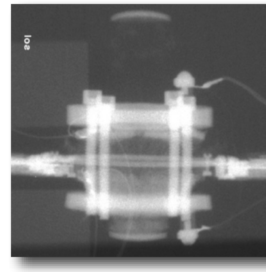
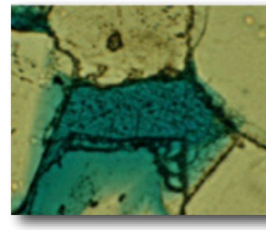
INDEX of PADSTE HIGHLIGHTS   June 3, 2009

BIOSCIENCE
Helper plasmid display technology licensed

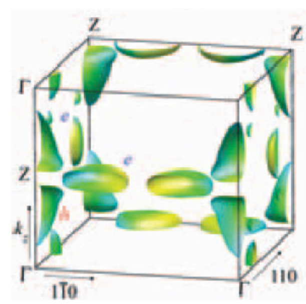


CHEMISTRY
X-ray radiography of internal, subsonic burning of explosives



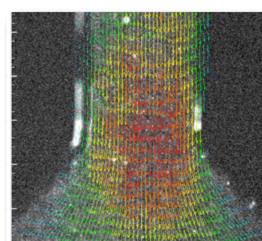
EARTH AND ENVIRONMENTAL SCIENCES
Low-frequency mechanical stress oscillations enhance particle release

LANSCE
American Physical Society's *This Week in Physics* highlights Lujan research

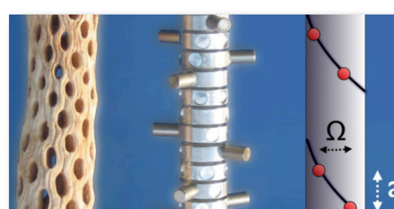


MATERIALS PHYSICS AND APPLICATIONS
Two LANL papers selected for Top Papers Collection of 2008

MATERIALS SCIENCE AND TECHNOLOGY
Understanding materials properties of radioactive waste forms



PHYSICS
New microfluidics facility in P-23



THEORETICAL
Mathematical regularities in plant structures and physics

PADSTE HIGHLIGHTS June 3, 2009

BIOSCIENCE

Helper plasmid display technology licensed

The German company MorphoSys acquired a full license for the use of "helper plasmid display technology" developed in B Division's Advanced Measurement Science Group. Andrew Bradbury (B-9) and his team developed the helper plasmid technology in 2006, to aid in antibody screening by simplifying the process and eliminating the need for helper phage (short for bacteriophage). [Reference: "Eliminating helper phage from phage display", ***Nucleic Acids Research*** *34, e145* (2006), doi:10.1093/nar/gkl772.] Biologists often make use of bacteria and bacteriophage (viruses that infect bacteria) in their research, taking advantage of their minimal genomes and rapid growth and reproduction. One such use is to create libraries of phages, each of which has a different receptor on the surface, allowing the selection of specific receptors that recognize targets of interest. However, because the process requires helper phage that contains all the genes needed for replication, the libraries are often "contaminated" with excess helper phage. The team's plasmid display technology eliminates this problem, making it possible to screen a library of phagemids—each displaying a different antibody—for a specific antibody of interest without contamination with helper phage. This technology results in a genetically pure library population.

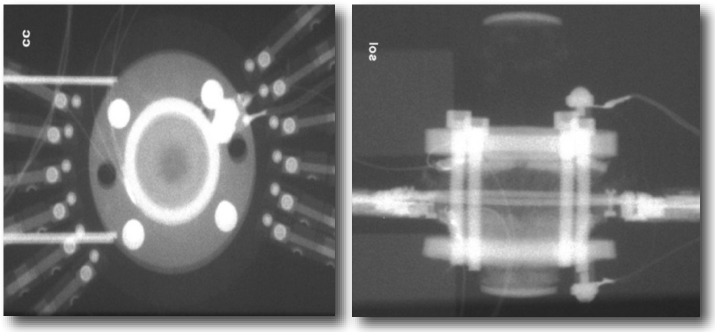
MorphoSys is a therapeutic antibody company using the display technology under a non-exclusive license with LANL. The company will incorporate it into their proprietary high-throughput platform to select antibodies for drug development. One such antibody-based drug is Herceptin, developed by Genentech, which is currently used for breast cancer therapy. Discussions to license the technology to biotech reagent companies are also ongoing. David Hadley (TT-DO) is the business development executive leading the licensing effort for this technology.

