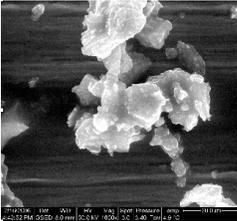


## INDEX of PADSTE HIGHLIGHTS November 7, 2007

### BIOSCIENCE

Improving metabolomic measurement and analysis

### CHEMISTRY



Complex processing salts

### EARTH AND ENVIRONMENTAL SCIENCES

Stardust sample return shockwave

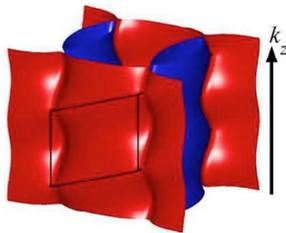
### HIGH PERFORMANCE COMPUTING

Roadrunner Critical Decision 3b package sent to NNSA

### LANSCE

“Training” shape-memory alloys

### MATERIALS PHYSICS AND APPLICATIONS



Interlayer coherence in an organic superconductor

### MATERIALS SCIENCE AND TECHNOLOGY

Hollow fiber propane/propylene separation  
Steve Valone appointed visiting research professor  
Uranium characterization

### PHYSICS



Dynamic proton radiography experiments

### THEORETICAL

Connections get you everywhere, but slowly

**PADSTE HIGHLIGHTS November 7, 2007****BIOSCIENCE****Improving metabolomic measurement and analysis**

Metabolomics, the study of small molecule biochemical components associated with metabolism, can greatly enhance researchers' fundamental understanding of how cells operate. This approach has a wide range of potential uses, from gaining insight into how a single-cell microorganism uses carbon and nitrogen, to identifying differences between cancer cells and healthy cells. Metabolomics technologies, in particular mass spectrometry (MS), are rapidly maturing and nearing high throughput status, when one would be able to measure the concentrations of a large fraction of metabolites with high precision, high temporal resolution, and low per-experiment cost. However, the experimental techniques, as well as data analysis protocols, are still far from perfection. In particular, the sensitivity of high throughput metabolic techniques currently allows determination of the concentrations of relatively abundant species only.

Taking advantage of Los Alamos expertise in stable isotope labeling and MS analysis, as well as in reverse engineering of biochemical interaction networks from metabolic data; researchers in B, CCS, ISR and T Divisions are developing a set of coordinated experimental and computational tools and protocols for improving the quality of high throughput metabolomic measurements and analysis. They will use this data for reconstruction of both small-scale metabolic pathways and system-wide metabolic networks. Specifically, they are working to improve MS metabolic profiling by developing stable isotope-enhanced metabolome analysis methods and improving the unique reverse engineering metabolic network inference software developed at Los Alamos. These methods will be applied to an evolving series of experimental studies using *in vitro* models of malignant tumor progression in standard 2-D and more complex 3-D cell culture systems. In addition to enhancing the technologies used in this area of research, the Los Alamos team will provide a large set of metabolic profiles to improve the basic understanding of the metabolomics of human cancer, a necessary step before such technologies will be applicable in diagnostics and therapy monitoring. The National Institutes of Health recently funded this research for five years in conjunction with the National Cancer Institute. James Freyer (B-9) and Ilya Nemenman (CCS-3) lead the project; other researchers include includes Pat Unkefer (B-DO) and Cliff Unkefer (B-8), Steven Brumby (ISR-2), and William Hlavacek and Fangping Mu (both in T-10).

**CHEMISTRY****Hygroscopic behavior of complex processing salts**

Surplus plutonium-bearing material within the Nuclear Weapons Complex that is packaged for up to 50 year storage under DOE's 3013 Standard is allowed to have up to 70% impurities by weight. One of the more common, and potentially problematic, impurities is electrorefining salts (ER salts), which typically are composed of 95% by

weight of an equimolar mixture of sodium chloride and potassium chloride with 5% by weight of anhydrous magnesium chloride. The 3013 Standard limits the amount of moisture to 0.5wt% or less to minimize both the radiolytic production of gases and corrosion. Moisture sorption by plutonium oxide materials containing ER salts is a complex process with known mechanisms including surface adsorption of approximately a monolayer, formation of hydrated salts, and deliquescence (absorbing so much moisture from the air that the salt ultimately dissolves in it to form a solution). Stephen Joyce (C-PCS) and Eduardo Garcia, Obie Gillespie, Kirk Veirs and Laura Worl (all in PMT-1) have examined the hygroscopic behavior (ability to attract moisture from the atmosphere) of various compounds that may be present in ER salts.

