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CALENDAR

7/9-13/2023
30th IEEE Symposium on Fusion Engineering, Oxford, UK

7/9-13/2023
12th International Conference on Dense Z Pinch Plasmas (DZP 2023), Ann Arbor, MI

7/16-20/2023
Computational Science Graduate Fellowship Annual Program Review, Washington, DC

7/17-28/2023
High Energy Density Summer School, San Diego, CA

8/9-11/2023
14th Z Fundamental Science (ZFS) with Pulsed Power: Research Opportunities and User Meeting, Hotel Andaluz in Albuquerque, NM

9/6-8/2023
11th Hardened Electronics and Radiation Technology, Zurich, Switzerland

INSIDE

*Contractor Support

It is my pleasure to welcome you to the latest issue of *Stewardship Science Today* (SST). The National Nuclear Security Administration (NNSA) has reorganized, and now Academic Programs is being administered by the Office of Chief Science and Technology Officer. We are pleased to have Academic Programs join with our other initiatives, and we look forward to continuing the outstanding efforts of supporting stewardship science with our academic partners and evolving the program to expand community outreach efforts.

This issue features the work of a recently established Center of Excellence (COE) focused on better understanding materials degradation and component life extension in the context of stockpile stewardship. The Materials Data Science for Stockpile Stewardship COE at Case Western Reserve University is employing novel data science tools, computational frameworks, and experimental research to better understand and predict material failure caused by aging and to inform the design and manufacture of replacement components. This is vital work for the stockpile and having a focused COE that synergizes efforts in this area is a great step forward for this crucial work.

We also feature a series of experimental campaigns being undertaken by a team of Massachusetts Institute of Technology researchers using the MAIZE pulsed-power facility at the University of Michigan designed to gain a clearer understanding of the process of magnetic reconnection by incorporating the guide field and manipulating the orientation of the system to non-idealized conditions. Understanding magnetic reconnection, predicting and quantifying the thermal and kinetic energy released, and being able to manipulate the process has vast implications for the field of astrophysics and for high energy density science and the stockpile.

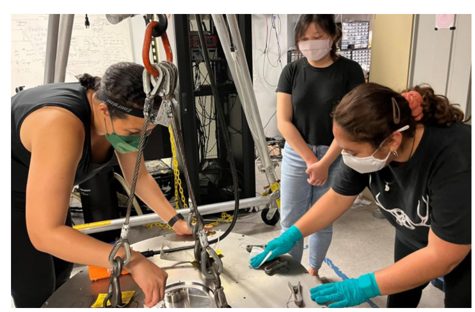
Congratulations to the eight universities that NNSA recently selected to receive cooperative agreements to support nine Stewardship Science Academic Alliances (SSAA) COEs. The SSAA program has been supporting academic institutions who conduct research and development in areas of importance to our stockpile stewardship mission since 2002.

Please enjoy this issue of SST. We look forward to bringing you news of continued innovations in stewardship science.

Dr. Kevin C. Greenaugh
Chief Science and Technology Officer
Defense Programs

NNSA to Award $100 Million for Stewardship Science Academic Alliances Centers of Excellence

The U.S. Department of Energy/National Nuclear Security Administration (DOE/NNSA) selected eight universities to receive cooperative agreements totaling $100 million to support nine Stewardship Science Academic Alliances (SSAA) Centers of Excellence focused on research activities in areas of physical sciences and engineering.



The University of California, San Diego (UCSD) is one of the eight universities selected to receive a cooperative agreement from NNSA to support research at its Center for Matter Under Extreme Conditions. Pictured are graduate student Apsara Williams, R&D engineer Samantha Fong, and undergraduate Kimberly Inzunza conducting maintenance on the Center's CESZAR machine (2021-2022 academic year).