CHEMISTRY

X-ray radiography of internal, subsonic burning of explosives

The rate of energy release in a thermal explosion begins with a very nonlinear thermal ignition, wherein chemical energy is released, temperature increases, and the rate depends on temperature. This nonlinear temporal evolution and acceleration of the process precluded the synchronization of a thermal explosion with any modern, fast radiographic method until the first demonstration using proton radiography at LANSCE in 2005. Laura Smilowitz, Bryan Henson, Cynthia Schwarz, Alex Saunders, Frank Merrill, Christopher Morris and others of the proton radiography team conducted the experiment. The result led to publication in ***Physical Review Letters*** *100*, 228301 (2008) and a ***Physical Review*** Focus story. Smilowitz developed a new technique for synchronizing the timing of a thermal ignition while preserving the inherent features in the subsequent evolution of the explosion.

Subsequently Smilowitz and Henson collaborated with Lawrence Livermore National Laboratory (LLNL) to expand the scope of these techniques to include X-ray radiography at LLNL's HYDRA facility. Fast observation of thermal runaway at the ignition volume was required for the timing of the images at HYDRA, and it was this technology, developed by LANL, that enabled the full suite of radiographic tools to be applied to an important class of subsonic, internal combustion problems. Scientists completed a thermal explosion experiment very similar to the one used in the 2005 LANL proton radiography demonstration using 450 keV and 1MeV X-rays in March 2009 (Figure 1). The

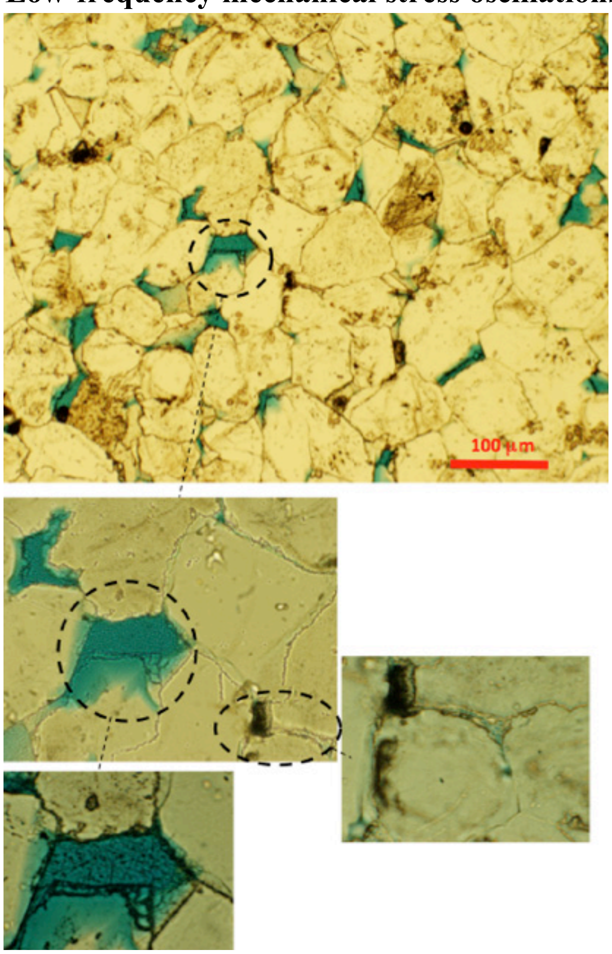


DOE/DoD Joint Munitions Program and the DOE Science Campaigns funded this work.

Figure 1. X-ray transmission images obtained at the HYDRA facility at LLNL. The two transmission images were recorded on the same experiment viewed down the long axis (1MeV) and side on (450 keV). The sample is a solid right circular cylinder of the explosive PBX 9501 encased on aluminum. The images were obtained at 10 ms and 60 ms after the fast thermocouple trigger; cracking, solid density loss, and case motion are observable.

