LA-UR-24-24742

Approved for public release; distribution is unlimited.

Title: Dynamic Mesoscale Materials Science at the Advanced Photon Source

Author(s): Bishop, Arthur Dick

Intended for: Presentation.

Issued: 2024-05-13

Los Alamos
NATIONAL LABORATORY

Dynamic Mesoscale Materials Science at the Advanced Photon Source

Thom Mason

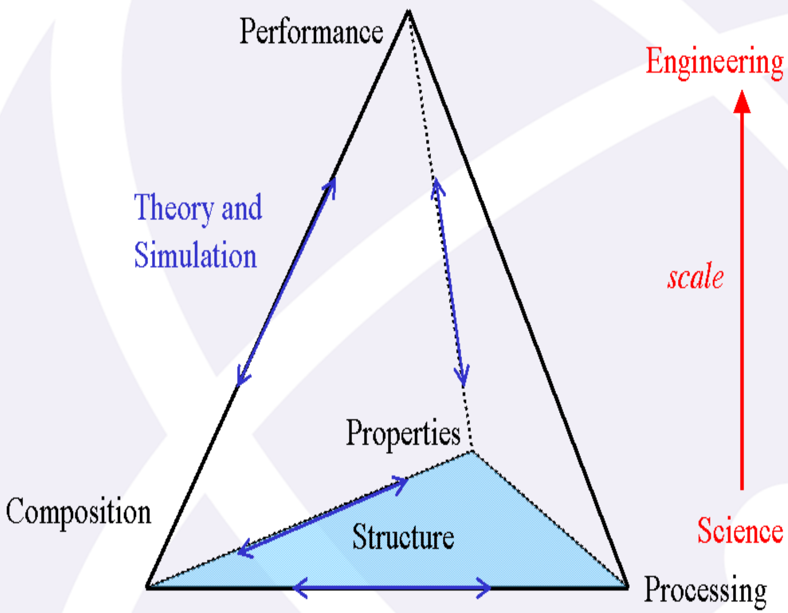
May 21, 2024

Mesoscale materials science and dynamic imaging are integral capabilities of our nuclear weapons missions.

- We are modernizing our 1980s nuclear deterrent, and moving beyond life extensions (W76, B61, W88) to systems that have more newly (differently) manufactured components (W80, W87).
- For the first time since the 1980s, we are doing truly new designs (W93) and there will likely be more to respond to emerging deterrence gaps.
- Whether due to aging, or new manufacturing processes and materials, we need to understand how changes in microstructure (compared to tested legacy systems) impact performance.
    - This understanding on how the mesoscale impacts macroscopic system performance needs to be in the extreme environments relevant weapons and on the length and timescale that matter.
- Experiments on materials we care about (Pu, U, plastics, HE, weird alloys,…) on those time and lengths allow us to link simulations with our test history, and enable ML/AI approaches to future qualification.

Filling the dynamic mesoscale materials science (DMMSC) gap today and in the future are institutional priorities

- The Dynamic Mesoscale Materials Science Capability (DMMSC) addresses a national unmet scientific need for understanding material performance and production at the mesoscale.
- The ultimate goal is the integration of material structure and processing to achieve desired material properties and ultimately desired performance – supporting production science.
- The mission need for the capability and the facility project are important timely priorities for DOE/NNSA and Los Alamos National Laboratory.

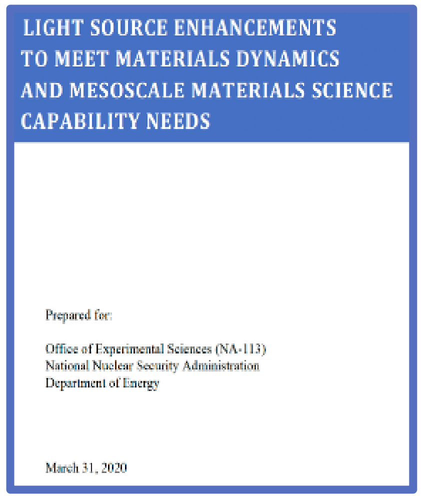


Understanding process-structure-property-performance relationships requires a research capability to explore mesoscale dynamics

NNSA's need to predict and control the microstructure of materials is also a science frontier…

2021

"The National Nuclear Security Administration (NNSA) has **an unmet capability need to improve our ability to predict how changes in a material's microstructure impact its performance in weapons environments.** Certification of the future stockpile; maintenance of the current, aging stockpile; and qualification challenges associated with materials and manufacturing changes will rely heavily on an understanding of materials in extreme environments."

