polycrystalline Iron" by Kai Kadau, Timothy C. Germann, Peter S. Lomdahl, Robert C. Albers, Justin S. Wark, Andrew Higginbotham, and Brad Lee Holian (Los Alamos National Laboratory and University of Oxford), PHYSICAL REVIEW LETTERS; MAR 30 2007; v.98, no.13, p.135701.

Because of its technological, geological, and sociological importance, iron is one of the most studied materials. In particular, phase changes due to pressure or temperature, be it from the ferromagnetic body-centered cubic (bcc) ground state into nonferromagnetic close-packed structures or vice-versa, are of interest, since they are the origin for many important properties of iron. It has been assumed that the same bcc to isotropic hexagonal-close-packed (hcp) transition occurred under dynamic shock loading. The propagation of shock waves through polycrystalline iron is explored by large-scale atomistic simulations. For large enough shock strengths the passage of the wave causes the body-centered-cubic phase to transform into a close-packed phase with most structure being hcp and, depending on shock strength and grain orientation, some fraction of face-centered-cubic (fcc) structure. The simulated shock Hugoniot is compared to experiments. By calculating the extended x-ray absorption fine structure (EXAFS) directly from the atomic configurations, a comparison to experimental EXAFS measurements of nanosecond-laser shocks shows that the experimental data is consistent with such a phase transformation. However, the atomistically simulated EXAFS spectra also show that an experimental distinction between the hcp or fcc phase is not possible based on the spectra alone.

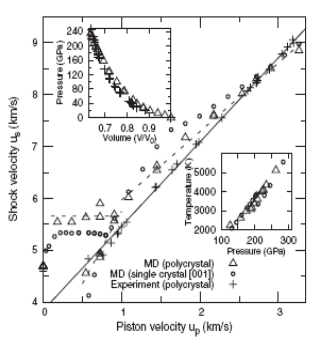

FIG. 2. Experimental and simulated Hugoniots for polycrystalline iron. The full line is a linear fit to the experimental data [19,20], the dashed lines are fits to the three different parts of the simulated Hugoniots: elastic precursor, transformation wave, and the overdriven part. As a reference, the $[001]_{bcc}$ single crystalline shock data are included [5].

"A Metastable Limit for Compressed Liquid Water" by D. H. Dolan, M. D. Knudson, C. A. Hall and C. Deeney (of Sandia National Laboratories), NATURE PHYSICS 3(5), 339 (2007).

The transformation of liquid water to solid ice is typically a slow process. To cool a sample below the melting point requires some time, as does nucleation from the metastable liquid, so freezing usually occurs over many seconds. Freezing conditions can be created much more quickly using isentropic compression techniques, which provide insight into the limiting timescales of the phase transition. Here, we show that water rapidly freezes without a nucleator under sufficient compression, establishing a practical limit for the metastable liquid phase. Above 7 GPa, compressed water completely transforms to a high-pressure phase within a few nanoseconds. The consistent observation of freezing with different samples and container materials suggests that the transition nucleates homogeneously. The observation of complete freezing on these timescales further implies that the liquid reaches a hypercooled state.

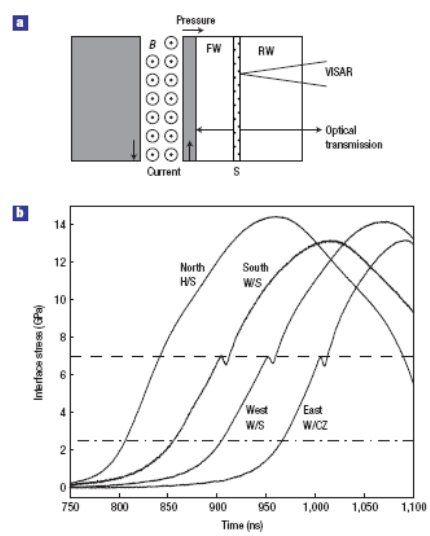

Figure 3 Ramp-wave compression experiments. a, Current from the Sandia Z machine generates continuous stress waves in a thin liquid sample (≈ 0.02 mm) confined between transparent windows (FW and RW). b, Interface stress histories for isentropically compressed water and hexane (experiment Z1580). The abbreviations indicate the sample (water, W, or hexane, H) and window (sapphire, S, or cubic zirconia, CZ) materials. The dashed line indicates the prompt transition threshold near 7 GPa, whereas the dash–dot line indicates the pressure at which liquid water becomes metastable. The plots have been time shifted by 50 ns for visual clarity; actual compressions are nearly coincident.

Other recently published articles include:

- **"Near-equilibrium polymorphic phase transformations in praseodymium under dynamic compression"** by Marina Basteaa and D. B. Reisman, APPLIED PHYSICS LETTERS 90, 171921 (2007).
- **"Isentropic Loading Experiments of a Plastic Bonded Explosive and Constituents"** by M. R. Baer, C. A. Hall, R. L. Gustavsen, D. E. Hooks, and S. A. Sheffield, JOURNAL of APPLIED PHYSICS 101, 034906 (2007).
- **"Structured Evolution and Formation of High-pressure Plasmas in X-pinches"** by J. P. Chittender et al, PHYSICAL REVIEW LETTERS 98, 25003 (2007).

New Appointment and Awards

Dr. Russell J. Hemley was appointed Director of the Geophysical Laboratory at the Carnegie Institution of Washington, effective July 2, 2007. He is the principal investigator of the NNSA supported Carnegie/DOE Alliance Center (CDAC), a center of excellence in the field of static high-pressure research. Dr. Hemley did his graduate work in physical chemistry at Harvard University (M.A., 1980; Ph.D. 1983). After a post-doctoral fellowship in theoretical chemistry at Harvard (1983-84), he joined the Geophysical Laboratory as a Carnegie Fellow (1984-86) and Research Associate (1986-87), and became a Staff Scientist in 1987. He has been a visiting Professor at the Johns Hopkins University (1991-92) and at the Ecole Normale Superieure, Lyon (1996). He is the recipient of the 1990 Mineralogical Society of AmericaAward, and is a Fellow of the American Physical Society, the American Geophysical Union, and the American Academy of Arts and Sciences. He was elected as a member of the National Academy of Sciences in 2001 and became a member of JASON in 2003. In 2005, he was awarded the Balzan Prize in Mineral Physics. He has been an author on over 440 publications.

Congratulations to **Kim Budil**, LLNL, and **Kevin Greenaugh**, NNSA HQ, for receiving the 2007 Top Minorities in Science "Trailblazer Award".

Congratulations to **Dr. Yitzak Maron** of The Weizmann Institute of Science on being awarded the Plasma Science and Applications Committee Award from the Institute of Electrical and Electronics Engineers, Inc. This work is partially funded by the Stewardship Science Academic Alliances Center at Cornell University and by Sandia National Laboratories.

Congratulations to our laboratories for winning twelve R&D 100 awards!