EARTH AND ENVIRONMENTAL SCIENCES

Low-frequency mechanical stress oscillations enhance particle release in sandstone



Peter Roberts (EES-17) and Amr Abdel-Fattah (EES-14) observed unique results of laboratory fluid flow experiments performed on a Fontainebleau sandstone core (Figure 2). The experiments demonstrate the ability of low-frequency (seismic band) mechanical stress oscillations to couple to micro-scale processes in a porous medium, enhancing the release and transport of sub-pore-size *in-situ* colloidal particles trapped in the pore space.

Figure 2. Photograph of a thin section for the Fontainebleau sandstone core used in the experiments, showing the open pore space filled with blue dyed epoxy. The inset figures at the bottom left show enlargements of one of the open pores where small particles are seen coating the bottom surface of the

pore. The inset at bottom right is an enlargement of a closed pore containing additional particles not accessible to water flow.

Experimental effluent particle concentration data (Figure 3) showed that release of *in-situ* particles (clays, silica fines, etc.) from Fontainebleau sandstone is enhanced by applying mechanical stress oscillations to the core at 26 Hz. The behavior of the post-stimulation particle release is distinctly different than the pre-stimulation behavior in that *a cyclical pattern with uniform periodicity is observed*. The scientists attributed this behavior, which is independent of particle size over the range of 50 to 800 nm, to stimulation causing a long-term change in the distribution of the rate coefficients for release of particles from the pore space. The rate change is likely not due to alteration of particle-wall interactions, which are sensitive to particle size. Size-independent release mechanisms that explain the stimulated rate change are 1) enhanced flushing or squeezing out of particles trapped in dead-end pores, and 2) forced particle detachment and exposing of new detachment sites on the pore walls. These observations are unique in that they indicate sub-pore-scale particle release and transport can be influenced by dynamic stress at wavelengths approximately 5 to 6 orders of magnitude larger than the average pore size. This phenomenon alters subsurface permeability and mass transport behavior in ways that could impact field applications, such as enhanced oil recovery, accelerated contaminant extraction from groundwater aquifers, and permeability control for improved geologic carbon sequestration. Reference: "Seismic Stress Stimulation Mobilizes Colloids in a Porous Rock", ***Earth and Planetary Science Letters***, in press. The DOE Office of Science, Office of Basic Energy Sciences, Geoscience Division funded the work.

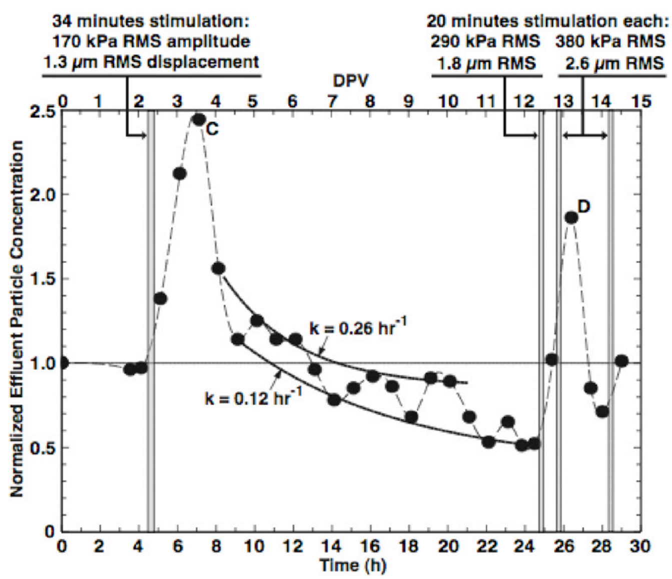


Figure 3. Normalized effluent particle number concentration vs. time and displaced pore volumes during 26-Hz dynamic stress stimulations of a Fontainebleau sandstone core. Solid curves are the least-squares fit of a first-order exponential particle release equation to the peaks and valleys of the cyclical particle concentration data after the first stimulation.