X-ray diffraction (XRD) of mixtures of calcined KCl, NaCl, and MgCl<sub>2</sub> have identified KMgCl<sub>3</sub>, K<sub>2</sub>MgCl<sub>4</sub>, and K<sub>3</sub>NaMgCl<sub>6</sub> as compounds that could be present in dry ER salts. The only reported hydrate of these salts is KMgCl<sub>3</sub>·6H<sub>2</sub>O (carnallite) which deliquesces at ~60% relative humidity. Pure samples of anhydrous KMgCl<sub>3</sub>, K<sub>2</sub>MgCl<sub>4</sub>, and K<sub>3</sub>NaMgCl<sub>6</sub> as well as an ER salt simulant were synthesized. These salts were examined in an environmental scanning electron microscope that has the ability to acquire images in the presence of water vapor. All four salts began to deliquesce at the same relative humidity of 58%, indicating that carnallite formed at lower humidities. XRD measurements confirm that the more complex K<sub>2</sub>MgCl<sub>4</sub>, K<sub>3</sub>NaMgCl<sub>6</sub>, and ER simulant do indeed phase separate at low relative humidity into KMgCl<sub>3</sub>·6H<sub>2</sub>O and the respective alkali halides. Upon deliquescence, further phase separation was observed due to the incongruent dissolution of carnallite into a Mg-rich solution and KCl crystallites. Upon lowering the humidity, this solution can become supersaturated, with recrystallization occurring at significantly lower humidities. Further phase separation into MgCl<sub>2</sub>·6H<sub>2</sub>O and the alkali halides was observed for the “dried” salt. A striking example is shown in Figure 1. The presence of MgCl<sub>2</sub>·6H<sub>2</sub>O is significant because once it is formed through a deliquescent cycle, the presence of a liquid phase within the material will be controlled by the lower deliquescent relative humidity (33%) of MgCl<sub>2</sub>·6H<sub>2</sub>O rather than by KMgCl<sub>3</sub>·6H<sub>2</sub>O. This possibility affects humidity control levels established to limit moisture uptake in support of criticality safety after a container is opened for surveillance. The Surveillance and Monitoring Program, DOE Office of Environmental Management, supported the work.

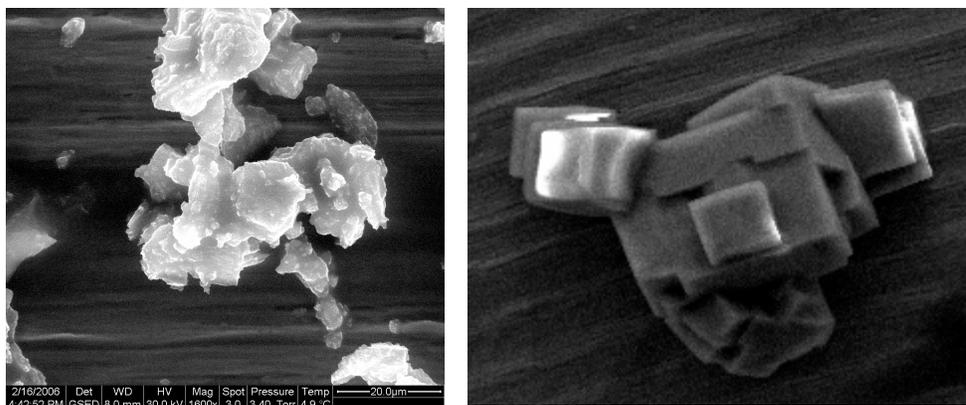


Figure 1. Images of ER simulation prior to deliquescence (left panel) and cubes of KCl

and NaCl (right panel).