The SSAA program funds research grants and cooperative agreements to provide opportunities for scientific collaboration between the academic community and scientists at the DOE and NNSA national laboratories. A main objective of the SSAA is to develop and maintain a long-term

(continued on page 3)

Materials Data Science for Stockpile Stewardship Center of Excellence

by Frank Ernst, Laura S. Bruckman, Yinghui Wu, and Roger H. French (Case Western Reserve University)

The mission of the Materials Data Science for Stockpile Stewardship (MDS³) Center of Excellence (COE) is to develop, demonstrate, and deploy novel data science tools, frameworks, codes, and computing infrastructure to advance the understanding of materials degradation and the failure of materials, parts, and subsystems and to deliver a diverse, data-enabled workforce for the future.

This effort is led by Case Western Reserve University (CWRU) in partnership with the University of Central Florida (UCF) and in collaboration with Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), Sandia National Laboratories (SNL), and the Kansas City National Security Campus (KCNSC). We are developing MDS³ COE tools and frameworks that will be applicable broadly across the major National Nuclear Security Administration (NNSA) programs.

The computational and experimental research components of the MDS³ COE will demonstrate the full lifecycle of data-science-enabled stockpile stewardship to address the challenging NNSA topics and missions in areas of material degradation and component reuse. This unified cycle of learning will integrate stockpile surveillance of materials' aging and lifetimes and will lead to actionable insights for advanced manufacturing design and production agency teams.

Understanding and transforming historical and newly-generated data to extract scientific knowledge and insights is a non-trivial task given both the complexity and size of the data. Advanced analytical tools and infrastructure are necessary to interpret and generate value from these datasets.

In the MDS³ COE, we develop the physical, computational, and intellectual resources to understand, process, and build models to predict the lifetime performance of materials in systems. The MDS³ COE has a matrix structure consisting of two Computer Science Thrusts, Computing Infrastructure (CI) and Knowledge Management & Learning (KML), that cross-cut two Materials Science Thrusts, Field-lab Aging & Reliability (AR) and Next-Generation Design Optimization & Production (DOP) (Figure 1).

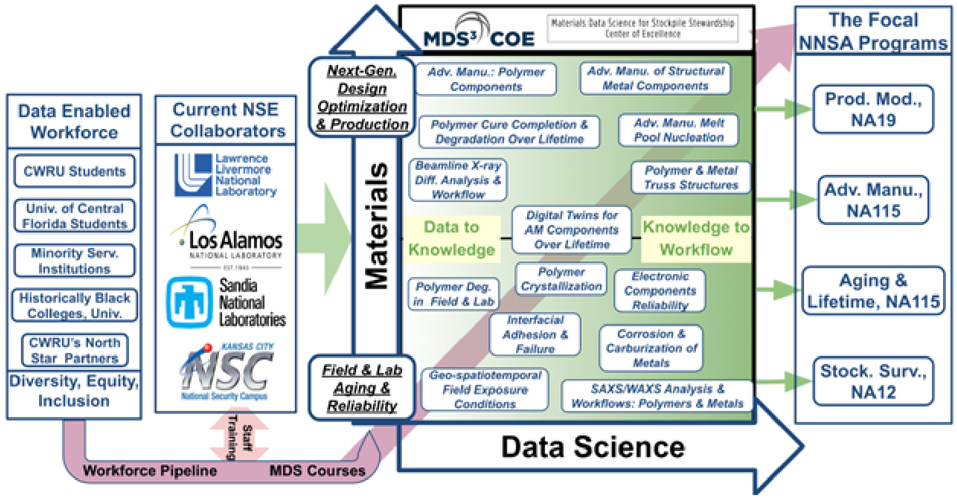


Figure 1. The structure of the MDS³ COE is focused on cross-cutting Materials Science and Computer Science research to develop tools and approaches for large scale materials data science applications for stockpile stewardship. MDS³ works closely with our NNSA collaborators, sites, and programs and focuses on producing data-enabled MDS³ researchers for the future NNSA workforce.

The intersection of these thrusts contain defined data science and materials science research projects and provide an avenue to explore and establish a suite of capabilities and tools. These projects can evolve over the course of the COE to fill the needs of our collaborators.

The NNSA can explore the approaches or workflow pipelines developed by CWRU and can tailor the applications to their specific classified needs.