LANSCE

American Physical Society's *This Week in Physics* highlights Lujan Center research

Anna Llobet's (LANSCE-LC) publication with collaborators on intrinsic localized modes in sodium iodide (NaI) was described in the American Physical Society's ***This Week in Physics***, which highlights exceptional physics research. A longstanding question in condensed-matter science and nonlinear dynamics is whether intrinsic three-dimensional (3D) localized modes can appear in an atomic lattice in *thermal equilibrium*. Although the presence of "intrinsic localized modes" was first proposed in the 1980s, there was no experimental evidence. Llobet and collaborators' inelastic neutron scattering measurements at the PHAROS-LANSCE spectrometer show that sodium iodide, a simple three-dimensional ionic crystal, can support a single intrinsic localized mode in thermal equilibrium above 555 K. The mode gains energy with increasing temperature, consistent with molecular dynamic simulations. The localized mode occurs at a single frequency of 299 meV, which lies near the center of a gap in the phonon spectrum. This is the first observation of a 3D intrinsic localized mode in a crystalline solid, and it suggests an important role for such modes in the high-temperature physical properties of solids. Collaborators include A.J. Sievers, S.A. Kiselev, N.I. Agladze (Cornell University), J.W. Lynn and (National Institute of Standards and Technology), and A. Alatas (Argonne National Laboratory). Reference: "Intrinsic localized modes observed in the high-temperature vibrational spectrum of NaI," ***Physical Review B*** 79, 134304 (2009), DOI: 10.1103/PhysRevB.79.134304. The work was performed under the auspices of the DOE.