## **EARTH AND ENVIRONMENTAL SCIENCES**

### **Stardust sample return shockwave**

A paper titled, “Calibrating Infrasonic to Seismic Coupling using the Stardust Sample Return Capsule Shockwave: Implications for Seismic Observations of Meteors,” was published in the *Journal of Geophysical Research*. This work is a continuation and an expansion of previous work published in *Meteoritics and Planetary Science* on the infrasonic and seismic monitoring of the NASA Stardust space capsule during its reentry into the atmosphere in January 2006. The velocity of the space capsule was the highest ever for an artificial object and is on the low end of the range typical of meteoroids. This work, a collaboration between D.O. ReVelle (EES-2) and researchers at the University of Western Ontario (Canada), is the first calibrated measurement of acoustic-seismic coupling efficiency for a meteor analog.

This research focuses on the interpretation and modeling of the seismic data measured during the reentry and its relationship to the recorded infrasound data. The ensemble of infrasonic data consisted of about 1-2 minutes of rumbling, which first began as a normal hypersonic boom from about 40 km altitude (which is also very near to the point of closest approach to the reentry trajectory) when the capsule was still moving at hyper/supersonic speeds. The delay time to the start of the hypersonic boom was totally normal and the “boom” was recorded well within the direct nominal “hypersonic sonic boom corridor”. This degree of normalcy was previously expected because the scientists had also monitored the NASA Genesis space capsule reentry in September 2004 at the same location (Wendover, Nevada). However some 10 sec after the onset of the initial boom, a second set of enigmatic infrasonic signals arrived that could not be interpreted as emanating directly from the entry trajectory. The subsequent detailed analysis and modeling shows that these signals indicate that acoustical energy from the reentry had penetrated directly into the ground and then subsequently reemerged into the air from below (referred to as higher order Airy phases). This set of observations is similar to the so-called earthquake sound phenomenon that has been known for many years. These observations also give new limiting values of the air-ground seismic coupling factor over desert playa regions. The Ground-Based Nuclear Explosion Monitoring program, the ISR RD Program Office, IGPP, and NASA supported the LANL work.

## **HIGH PERFORMANCE COMPUTING**

### **Roadrunner Critical Decision 3b package sent to NNSA**

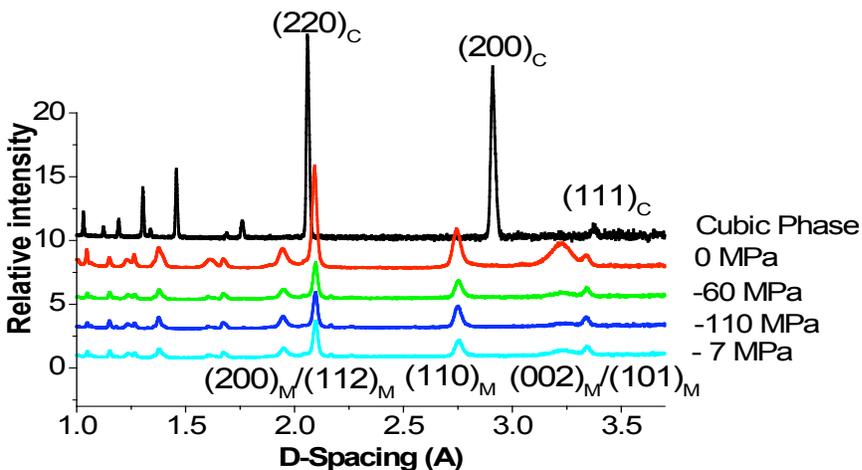
The Execution Readiness Package (Critical Decision 3b) for the ASC Roadrunner Final System has been completed and was sent to NNSA on November 6. This is the first NNSA review of Critical Decision 3b. This package is to request approval to proceed with the procurement and deployment of the Final System. It includes the project performance baselines for scope, cost, and schedule.

