

Stewardship Science Today

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

VOLUME 1 | NUMBER 4 | DECEMBER 2019

Stewardship Science Today (SST) highlights the stewardship science and academic programs supported by the Department of Energy/National Nuclear Security Administration (DOE/NNSA). SST is published quarterly by the NNSA Office of Research, Development, Test, and Evaluation. Questions and comments regarding this publication should be directed to Terri Stone via email at terri.stone@nnsa.doe.gov.

FEDERAL PROGRAM MANAGER
Dr. Tod Caldwell

MANAGING EDITOR
Terri Stone

TECHNICAL EDITORS
Dr. Joseph Kindel*, Jennifer Dieudonné*

PUBLICATION EDITOR & DESIGN
Millicent Mischo*



CALENDAR

2/23-27/2020

TMS2020: 149th Meeting and Exhibition, The Minerals, Metals & Materials Conference, San Diego, CA

2/26-27/2020

2020 Stewardship Science Academic Programs Symposium, Washington, DC

3/2-6/2020

American Physical Society March 2020 Meeting, Denver, CO

3/22-26/2020

American Chemical Society Spring National Meeting and Exposition 2020, Philadelphia, PA

INSIDE

- 2 Collisionless Shocks in NLUF Omega Experiments Mirror Conditions of Shocks in Supernova
- 3 Near Room Temperature Superconductivity at Extreme Conditions: Centerwide Discoveries at the Capital/DOE Alliance Center
- 4 DOE/NNSA Fellowships

*Contractor Support

Welcome to this latest issue of *Stewardship Science Today (SST)*. A large contingent of our team recently attended the American Physical Society Division of Plasma Physics meeting in Fort Lauderdale at which we hosted a Town Hall Meeting. We hoped to reach a wider sector of the scientific population with this meeting to let people know who we are, what we do, and the future opportunities available through our programs. If we didn't have the pleasure of meeting you there, we hope to meet you at another event in the near future.

Stewardship science is exciting, and the research that we support often is groundbreaking. This issue features a new breakthrough in superconductivity at more accessible temperatures. Much of this work has been carried out at our Capital/DOE Alliance Center and at the Advanced Photon Source. The breakthrough involves a new understanding of the lattice structures in materials that raises the temperature at which certain compounds become superconducting. Stay tuned for additional advances in this important field, as this new development is sure to be a game-changer.

We also feature work undertaken at the Omega Laser Facility to generate

electromagnetic, collisionless shocks in the laboratory! The success of these experiments now provides the potential to further study important, basic physics phenomena relevant to astrophysics and to the stockpile.

The call has gone out for the latest round of our graduate student fellowship opportunities. These are prestigious awards that come not only with a stipend but also with the coveted opportunity to conduct research at our national nuclear laboratories. Awardees of our fellowships are the top talent in our nation and go on to esteemed, scientific careers. Please pass this issue of SST on to rising graduate students, point them to the last page, make note of the deadlines, and encourage them to apply. We strive to identify young talent and to help those individuals succeed in their studies and move on to productive careers in fascinating scientific disciplines.

Happy new year!



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

2019 Annual Meeting of the American Physical Society Division of Plasma Physics and NNSA Town Hall

The Office of Experimental Sciences (OES) held a NNSA Town Hall at the 61st Annual Meeting of the American Physical Society (APS) Division of Plasma Physics (DPP) held in Fort Lauderdale, Florida, October 21-25. Open to all APS DPP attendees, OES Director Dr. Njema J. Frazier and Deputy Director Dr. Sarah Nelson Wilk led the well-attended Town Hall the evening of October 22. Along with NNSA Program Managers, Drs. Frazier and Wilk discussed current high energy density physics efforts as well as future opportunities and plans. The program ended with a question and answer session.

The 62nd Annual Meeting of the APS DPP will be held in Memphis, Tennessee, November 9-13, 2020.



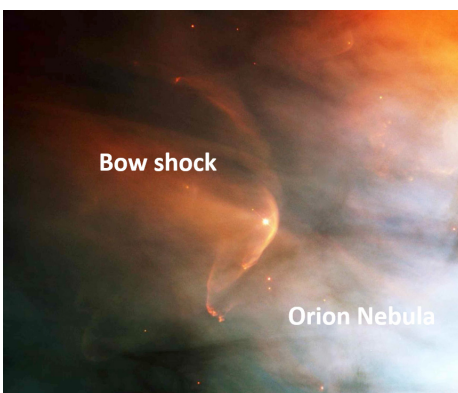
Dr. Charles P. Verdon, NNSA Deputy Administrator for Defense Programs, was among the distinguished guest speakers at the High Energy Density Science Association (HEDSA) Symposium held October 20. Dr. Verdon spoke about high energy density physics programs and activities at NNSA.