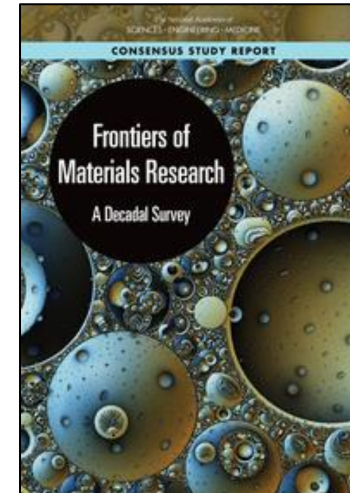

LIGHT SOURCE ENHANCEMENTS TO MEET MATERIALS DYNAMICS AND MESOSCALE MATERIALS SCIENCE CAPABILITY NEEDS

Prepared for:

Office of Experimental Sciences (NA-113)
National Nuclear Security Administration
Department of Energy

March 31, 2020

"Collectively, these new ultrabright sources will drive further advances in the techniques, enabling the **transformative studies of materials with nanoscale resolution while under operating conditions and on ultrafast time scales.** The United States had a significant fraction of all the world-leading capabilities 20 years ago, but that lead has eroded and today's landscape is one of intense competition from both Europe and Asia."

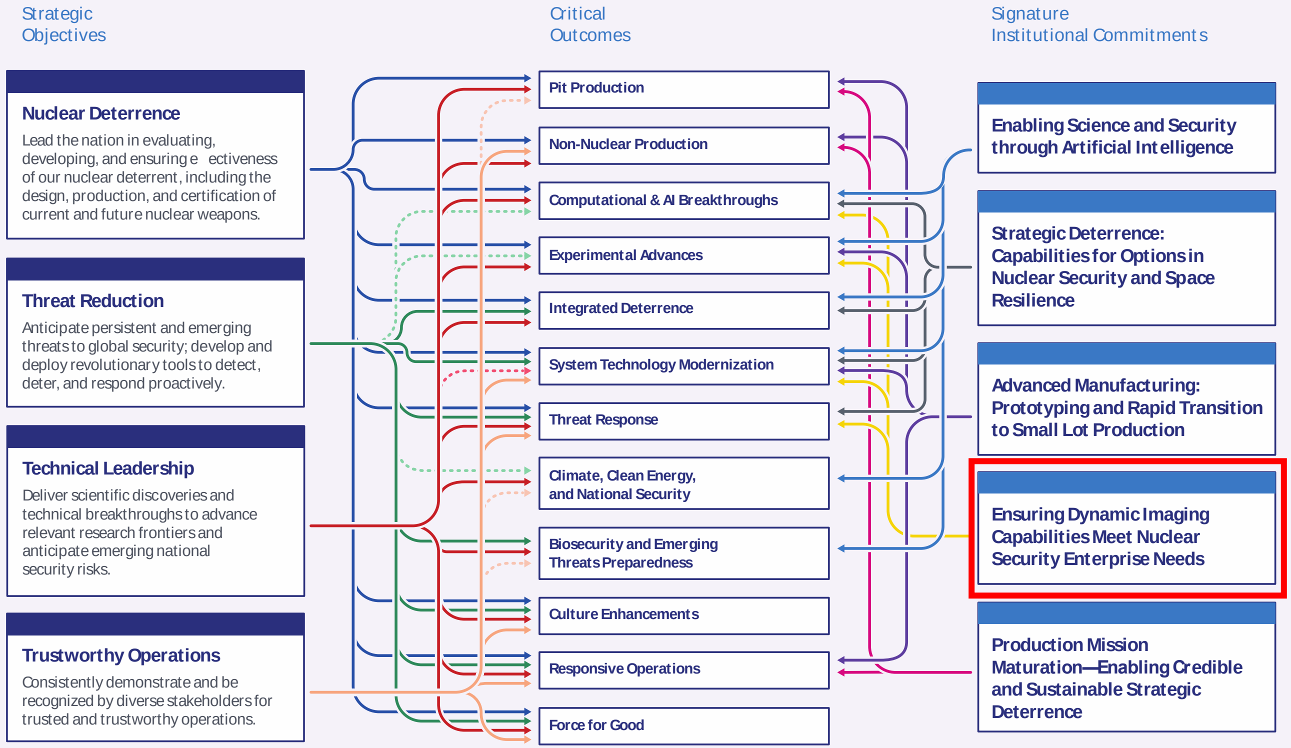


…that motivates new capabilities and will demand co-design for success

Lab Agenda Snapshot

January 2024

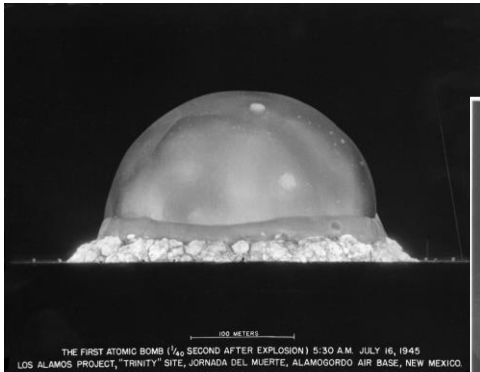
The Laboratory Agenda provides a structured framework that identifies the strategic objectives, critical outcomes, near-term R&D, and production and mission-support activities needed to accomplish our mission