## LANSCE

**“Training” shape-memory alloys**

A China-US research team at the Lujan Center has direct evidence for how microscopic stress influences the choice of crystal structure in magnetic alloys that remember their shape while undergoing a phase transition. This insight suggests ways to “train” materials for selected response in applications requiring adaptive response to environmental conditions. In ferromagnetic shape memory alloys, the distribution of crystallographic variants should be equally partitioned after a phase transition without applied external fields; but often some variants are favored, while others are suppressed. Although residual stress inside the materials was suspected, no direct experimental evidence was seen owing to the lack of effective experimental tools. Using the Spectrometer for Materials Research at Temperature and Stress (SMARTS) instrument at the Lujan Center, D. W. Brown (LANSCE) and Y. D. Wang (Northeastern University, China and the University of Tennessee) characterized the structure of Ni<sub>2</sub>MnGa ferromagnetic shape-memory alloy under a uniaxial stress field by neutron scattering.

The ratios of intensity for the two texture components (the two variants belonging to the same orientation of parent phase) are taken as the simple indicators to evaluate the influence of external stress on the selections of variants. The experimental values are shown in Figure 2. The experimental values at 0 MPa obviously deviates from the linear relationship and are not equal to 1. This indicates that the present alloy does not obey the equivalent partition of variants at the initial state. The result can be attributed to the existence of intergranular stress or the influence of lamellar microstructures in the cast alloy. However, a stress of -60 and -110 MPa obviously disturbed the distributions of variants. When the stress was released to -7 MPa, the initial partition of variants was not recovered. Thus, a small stress applied during phase transformation may cause obvious redistribution of variants. The neutron experiments further verified that the texture in the specimen was not changed by just a simple cyclic heat-treatment, i.e., repeatedly heating (up to 973 K) and cooling under no external stress field. Thus, the present observation on



the “broken” memory or reselections of variants during the phase transformation under the external stress provides direct and unique experimental evidence on the “training” mechanisms by changing the internal stress field that lead to the redistribution of the variants.

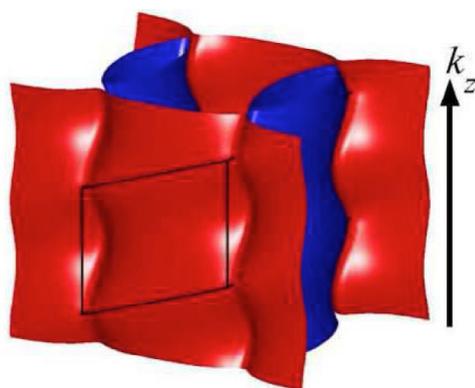
Figure 2. SMARTS data for the shape-memory alloy.

## MATERIALS PHYSICS AND APPLICATIONS

### Interlayer coherence in an organic superconductor

The past two decades have seen a blossoming of interest in compounds with quasi-two-dimensional electronic band structures; examples include layered oxides and crystalline organic metals. These materials may be described by a tight-binding Hamiltonian in which the ratio of the interlayer transfer integral to the average intralayer transfer integral is much less than 1.

The question arises as to whether the interlayer charge transfer is coherent or incoherent in these materials; i.e., whether or not the Fermi surface is three dimensional, extending in the interlayer direction. For example, a widely held view (even quoted in P.W. Anderson's book on cuprate superconductivity) is that a layered material will lose its three dimensionality when the temperature exceeds the interlayer transfer integral. By measuring the magnetoresistance of an organic superconductor in fields of up to 45 T, LANL researchers and collaborators have demonstrated that this view is false. The material retains its three-dimensional electronic properties even when the temperature is some 30 times the interlayer transfer integral.



The experiments have also allowed measurement of the electronic scattering rate on different parts of the Fermi surface for the first time. The scattering rate was found to be rather uniform and determined by electron-electron interactions; these observations provide stringent tests for certain models of superconductivity in the organics and cuprates.

Figure 3. A 3D representation of the Fermi surface of the superconductor. Quasi 1D and 2D Fermi surface sections are shown in red and blue, respectively.