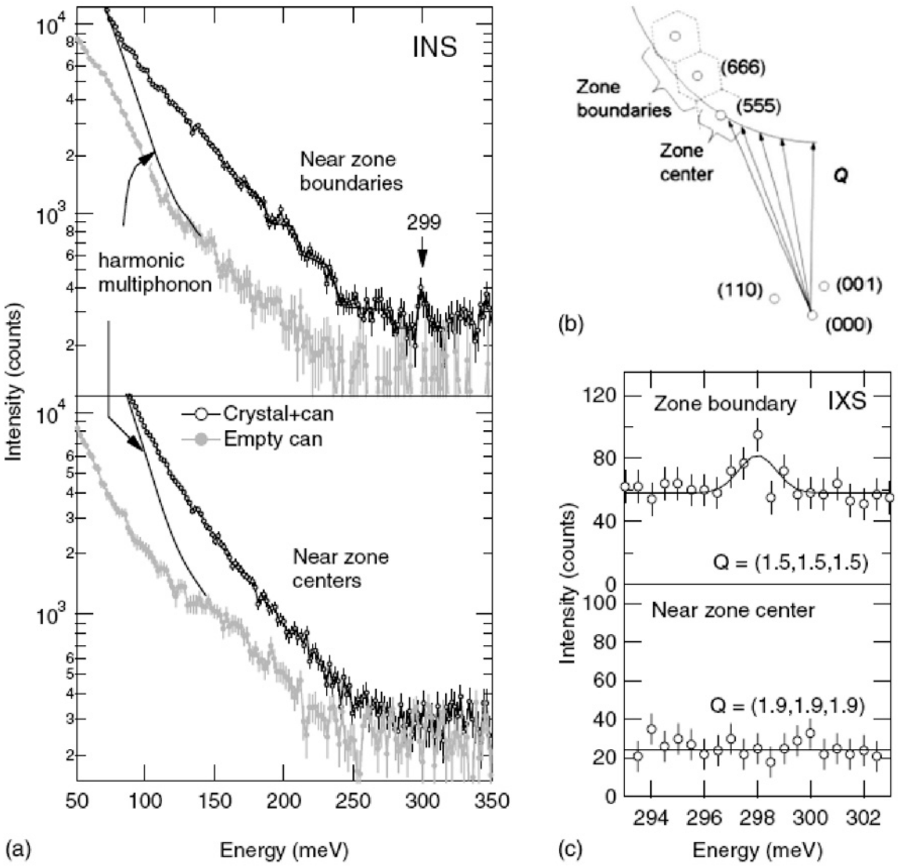


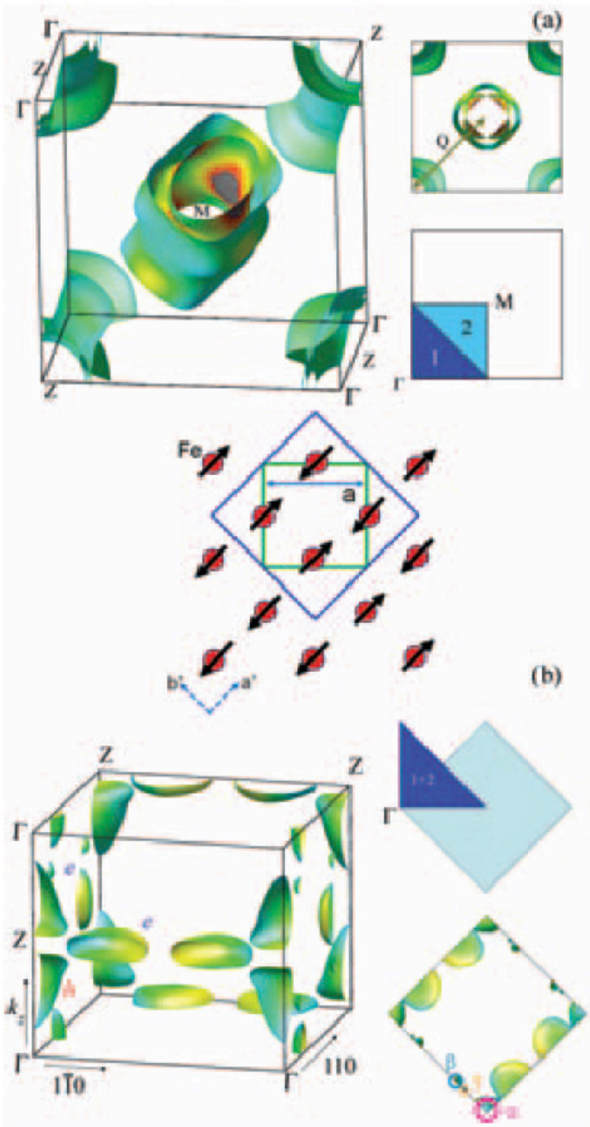
Figure 4. High-energy inelastic lattice response along for a room-temperature sodium iodide crystal probed using neutron and x-ray scattering. (a) Inelastic neutron scattering using 441 meV neutrons on the PHAROS-LANSCE spectrometer summed near zone boundaries (top panel) and near zone centers (bottom panel). The harmonic multiphonon contribution, which cuts off around 140 meV, was calculated in the incoherent approximation using the measured room-temperature phonon density of states. (b) Reciprocal space sampled by the PHAROS spectrometer. Here a neutron energy loss of 299 meV is assumed and this cut in *Q* space is illustrated, along with the regions near and away from the zone boundaries as applied in the detector sums. (c) Inelastic x-ray scattering collected near the 299 meV peak on the zone boundary (top panel) and near the zone center (bottom panel).

MATERIALS PHYSICS AND APPLICATIONS

Two LANL papers selected for Top Papers Collection of 2008

Two papers describing research performed in MPA-10, MST-8, and MPA-NHMFL were selected to be part of ***The Journal of Physics: Condensed Matter*** Top Papers Collection of 2008. The collection of 20 papers is a selection of articles that best represent the high quality and breadth of the contributions that were published in the journal last year, as chosen by the editorial board and publishing team. The LANL papers are described in the following paragraphs.

Quantum oscillations of $SrFe_2As_2$



Neil Harrison and Charles Mielke (MPA-NHMFL), S.E. Sebastian, J. Gillett, P.H.C. Lau, and G.G. Lonzarich (University of Cambridge, UK); and D.J. Singh (Oak Ridge National Laboratory) report measurements of quantum oscillations in $SrFe_2As_2$, which becomes superconducting under doping and the application of pressure. Knowing the nature of elementary excitations and their interplay with the Fermi surface is essential for understanding the origin of unconventional pairing in high temperature superconductors. The magnetic field and temperature dependences of the oscillations between 20 - 55 T in the liquid helium temperature range suggest that the electronic excitations are those of a Fermi liquid. The scientists show that the observed Fermi surface comprising small pockets is consistent with the formation of a spin density wave. This result demonstrates that high-T_c superconductivity can occur on doping or pressurizing a conventional metallic spin density- wave state. The observation indicates that strong correlations in the parent high- T_c antiferromagnetic phase $SrFe_2As_2$ are no obstacle to the establishment of conventional metallic behavior. Reference: "Quantum Oscillations in the Parent Magnetic Phase of an Iron Arsenide High Temperature Superconductor", ***The Journal of Physics: Condensed Matter*** *20*, 422203 (2008), DOI:10.1088/0953-8984/20/42/422203. DOE supported the LANL work.