Furthermore, there is a Data Enabled Workforce (DWE) Thrust that focuses on building and training a new generation of a data-enabled workforce that is both diverse and inclusive.

With the facilities of the Department of Energy (DOE)/NNSA, there are phenomenal instruments like the synchrotron beamlines that provide terabytes of data. The magnitude of these data sets does not support analyses on the scale of personal computers. Instead, there is an opportunity to create organized materials data science framework that can be analyzed using distributed and high performance computing. The evident need of such data framework is highlighted by a project in the MDS³ COE on beamline powder X-ray diffraction at the Advanced Photon Source (APS), in collaboration with LANL, looking at metal alloys *in situ* using deep neural nets. A major challenge is to generalize and scale these models into general-purpose computational frameworks to support large-scale materials analytical pipelines.

In order to understand and control the properties of a metal part, we need to understand how defects at a very small scale are introduced in the part as the part is forming from liquid metal to solid metal. This can be hard to imagine. Beamline X-ray diffractometry, for which a high-energy X-ray beam is transmitted through the material and video recordings of two-dimensional (2D) diffraction patterns are obtained, provides data of the inside of the metal part. Diffraction patterns present information in a less intuitive form than images and, traditionally, scientists have been struggling with extracting useful information from these patterns show. The features in the diffraction patterns show different components of the metal microstructure.

Figure 2 shows the simulated 2D diffraction patterns of beta-Ti for 1,000 randomly oriented grains with

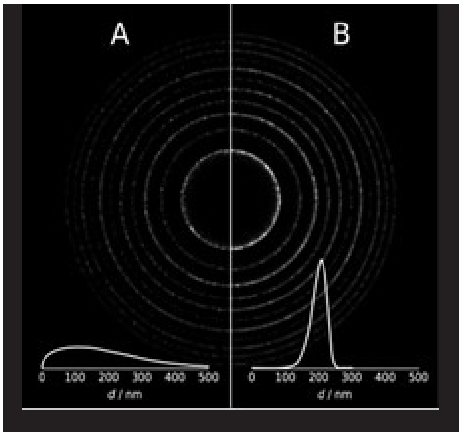


Figure 2. Simulated 2D diffraction patterns of beta-Ti for 1,000 randomly oriented grains with the same mean grain size of 200 nm, but different standard deviation in A and B, causing different variation of spot intensities.

the same mean grain size of 200 nm, but with different standard deviations in A and B, causing different variation of spot intensities. Whereas for a human observer, these two different effects are difficult to decouple, neural networks can be trained to reliably classify different grain-size distributions and corresponding unknown patterns, each belonging to one grain size distribution. Developing this approach further will provide an entirely new way to extract massive data from a series of 2D diffraction patterns.

Materials data science advances, such as X-ray diffraction pathways, illustrate the benefits MDS[3] COE brings to the NNSA's stockpile stewardship mission in a number of ways:

- Streamlining and accelerating the development and utilization of data science across the DOE/NNSA programs to improve nuclear weapon surveillance and production for more effective and efficient decision making;
- Improving the competitiveness of the national laboratories;
- Providing a concrete demonstration of forefront data science techniques;
- Developing data standards, information quality assurance, and privacy-preserving mechanisms that enable automated analyses and protect against cyber-risks;
- Establishing workforce pathways with deep expertise in advanced data science and analytics;
- Accelerating and deepening analyses of specific collaborator data resources.

Stewardship Science Academic Alliances Centers of Excellence *(continued from page 1)*

recruiting pathway supporting the DOE/NNSA national laboratories by training and educating the next generation of scientists in critical areas of science and technology research relevant to stockpile stewardship.

"These grants will allow NNSA to train the brightest and most skilled individuals while creating a direct pathway into our workforce with a diverse group of experts that can meet the evolving needs of the nuclear security enterprise," said Dr. Kevin Greenaugh, Chief Science and Technology Officer for Defense Programs.