The research by John Singleton, Paul Goddard, and Ross McDonald (all in MPA-NHMFL); A. Ardavan and S.J. Blundell (University of Oxford); A.I. Coldea (Bristol University); S. Tozer (NHMFL, Florida); and J.A. Schlueter (Argonne National Laboratory), was published in *Physical Review Letters* **99**, 027004 (2007). LDRD funded the Los Alamos portion of this work. The National Science Foundation, DOE, and the State of Florida support the National High Magnetic Field Laboratory (NHMFL).

## MATERIALS SCIENCE AND TECHNOLOGY

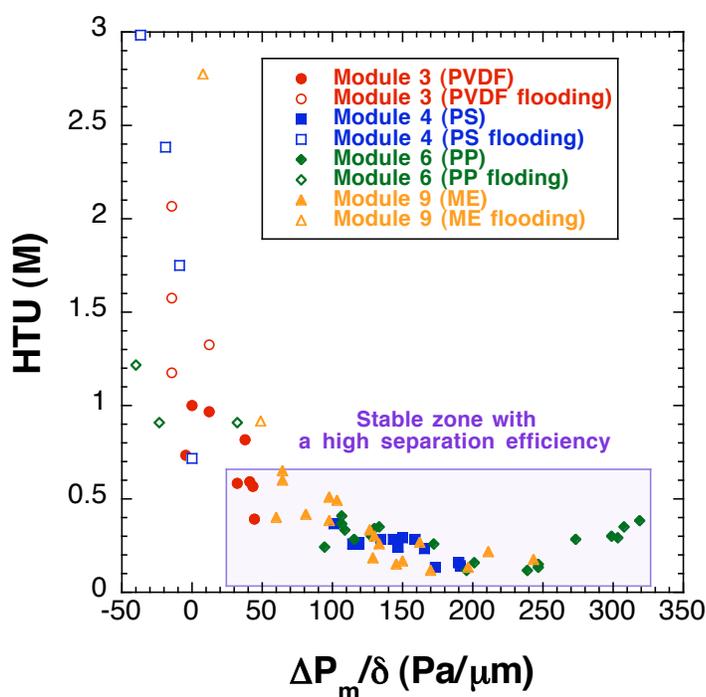
### Hollow fibers improve efficiency of propane/propylene distillation

The light hydrocarbon mixtures of ethylene and propylene (olefins) are two of the largest commodity chemicals in the U.S. and are major building blocks for the petrochemicals

industry. With than 75 billion pounds of these chemicals distilled annually in the U.S. at an estimated energy requirement of 400 trillion BTUs, intensive efforts are being dedicated to reducing the energy consumption in this distillation process.

Improving separation efficiency of structured packing materials is an approach to improve the energy efficiency of distillation. Micro-porous membranes with a large specific area within a small volume, constructed in the geometry of hollow fibers become attractive materials for providing an effective contact area between two phases (e.g. liquid-gas and liquid-liquid). The column packed with hollow fibers may operate above the normal flooding and below the normal loading limits.

Dali Yang, David Devlin and Robert Barbero (all in MST-7) used hollow fibers as structured packing materials to investigate the effects of morphology and compatibility of



hollow fibers on separation efficiency and operation stability in the propane/propylene distillation process. The scientists found that there is a stable zone in which high separation efficiency and operation stability can be achieved for the hollow fiber modules (Figure 4). Their work demonstrates that while a hydrophobic micro-porous membrane may seem preferable for this application, an asymmetric membrane with sub-micron pore size on the liquid side may be more suitable for long-term stability of the distillation operation with a high separation efficiency. The hollow fiber modules may be over 10 times more productive per equipment volume than conventional packing.

Figure 4. Correlation between pressure drop across the membrane wall and separation efficiency for a propane/polypropylene mixture.

The researchers conclude that a highly connective porous structure will promote the intimate interaction between the vapor and liquid phases, and enhance the mass transfer rate. However, as the pore size increases, the potential for the two phases to interfere with each other's flow increases. To overcome this problem, a membrane with an asymmetric structure seems to be a good choice (Figure 5). The research was published in *Journal of Membrane Science* 304, (2007). The DOE Energy Efficiency and Renewable Energy, OIT, Industrial Technology Program supported the work.