Figure 5. a) The paramagnetic (unreconstructed) Fermi surface of $SrFe_2As_2$ calculated using the local-density approximation, together with a top–down view showing the relative sizes of the sections within the Brillouin zone. b) The reconstructed Fermi surface resulting from folding together with a top– own view of the antiferromagnetic Brillouin zone. The sizes of the experimentally observed α, β and γ pockets are shown for comparison. The color graduation of the Fermi surface represents the local Fermi velocity with red and blue corresponding to high and low velocities respectively.

Pressure-induced superconductivity in $CaFe_2As_2$

Joe D. Thompson, Tuson Park, Filip Ronning and Eric D. Bauer (MPA-10); Tomasz W. Klimczuk (MST-8); and E. Park and H. Lee (Sungkyunkwan University, Korea) report pressure-induced superconductivity in a single crystal of $CaFe_2As_2$. At atmospheric pressure, this material is antiferromagnetic below 170 K. Under an applied pressure of 0.69 GPa, it becomes superconducting, with a relatively high transition temperature T_c exceeding 10 K. The observations show that pressure offers a new route to superconductivity in these and possibly the related ZrCuSiAs materials without the need to introduce extrinsic chemical disorder. Reference "Pressure-induced Superconductivity in $CaFe_2As$", ***The Journal of Physics: Condensed Matter*** *20*, 322204 (2008), DOI:10.1088/0953-8984/20/32/322204. The DOE Office of Science and LANL LDRD supported the work.

MATERIALS SCIENCE AND TECHNOLOGY

Advances in understanding materials properties of radioactive waste forms

MST-8 researchers Chao Jiang, Chris Stanek, Kurt Sickafus, and Blas Uberuaga performed theoretical and calculational investigations of potential materials for radioactive waste forms. Two papers reporting their research were published in ***Physical Review B***. The papers, which feature the work of postdoctoral researcher Jiang, are described in the following paragraphs.

Chao Jiang, Chris Stanek, Kurt Sickafus, and Blas Uberuaga (MST-8) and collaborator N. Marks (Curtin University of Technology, Australia) used density functional theory to demonstrate "radioparagenesis", formation of new atomic structures due to the radioactive decay of one or more of the original structure's constituents. As cesium-137 chloride decays to barium-137 chloride, the resulting barium chloride (BaCl) structure is mechanically stable. The new phase for the Ba-Cl system was previously thought to be impossible to form, since Ba is a 2+ cation and Cl is a 1- anion. This result gives insight into how crystalline radioactive waste materials evolve with time, provides an understanding to develop new waste materials, and suggests synthesis routes for crystalline materials that cannot be created by conventional methods. Reference: "Predicting from First Principles the Chemical Evolution of Crystalline Compounds Due to Radioactive Decay: The Case of the Transformation of CsCl to BaCl", ***Physical Review B*** *79*, 132110 (2009), DOI: 10.1103/PhysRevB.79.132110. The DOE Office of Basic Energy Sciences funded the work.

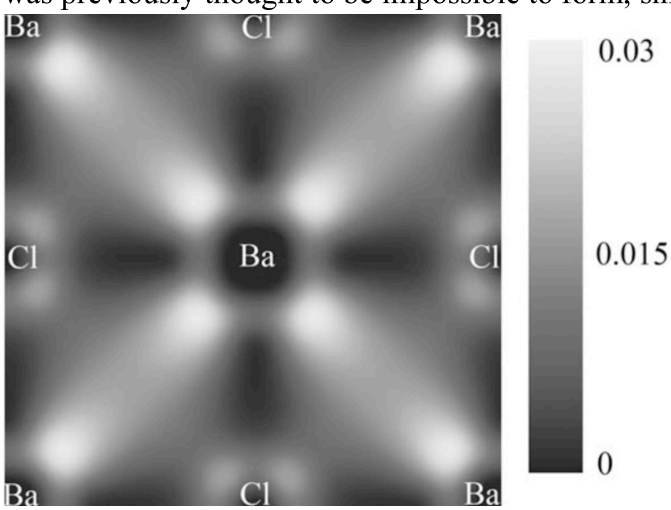


Figure 6. Conduction band-charge density (in e/Å3) on the (001) plane of rocksalt BaCl.