Collisionless Shocks in NLUF Omega Experiments Mirror Conditions of Shocks in Supernova Remnants

by Richard D. Petrasso (Massachusetts Institute of Technology)

For the last several decades, generation of electromagnetic collisionless shocks in the laboratory has been an important goal for elucidating large-scale astrophysical phenomena: supernova remnants, protostellar jets, accreting compact objects, and studying a broad range of fundamental physics phenomena. In this context, massive clouds of interstellar gas collide at non-relativistic speeds well in excess of 1,000 km/s, yet the plasma particles within these clouds still are so rarefied that most actually miss each other. Nevertheless, they interact electromagnetically or in other ways to produce visible shock waves and filaments (see Figure 1). These high-energy events, thought to be responsible for producing high-energy-cosmic rays, have been difficult to reproduce under laboratory conditions leading to disagreements among physicists as to the mechanisms at work.

To this end, Massachusetts Institute of Technology's (MIT's) Chikang Li and a large international collaboration succeeded in generating these collisionless shocks in innovative experiments performed at the Omega Laser Facility at the University



An example of an interstellar collisionless shock is seen in this photo of a bow shock in the Orion Nebula. Experiments recently performed at the Omega Laser Facility were able to mirror critical collisionless conditions found at the shock boundary. Image credit: NASA and the Hubble Heritage Team (STScI/AURA)

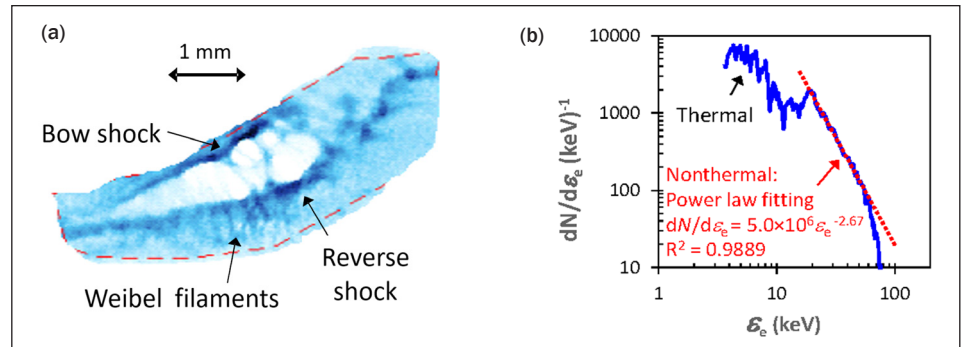


Figure 2. (a) Two-dimensional reconstruction of proton radiograph at $t = 6.4$ ns shows a double shock structure and filaments that characterize the collisionless shock conditions of the Omega experiments. (b) Electron spectrum measured in a direction perpendicular to the jet propagation shows a structure of two components: thermal and nonthermal. The nonthermal component has energies 2 orders of magnitude greater than the thermal component, a feature that indicates significant acceleration of the electrons through their interaction with the shocked region.

of Rochester Laboratory for Laser Energetics. This work, sponsored by the National Laser Users' Facility (NLUF) program and an NNSA Center of Excellence, recently was published in *Physical Review Letters* (PRL 123; 2019). As discussed in the journal article, electromagnetic collisionless shocks were formed (see Figure 2a), leading to the first definitive demonstration that the structure and dynamics of non-relativistic, astrophysically-relevant collisionless shocks can be reproduced in the laboratory. To achieve these special conditions, it was necessary to have compressed Biermann-generated magnetic fields associated with a gaseous magnetic piston from an exploding gas bag interact with Weibel magnetic fields generated within the colliding gas bag plasma and a counter-streaming jet plasma. This enhanced interaction enables the collisionless shock to be formed on a time scale that is orders of magnitude faster than if the Weibel magnetic filaments only were present. For more information about Biermann-generated magnetic fields, visit <https://www.energy.gov/science/fes/articles/biermann-battery-effect-spontaneous-generation-magnetic-fields-and-their>.

Under these conditions, one of the key signatures of these collisionless shocks is the generation of very energetic electrons, something that along with other important conditions and signatures, was observed in these experiments (see Figure 2b). In explaining these observations, it is

hypothesized that turbulent magnetic irregularities across the shock front could trap and accelerate, via a first-order Fermi mechanism, electrons to energies orders of magnitude above their thermal energy (see Figure 2b).

In an invited talk at the American Physical Society Division of Plasma Physics annual meeting in Fort Lauderdale in October, Li described details of these laboratory experiments and their close kinship to non-relativistic astrophysical phenomena. He posited that these experiments demonstrate that laser-matter interactions offer a unique platform, such as found at the Omega Laser Facility, for exploring collisionless shocks in a broader and more quantitative fashion. Working with Dr. Li, Associate Director of the High-Energy-Density Physics Division at the MIT Plasma Science and Fusion Center, PhD student Tim Johnson is further characterizing the conditions and details of these collisionless laboratory experiments. This will be accomplished through upcoming NLUF Omega experiments involving Thomson scattering.