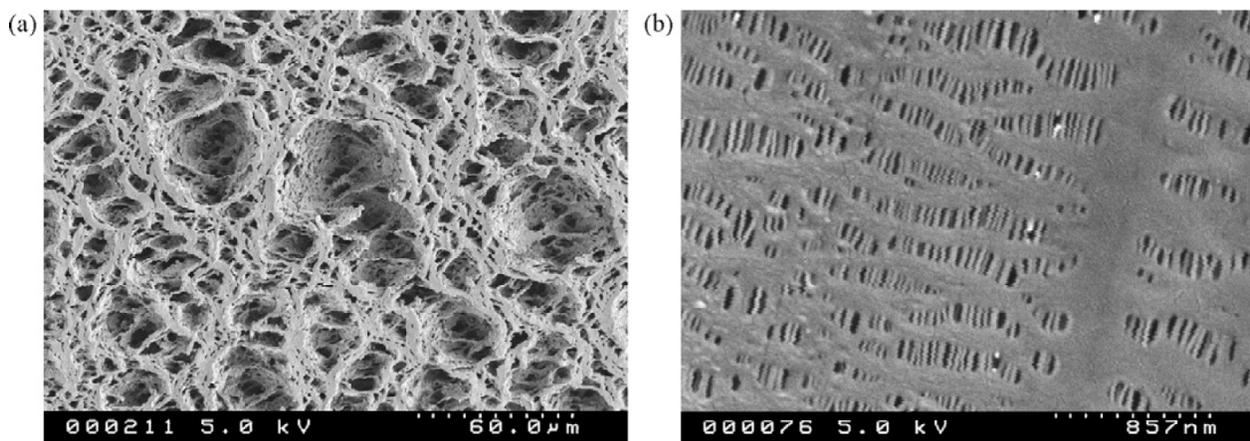


Figure 5. SEM images of the porous structure of the outer surface with a large pore size (a) and the inner surface with a small pore size (b) of the proposed asymmetric membrane.

#### **Steve Valone appointed visiting research professor at UNM**

Steve Valone (MST-8) has been appointed a visiting research professor in the Department of Physics and Astronomy at the University of New Mexico. During his three-year appointment, Valone will promote his long-time collaboration with Professor Susan Atlas in the same department. Over the last five years, the collaboration has netted a National Science Foundation grant on dynamical potentials for charge transfer in molecular motors, several publications, and the mentoring of two students and a postdoctoral researcher. Valone and Atlas will write a follow-on NSF proposal focusing on charge transport in proteins at an atomistic level. He will also give lectures on special topics as requested by the department.

#### **Uranium characterization**

MST-6 completed uranium characterization studies on both depleted, uranium-238, and highly enriched, 93% uranium-235, uranium metal in support of uranium process development activities at Y-12. This was associated with a high-level Y-12 milestone, which provides direction for future investments in uranium manufacturing capabilities at Y-12. While the depleted uranium measurement was routine, the measurement of the highly enriched uranium required significant efforts to ensure that (1) accountability was maintained and (2) the location of the experiment was authorized to handle the amount of material involved. The anisotropy in linear coefficient of thermal expansion (CTE) was measured on small polycrystalline specimens with induction dilatometry; this anisotropy can be considerable and potentially deleterious given the huge CTE anisotropy in single grains of alpha-uranium. The anisotropy measured were correlated with and consistent with microstructure (light optical microscopy) and microtexture (orientation microscopy) measurements done on the same CTE specimens. The data showed the extent to which changes in uranium processing will result in changes in the resulting thermal expansion, microstructure and texture, as requested by the stakeholders. In addition, this work has filled in key gaps in the data set for enriched uranium, a material that historically has

been examined and measured much less than depleted uranium. MST-6 employees contributing to this effort include Lydia J. Apodaca, John.A. Balog, Timothy V. Beard, Ross S. Casey, Issac P. Cordova, Robert T. Forsyth, Robert E. Hackenberg, Ann M. Kelly, Deniece R. Korzekwa, Rodney J. McCabe, David F. Teter, and Chastity J. Vigil.