Chao Jiang, Chris Stanek, Kurt Sickafus, and Blas Uberuaga (MST-8) used first-principles calculations to describe the tendency for structural disorder versus composition of various pyrochlores. Pyrochlores are a family of complex oxides that has attracted great attention due to their potential as nuclear materials. The team's earlier work found that oxides with an ability to accommodate lattice disorder would be less susceptible to detrimental radiation damage effects. Therefore, the scientists examined the order-disorder phase transition under equilibrium conditions. Their work focuses on the similarities and differences between different pyrochlore compounds and should guide experimental studies for radiation tolerant materials. Reference: "First-principles Prediction of Disordering Tendencies in Pyrochlore Oxides," published in ***Physical Review B*** *79*, 104203 (2009), DOI: 10.1103/PhysRevB.79.104203. The DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering sponsored the work.

PHYSICS

New microfluidics facility in P-23

B. J. Balakumar (Fluid Mechanics Research Team, P-23) developed a new microfluidics facility that is capable of performing high-resolution velocity measurements in fluid flows at micron scale. The facility uses a micro-PIV (Particle Image Velocimetry) diagnostic and an epifluorescent microscope. Micro-PIV utilizes a dual head Nd:YAG pulsed laser to illuminate and track fluorescent particles embedded in the fluid. Cross-correlation techniques convert particle displacements into instantaneous fluid velocity fields. The facility is currently being used to study fluid and particle motion through micro-nozzles maintained under large pressure differentials. Data from the experiments are used to model hyperbaric chemical vapor deposition processes to make ultra-strong nanofibers for the Laser-weave project (R&D 100 Award recipient). The facility can also be used to perform experiments in biofluidics for threat reduction, porous media flows for environmental applications, explosives detection, and in micro-shock flows. Kathy Prestridge (P-23), Will Fox (IAT-2), John George (P-21), Luca Maciucescu (IAT-2/W-13) and James Maxwell (IAT-2) provided support. The LANL International and Applied Technology Division funded the work. Technical contact: *(Bala) B. J. Balasubramaniam*