The SSAA Centers of Excellence funding opportunity announcement is posted every five years. The proposals, submitted in response to a solicitation published last year, went through a competitive application process with an extensive peer review by subject matter experts. Overall, nine proposals were selected to receive cooperative agreements in the research areas of advanced characterization of material properties under extreme conditions, low energy nuclear science, radiochemistry, or high energy density physics.

The grants will be awarded between May 2023 and June 2024. The total funding is $17 million in Fiscal Year 2023 with $83 million allocated in outyear funding contingent on congressional appropriations.

Launched in 2002, the SSAA supports areas of fundamental research and development relevant to NNSA's stockpile stewardship mission and works to recruit the next generation of highly trained technical scientists and engineers for careers with the nuclear security enterprise.

The SSAA program includes the Laboratory Residency Graduate Fellowship and the Stewardship Science Graduate Fellowship and is one of five academic programs under NNSA along with the Minority Serving Institutions Partnership Program, including the Tribal Education Partnership Program, the High Energy Density Laboratory Plasmas, the Computational Science Graduate Fellowship, and the Predictive Science Academic Alliance Program.

The SSAA Centers of Excellence that were selected under this solicitation are as follows:

- Advanced Characterization of Metals under Extreme Environments (ACME[2]), Colorado School of Mines
- Transuranic Chemistry Center of Excellence, Georgia Institute of Technology
- CENTAUR: Nuclear Science in Service to the Nation, Texas A&M University
- Center for Additively Manufactured Complex Systems under Extremes (CAMCSE), University of Alabama at Birmingham
- The Center for Matter Under Extreme Conditions, University of California, San Diego
- Chicago/DOE Alliance Center – A Center of Excellence for Materials at Extremes, University of Illinois Chicago
- The Center for Magnetic Acceleration, Compression, and Heating (MACH), University of Michigan
- Center for High Energy Density Laboratory Astrophysics Research, University of Michigan
- The Wootton Center for Astrophysical Plasma Properties, University of Texas at Austin

Magnetic Reconnection Experiments on the MAIZE Pulsed-Power Generator

by Jack Hare (Massachusetts Institute of Technology)

Magnetic reconnection is a ubiquitous process that happens anywhere in the Universe when non-aligned magnetic field lines are brought together inside a plasma. As the field lines are pushed closer and closer together, an intense sheet of electrical current forms between them which breaks the frozen-in condition of ideal magnetohydrodynamics. This enables the magnetic fields lines to break and reconnect, changing their topology and explosively unleashing the magnetic energy as kinetic and thermal energy.

Reconnection can be studied in the laboratory using a range of techniques from low density, magnetically-dominated devices that resemble the conditions found inside of tokamaks to high energy density, magnetically sub-dominant plasmas created at laser facilities such as the Omega Laser Facility at the University of Rochester and the National Ignition Facility at Lawrence Livermore National Laboratory.

In the last few years, new experiments driven by pulsed-power also have emerged that enable magnetic reconnection to be studied in a new regime of parameter space in which the magnetic, thermal, and kinetic pressures all are roughly equal. This regime is particularly relevant astrophysically. Previous pulsed-power reconnection experiments on MAGPIE at Imperial College London and on the Z Machine at Sandia National Laboratories have studied magnetic reconnection using exactly anti-parallel magnetic fields. However, in nature magnetic fields rarely are so neat and orderly. There is a component of the magnetic field perpendicular to the anti-parallel components known as the guide field, because electrons and ions can be magnetized and guided by it.

In recent experiments on the MAIZE pulsed-power generator at the University of Michigan, a group of researchers from the Massachusetts Institute of Technology (MIT) developed a new pulsed-power-driven reconnection platform that attempts to incorporate this guide field, either by applying a large external magnetic field using a set of pulsed Helmholtz coils or by rotating the wire arrays that produce the reconnecting plasma flows so that the magnetic fields are tilted.