This work is supported in part by the Department of Energy/National Nuclear Security Administration under Award Numbers DE-NA0002949 and DE-NA 0003539. ♦

Near Room Temperature Superconductivity at Extreme Conditions: Centerwide Discoveries at CDAC

by Eva Zurek (University at Buffalo, State University of New York) and Maddury Somayazulu (HPCAT, X-ray Science Division, Argonne National Laboratory)

Ever since the observation of superconductivity in mercury below a critical temperature, (T_c), of 4.2 K in 1911, scientists have searched for a material whose T_c approaches room temperature. Superconductors are employed in magnetically levitating trains, in strong electromagnets, and in particle accelerators. Moreover, because electricity passes through a superconductor without any resistance, replacing copper wires with superconducting power lines could save a tremendous amount of energy. Unfortunately, the materials that are commercially employed need to be cooled by liquid helium or nitrogen to below their T_c to realize their superconducting properties. Recent breakthroughs at the Capital/DOE Alliance Center (CDAC) may change this state of affairs, leading ultimately to the century-old dream of creating useful materials that superconduct at or near room temperature.

In 1968, Neil Ashcroft predicted that hydrogen in a hypothetical atomic metallic state at very high pressures, would be a conventional (i.e., electron-phonon), high-temperature superconductor. In 2004, he predicted that doping hydrogen with a second element could lower the metallization pressure required but still keep all of the properties conducive to high T_c superconductivity. Since then, the development of computational methods for crystal structure prediction using quantum-mechanical calculations and dramatic increases in supercomputing capabilities has made it possible for researchers to study theoretically the compounds that can be synthesized under high pressure and their properties.

The breakthroughs at CDAC began with the prediction of new classes of superhydride materials that have calculated T_c s near room temperature.¹ The work was performed by Hanyu

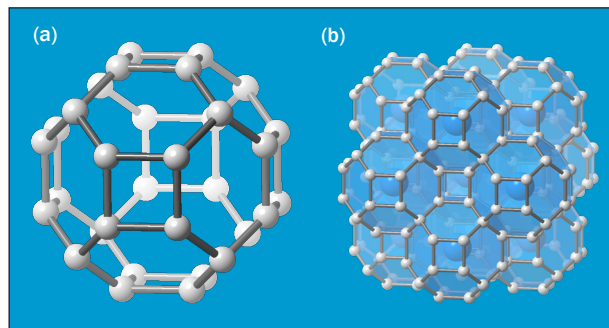


Figure 1: (left) The hydrogenic clathrate cage that is found within $Fm\text{-}3m$ LaH_{10} and (right) its extended crystal structure.

Liu under the direction of Center director Russell Hemley and CDAC research scientist Ivan Naumov. One of the most promising materials, LaH_{10} , then was synthesized by the team very close to the predicted pressures of 180 GPa (about half of the pressure in the Earth's core) using diamond anvil cell techniques.² These experiments were led by CDAC postdoc (and former Center student at Berkeley) Zachary Geballe at the NNSA-funded HPCAT synchrotron x-ray facility at the Advanced Photon Source. The team then spent a year developing new experimental techniques to both carefully synthesize and measure the superconducting properties by electrical conductivity and magnetic susceptibility at megabar pressures. This work was led by former CDAC research scientists Maddury Somayazulu and Muhetaer Ahart. The team then confirmed in multiple measurements the predicted very high T_c value of 260 K near 200 GPa, which is the current highest temperature superconductor yet found experimentally.³

These developments in CDAC have led to a broader Center-wide research initiative involving theory and experiment. In a recent article, CDAC university partner Eva Zurek and her student Tiange Bi, have reviewed the theoretical investigations that have searched for superconductivity in binary hydrides under pressure.⁴ The highest T_c values have been predicted for a subset of the alkaline and rare earth polyhydrides, such as MgH_6 , LaH_{10} , YH_9 , and YH_{10} . In these compounds, the hydrogen lattices resemble chemical compounds called clathrates, and these unique structures turn out to be key for

the extremely high T_c values. The LaH_{10} crystal structure is composed of face-sharing hydrogenic polyhedra that contain square and hexagonal faces, and the lanthanum atom lies in the center of each polyhedron (see Figure 1). The effort is being extended in CDAC to other areas of ‘materials by design’—the new paradigm in

materials science—taking advantage of the diverse capabilities and expertise across the Center.