## PHYSICS

### Dynamic proton radiography experiments study plutonium damage

A series of six proton radiography experiments were completed at LANSCE to study the damage evolution of small samples of plutonium driven by small quantities of high explosives. These experiments were an extension of the Thermos series of experiments previously fired at the Nevada Test Site. Three dynamic experiments were performed as confirmatory experiments in preparation for the plutonium series. Early time radiographs from one confirmatory experiment, in which a lead sample was used, is shown in Figure 6. These radiographs were collected at 200 ns intervals and have been divided by a static radiograph to compress the dynamic range for display purposes. In these radiographs the expanding high explosives products can be seen as well as the resulting shock passing through the lead sample.

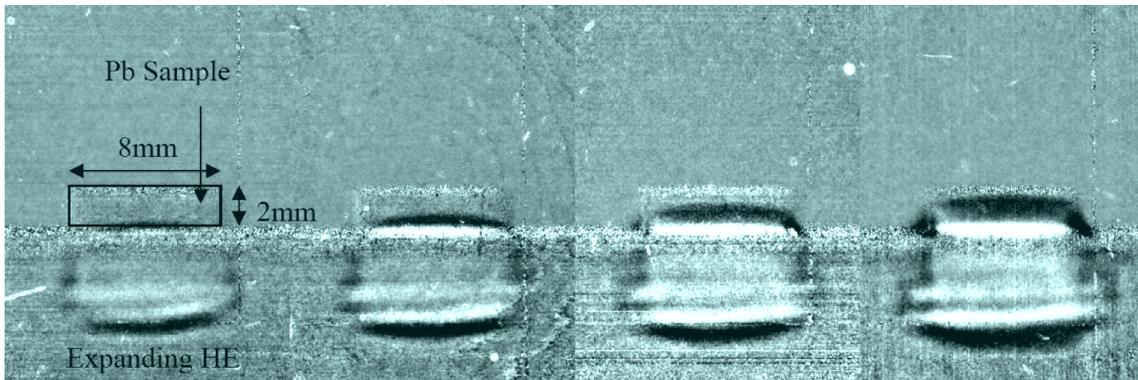


Figure 6. Early time radiographs, divided by a static radiograph, collected at 200 ns spacing showing the high explosives expansion and resulting shock traversing the lead sample.

Late time radiographs from the same dynamic event are shown in Figure 7. In this series of radiographs, the damage process formed multiple spall layers in the lead sample. The lead and plutonium samples were stopped in a foam recovery system for post-shot analysis of the damaged material.