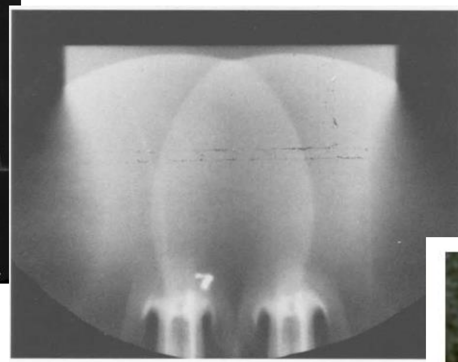
Los Alamos NATIONAL LABORATORY

LA-UR-24-20391

The Laboratory recently announced a signature institutional commitment to our dynamic imaging science and capabilities.



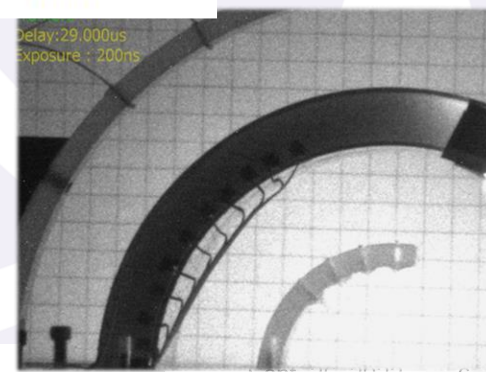
Trinity, 1945



Phermex, 1969

- Dynamic imaging has always been central to our missions.

DARHT, 2009
(first 2-axis explosive test)



pRad, 2023

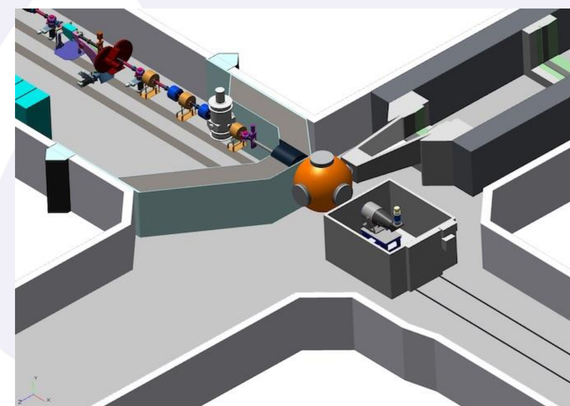
- The future priorities will include modernizing capabilities (U1a, DARHT, LAMP, NIF, DMSS) and applying data science methods to be more agile in our use of qualification and certification tools.

Enhanced Capabilities for Sub-critical Experiments (ECSE)

- **ESCE** is currently under construction at U1a (PULSE):
  - Scorpius radiography
  - Neutron-diagnosed SCEs (NDSE)
  - Multi-point PDV

- Scorpius will be located at U1a, where scientists and engineers have been conducting subcritical experiments since 1995.

- The aim of Scorpius is to provide a radiographic capability, using particle accelerator technology to generate x-rays and to “see” what's happening to plutonium.