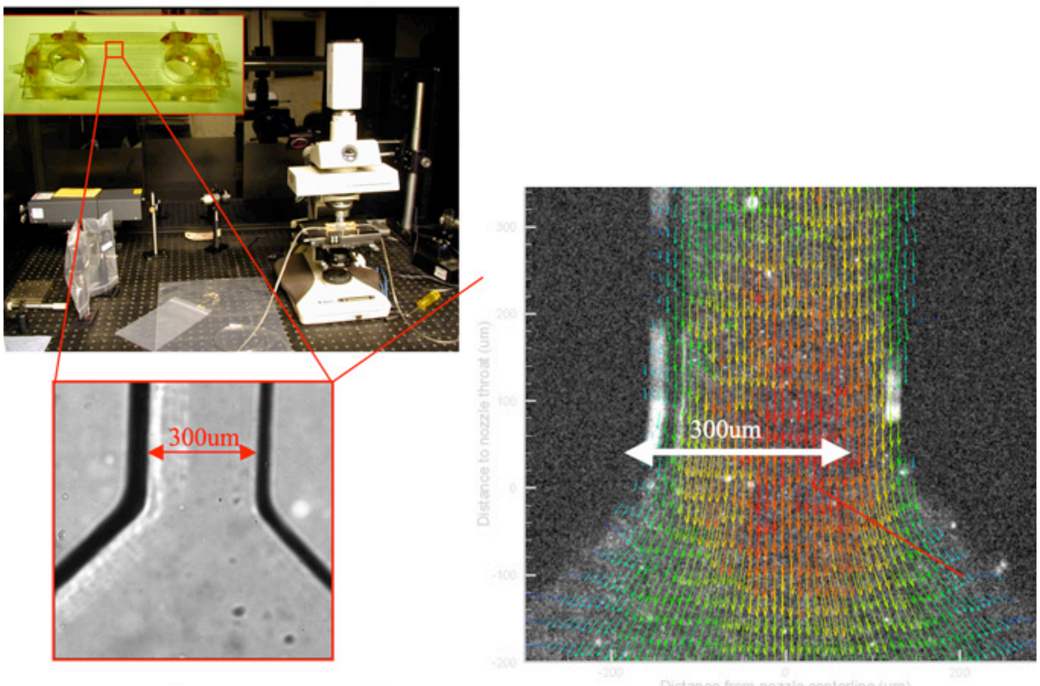


Figure 7. *Top:* photo of the microfluidics apparatus. *Bottom left:* polydimethylsiloxane micronozzle. *Right:* micro-PIV velocity field (9 micron resolution; Re=30).

THEORETICAL

Mathematical regularities in plant structures and physics

Phyllotaxis, the study of mathematical regularities in plants, challenged Kepler and Leonardo da Vinci, inspired the Bravais lattice of crystallography, and may have motivated humanity's first mathematical inquiries. S.L. Levitov proposed that the appearance of the Fibonacci sequence and golden mean in the disposition of spines on a cactus is replicated in physics, in the statics of cylindrically constrained, repulsive objects.

Cristiano Nisoli (T-4) and collaborators from Pennsylvania State University and Cornell University experimentally prove Levitov's model and describe for the first time the intriguing collective excitations of the phyllotactic geometry: multiple classical rotons and a huge family of interconverting topological solitons. The researchers constructed a magnetic cactus consisting of 50 outward-pointing, dipolar permanent magnets (spines) mounted on stacked coaxial bearings free to rotate about a vertical axis (stem), shown in Figure 7. They annealed the system into a lower-energy state by mechanical agitation. The spines on the magnetic cactus, like those of the plant, form phyllotactic spirals, generating a Farey tree of unfavorable angles. The unfavorable angles are fractional multiples of 2π. The spines on the magnetic cactus, analogous to those of the plant, form a helix around the cylindrical stem by growing around these particular angles. The scientists made the first investigations of dynamic linear and nonlinear phyllotaxis. A simple geometrical mismatch underpins both static and dynamic phyllotaxis phenomena: nearest neighbors in one dimension (i.e., along the axis) are not nearest neighbors in the full three dimensions. The scientists conclude that because dynamical phyllotaxis is purely geometrical in origin, this rich phenomenology could appear across many areas of physics.

Reference: "Static and Dynamical Phyllotaxis in a Magnetic Cactus", ***Physical Review Letters*** *102*, 186103 (2009), DOI: 10.1103/PhysRevLett.102.18610.3 .

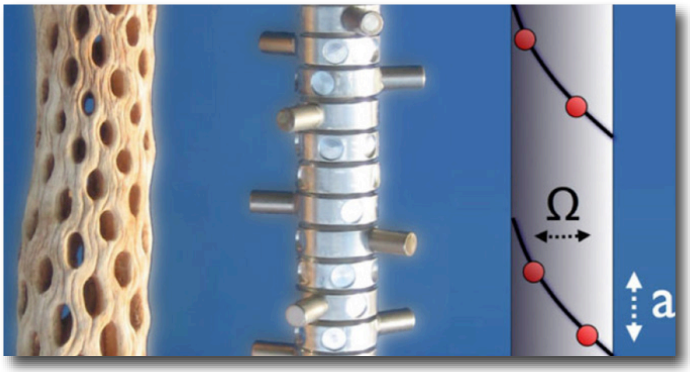


Figure 7. *Left:* a specimen of *Mammillaria elongata* cactus displaying a helical morphology ubiquitous to nature. *Center:* a magnetic cactus of dipoles on stacked bearings assumes phyllotactic spirals, similar to the cactus. *Right:* a schematic of a wrapped Bravais lattice showing the angular offset (screw angle) Ω and the axial separation *a* between particles.