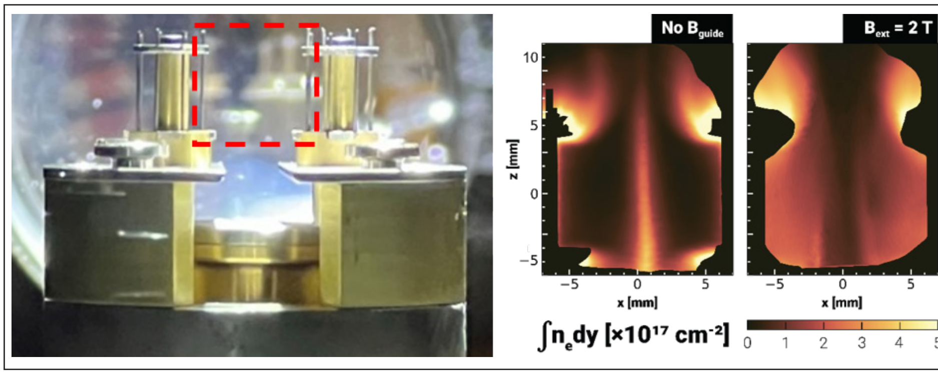


Figure 1. The reconnection platform with external applied magnetic fields. The region viewed by the interferometer is shown as a dashed red line. The interferometer shows the formation of a dense reconnection layer in the absence of an external field and the formation of a void between the plasma flows when a 2 T external field is applied.

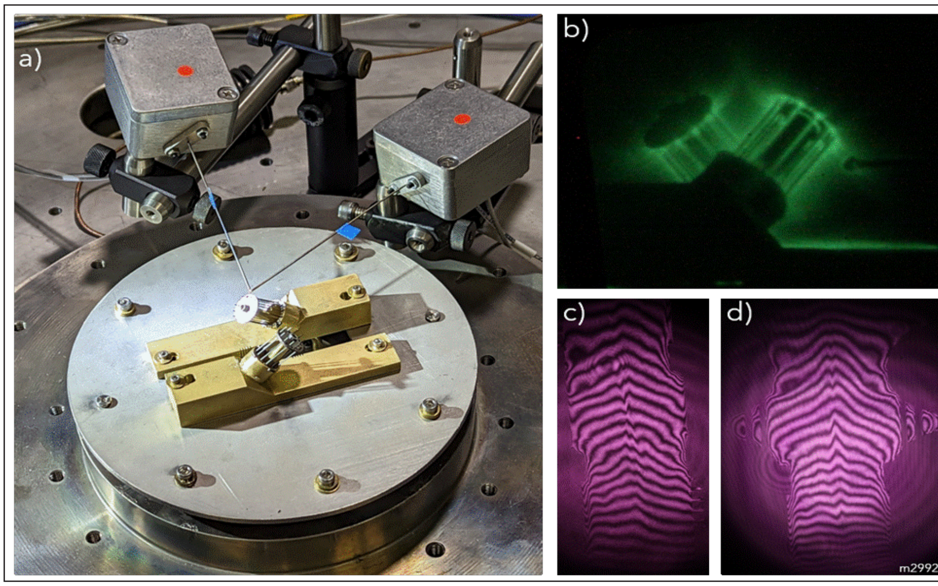


Figure 2. The reconnection platform with tilted wire arrays. a) Photograph of the hardware in chamber. b) An extreme ultraviolet (XUV) image of the two wire arrays. c) End-on interferometry and d) side-on interferometry, showing a reconnection layer.

The first series of experiments took place in January 2022 and was led by graduate student, Thomas Varnish of the MIT Nuclear Science and Engineering department. The load hardware is shown in Figure 1. The main result was that applying a large external magnetic field prevented the reconnection layer from forming, as the plasma flows "froze-out" the external field.

The second series of experiments ran in March and April of 2023 and was led by Thomas Varnish with two other MIT graduate students, Simran Chowdhry and Lansing Horan. These experiments used tilted wire arrays. Preliminary data from these experiments are shown in Figure 2, where a reconnection layer clearly is visible in the two orthogonal interferometry images.

We are grateful to the National Science Foundation and the National Nuclear Security Administration for funding this research under award PHY2108050.