M. Crawford, J. Barraza, Scorpius: The Development of a New Multi-Pulse Radiographic System, Los Alamos National Laboratory.

We are actively doing 'DMMSC science' today using existing capabilities

- Active and growing engagement at APS, LCLS, EuXFEL, …
- Focus on production science and advanced manufacturing
- Developing future predictive capabilities of materials performance under extreme environments: phase-, microstructure-, and age-aware
- Continuing to leverage LANSCE's unique capabilities
- Exploring accelerator technology alternatives, including detectors and drivers, while also delivering ECSE

LANL is performing mesoscale materials science relevant to our missions today at LANL and national facilities.

CINT: Nanomaterials synthesis and characterization

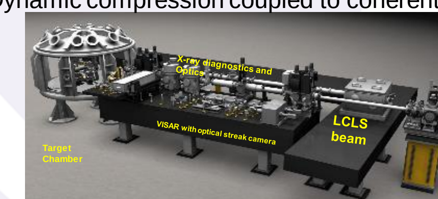
NHMFL-PFF: Research with high magnetic fields

Materials-Centric National User Facilities

LCLS

Current MEC at LCLS

Dynamic compression coupled to coherent x-rays



Advanced Photon Source

HPCAT

DCS@APS

WASHINGTON STATE UNIVERSITY

LANSCE Los Alamos Neutron Science Center

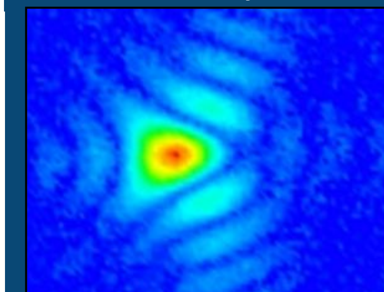
SNS SPALLATION NEUTRON SOURCE

DOE/NNSA has been a partner at APS for over 20 years.

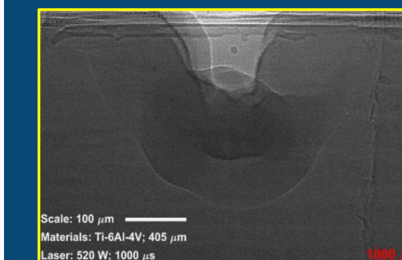
Advanced Photon Source Key Characteristics

High Energy
Penetrating bulk materials and operating systems

Brightness/Coherence
Highest possible spatial resolution/dynamics



Time-Resolved Studies
Measurements from ~100ps to seconds

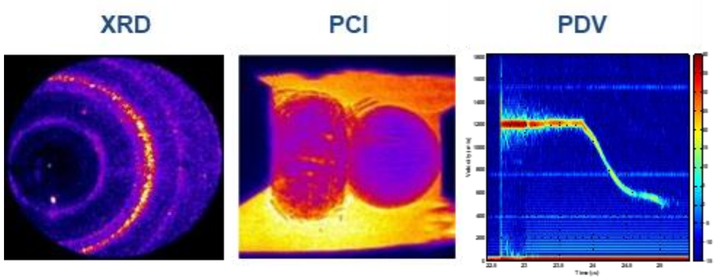


Argonne National Lab

Leverage ANL core research programs & advanced computing facilities to enhance x-ray capabilities & scientific productivity