Researchers worldwide are studying these exciting compounds. The findings of the CDAC scientists were soon confirmed by the theoretical group of Yanming Ma and the experimental group of Mikhail Eremets who, in addition, observed other characteristic signatures of superconductivity. The Meissner effect (the expulsion of a magnetic field by the superconductor) still must be demonstrated, and experiments are underway to verify the theoretical predictions of high-temperature superconductivity in other binary hydrides under pressure. Meanwhile, theoretical groups have started finding related materials that will be very high T_c superconductors at lower pressures and, potentially, even higher temperatures, for example in ternary hydride systems.

References

- ¹H. Liu, I.I. Naumov, R. Hoffmann, N.W. Ashcroft, and R.J. Hemley. “Potential High- T_c Superconducting Lanthanum and Yttrium Hydrides at High Pressure,” *Proc. Natl. Acad. Sci.*, 114, 6990–6995 (2017).
- ²Z.M. Geballe, H. Liu, A.K. Mishra, M. Ahart, M. Somayazulu, Y. Meng, M. Baldini, and R.J. Hemley. “Synthesis and Stability of Lanthanum Superhydrides,” *Angew. Chem. Int. Ed.* 57, 688–692 (2018).
- ³M. Somayazulu, M. Ahart, A.K. Mishra, Z.M. Geballe, M. Baldini, Y. Meng, V.V. Struzhkin, and R.J. Hemley. “Evidence for Superconductivity Above 260 K in Lanthanum Superhydride at Megabar Pressures,” *Phys. Rev. Lett.* 122, 027001 (2019).
- ⁴E. Zurek and T. Bi. “High-Temperature Superconductivity in Alkaline and Rare Earth Polyhydrides at High Pressure: A Theoretical Perspective,” *J. Chem. Phys.* 150, 050901 (2019).

This work is supported by the Department of Energy/National Nuclear Security Administration under Award CDAC DE-NA0003858. ♦

DOE/NNSA Fellowships

Stewardship Science Graduate Fellowship (SSGF)

The SSGF provides outstanding benefits and opportunities to students pursuing a PhD in areas of interest to stewardship science, such as properties of materials under extreme conditions and hydrodynamics, nuclear science, or high energy density physics. The fellowship includes a 12-week research experience at one of the NNSA national laboratories: Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), or Sandia National Laboratories (SNL). Visit www.krellinst.org/ssgf to learn more.

Computational Science Graduate Fellowship (CSGF)

The CSGF is open to senior undergraduates and students in their first year of doctoral study. It provides up to four years of financial support for students pursuing doctoral degrees in fields that use high-performance computing to solve complex problems in science and engineering. The program also funds doctoral candidates in applied mathematics, statistics, or computer science who are pursuing research that will contribute to more effective use of emerging high-performance systems. Details and a listing of applicable research areas can be found on the DOE CSGF website, www.krellinst.org/csgf.

Laboratory Residency Graduate Fellowship (LRGF)

The LRGF provides outstanding benefits and opportunities to U.S. citizens who are entering their second (or later) year of doctoral study to work at premier national laboratories while pursuing degrees in areas relevant to the National Stockpile Stewardship Program. It includes at least two 12-week research residencies at LLNL, LANL, SNL, or the Nevada National Security Site. Details are available at www.krellinst.org/lrgf.

Applications are due March 4, 2020.

2020 Stewardship Science Academic Programs Symposium

The Department of Energy/National Nuclear Security Administration 2020 Stewardship Science Academic Programs (SSAP) Annual Review Symposium will be held at the Wardman Park Marriott, 2660 Woodley Road NW, Washington, DC February 26-27, 2020. This Symposium features overviews of work-to-date from ongoing grants and cooperative agreements in the Stewardship Science Academic Alliances Program, the High Energy Density Laboratory Plasmas Program, and the National Laser Users' Facility Program. Presentations on topics of general interest also will be given by National Laboratory and/or NNSA personnel. For more information and to register, visit <https://www.orau.gov/ssap2020>. ♦

2020 High Energy Density Summer School

The 2020 High Energy Density Summer School will be held at the University of Michigan in June. This course provides an in-depth introduction to the field of high energy density physics and includes 40 hours of lecture. The course is aimed primarily at graduate students, young scientists, and experienced scientists who are just entering the field of high-energy-density physics. The exact dates and more details will be available at <http://clasp-research.engin.umich.edu/workshops/hedss/>. The HED Summer School is sponsored by the Department of Energy/National Nuclear Security Administration and by the Department of Climate and Space Sciences at the University of Michigan. ♦

Diagnostics for Subcritical Experiments

New Federal Program Manager Dr. Samantha Calkins, Office of Experimental Sciences, met with Nevada National Security Site's Management & Operating Contractor Mission Support and Test Services team in late October to discuss their contributions to the NNSA Advanced Diagnostics program. Topics included subcritical experiments and high-frame-rate imaging for the Proton Radiography facility. Photos courtesy of Stuart Baker, Nevada National Security Site.