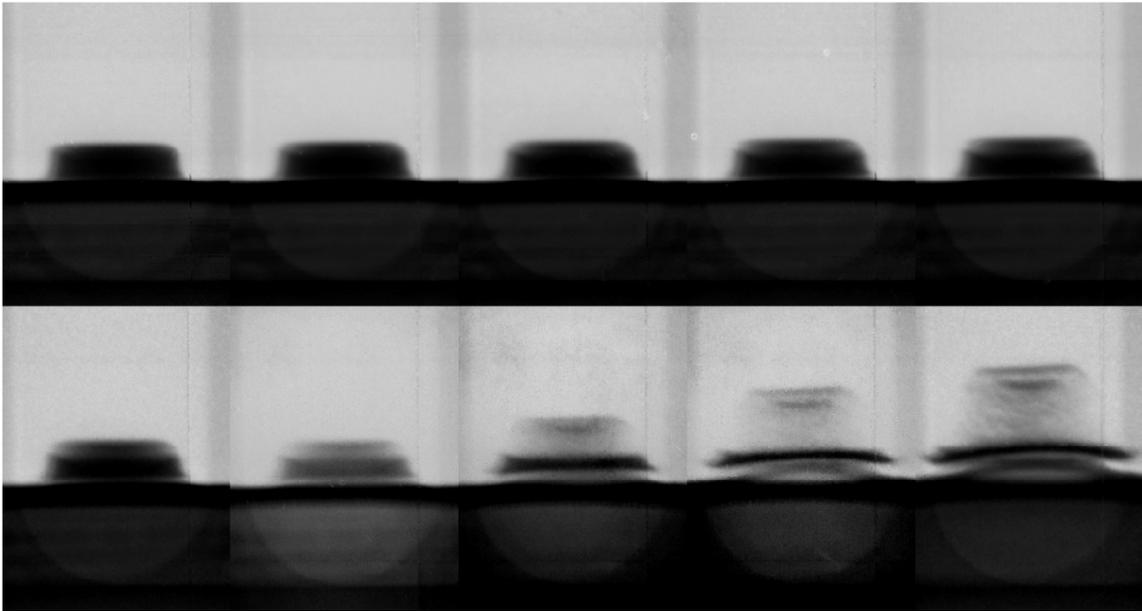


Figure 7. Late time radiographs of the same dynamic event as shown in Figure 6, shows the damage evolution of the lead sample.

Surface velocities of each sample were also measured for each of these six experiments using VISAR and photon Doppler velocimetry. This suite of data provides a fully diagnosed set of dynamic experiments for comparison to model predictions. Scientists expect to learn valuable information about the dynamic damage evolution of plutonium from the radiographs and velocimetry, in combination with results from the post-shot studies of the damaged materials. This new capability will provide new insights into the dynamic properties of high explosives driven materials of interest to the weapons program. The team that executed these experiments composed of personnel from P, HX, WT, W, T, LANSCE and RP Divisions at LANL as well as support from NSTech and SNL. This team worked closely with the LANSCE FOD to gain approval from the DOE to execute these small explosives driven experiments using plutonium. MST personnel were instrumental in preparing the small plutonium samples, as was SMS leadership.

## **THEORETICAL**

### **Connections get you everywhere, but slowly**

A network is any collection of things linked together by connections of some sort. The Internet is a collection of computers linked by communication lines. In mathematical terms, researchers know that it takes surprisingly few links to integrate isolated islands into one connected whole. An important question regarding networks is their stability; i.e. under what conditions the network break down. In communications, a network breakdown means information cannot be transmitted to most nodes. The Internet and other large networks can hang together as connected wholes even when 10% or more of their communication links are knocked out, according to some mathematical studies.

But Eduardo Lopez (CNLS and T-7) and collaborators from Bar-Ilan University (Israel) and MIT researchers suggest that some networks may not be so resilient. Networks must provide more than mere connection; they have to let information or other resources move from point to point quickly and effectively. The researchers argue that after a few links fail, the routes between some points can become so long as to be unusable. The effect could make networks fail even when simpler analyses would suggest they would continue to work.

To explore this effect, the scientists monitored how the distance between elements in simulated networks increased as they destroyed network links at random. They supposed that if the shortest path between two points became too large, the path between would become effectively useless. They found that a network can become disconnected, in practical terms, long before it becomes physically disconnected. For example, in a typical simulation, a network that mostly hung together as a connected whole even after 60% of its links were removed, fell apart in practical terms after only 30% were removed.

However, this effect can be positive as well as negative. While long paths in communication are inefficient, in epidemics disease spreading often decays in time because of decays in time due to effects of seasonality or pathogen mutation. Thus for long paths, the epidemic may die out before total network infection. These considerations indicate that these results are important for network design, routing protocols, and immunization strategies, where short paths are most relevant.

LDRD and the DOE Office of Science funded the work. This research has been published: Eduardo López, Roni Parshani, Reuven Cohen, Shai Carmii, and Shlomo Havlin <<http://link.aps.org/abstract/PRL/v99/e188701>> [Phys. Rev. Lett. 99, 188701](http://dx.doi.org/10.1103/PhysRevLett.99.188701) and featured in a Physical Review Letters focus story: <http://focus.aps.org/story/v20/st15>



Figure 8. A map of a portion of Mbone, an Internet overlay network for video and other high-bandwidth uses (height of arcs represents distance). Networks like this can remain connected even after many broken links, but they may no longer be effective. (graphic credit: T. Munzner/Stanford Univ.)