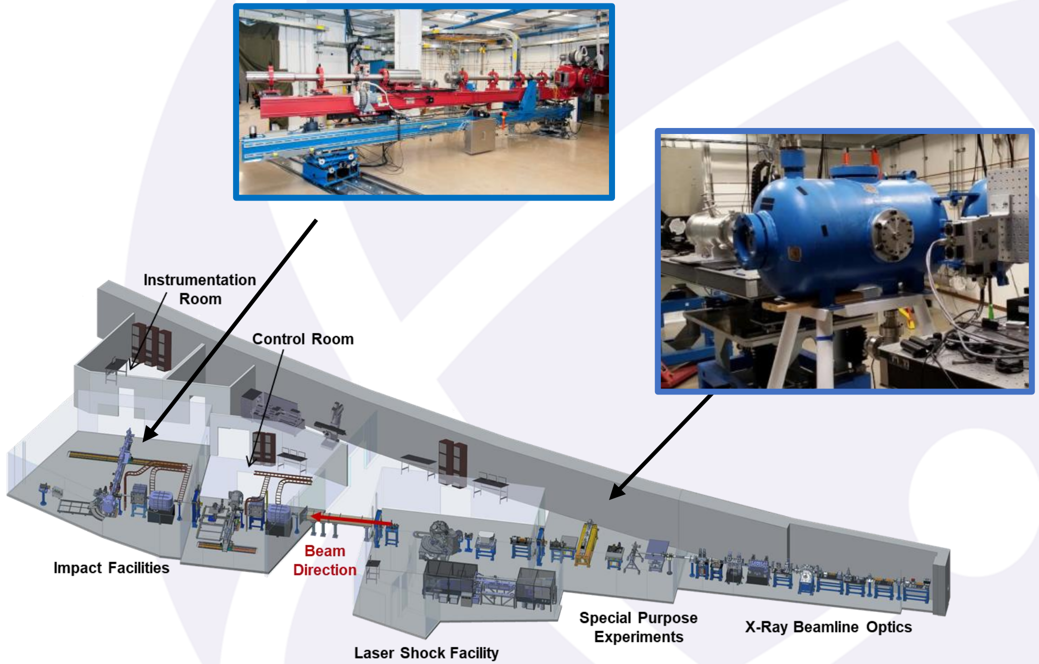
The Dynamic Compression Sector brought new X-ray based diagnostics coupled to dynamic driver platforms.

- **Dynamic Compression Sector (DCS)**
  - APS Sector 35
  - Focus on dynamic compression science
  - Commissioned in ca. 2013-2014
  - Managed by Washington State University



- Many “firsts” in dynamic compression science
- Countless contributions to NNSA missions and milestones

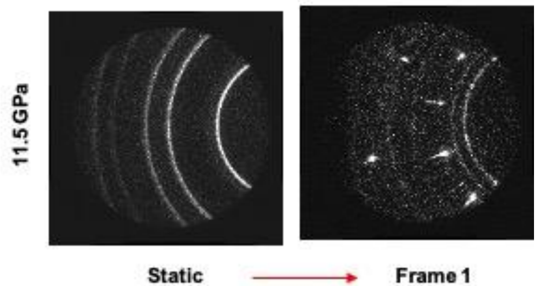
Diffraction, scattering and imaging under dynamic loading



Congratulations on 10 years!

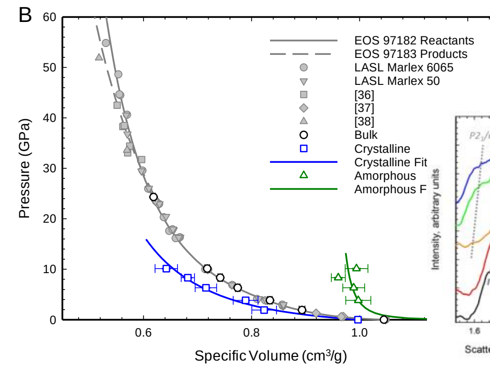
NNSA Laboratories are successfully using capabilities at the APS and DCS and acquiring data that are impacting NNSA Missions…

XRD to study phase transformation in Ce

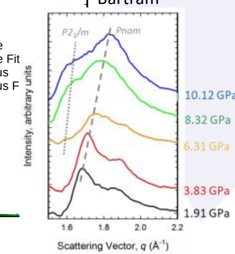


J. Apply. Phys. **128**, 165107 (2020).

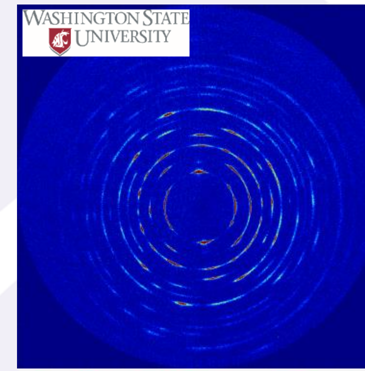
Gas gun driven polymer chain compression and decomposition studied with XRD



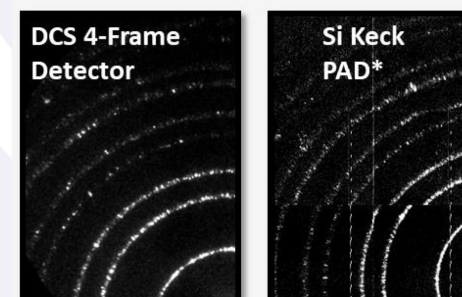
R. Huber, E. Watkins, J. Jordan, R. Gustavsen, D. Dattelbaum, L. Gibson, B. Bartram



Single-bunch image using the Rayonix detector from 25µm thick Ta

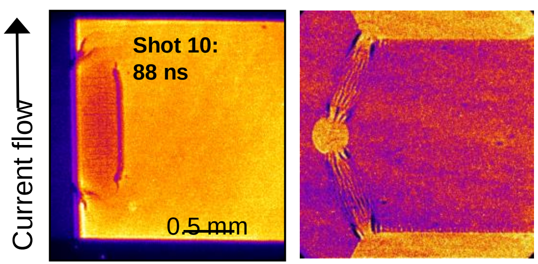


Single Bunch XRD Patterns (Si Target)



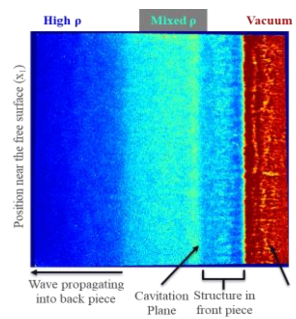
* Prototype detector with some damage (vertical lines)

Example X-ray Imaging data for EFIs that show early stages of the initiator

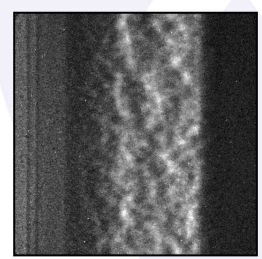


J. Appl. Phys. 119, 235901 (2016)
AIP Conference Proceedings **1979**, 160023 (2018)

Cavitation in Mg



Spall in Mg



M. Beason, S. Fensin, B.J. Jensen, D. Jones

Many more examples could be highlighted…

Today we can only *partially* fill the mission needs…

- **Progress on energetics, low Z materials**
  - Need higher energy photons for e.g., U and Pu, and thicker samples

- **Progress with single shot imaging**
  - Need enhanced time structure with coherence and brilliance for dynamics

- **Need closer coupling between production & measurement**
  - Co-location with an ultimate goal of real-time feedback

- **Opportunity to study hazardous materials and classified experiments would enhance impact**

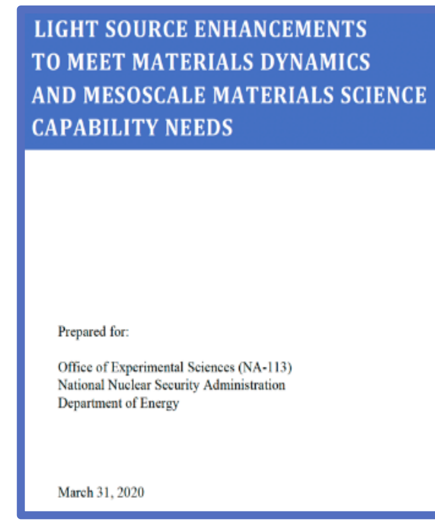
In response to NA-113 tasking, the Tri-lab with DOE SC partners presented three concepts to meet portions of the DMMSC mission need.

Collectively, the top two items are known as the U.S. Light Source investments, now "**M^3**", and NNSA has just initiated its formal study.

"DMSS"

"DMPL"

Concept	Brief description	Partnerships
Defense Materials Science Sector at the Advanced Photon Source	Long beamline extension and new building with materials qualification hutch, HE vessel and Thor-200 pulse power	Argonne National Laboratory, DOE Office of Basic Energy Sciences
Partnership in the new Matter in Extreme Conditions Endstation	Contribution of a 5 kJ Long-pulse laser	SLAC, DOE Offices of Basic Energy Sciences and Fusion Energy Sciences
Partnership in HEX and MRE beamlines at NSLS-II	Dedicated experimental platforms for rad/SNM and partner beamtime	Brookhaven National Laboratory, DOE Office of Basic Energy Sciences and DOE Office of Nuclear Energy


LIGHT SOURCE ENHANCEMENTS TO MEET MATERIALS DYNAMICS AND MESOSCALE MATERIALS SCIENCE CAPABILITY NEEDS

Prepared for:

Office of Experimental Sciences (NA-113)
National Nuclear Security Administration
Department of Energy

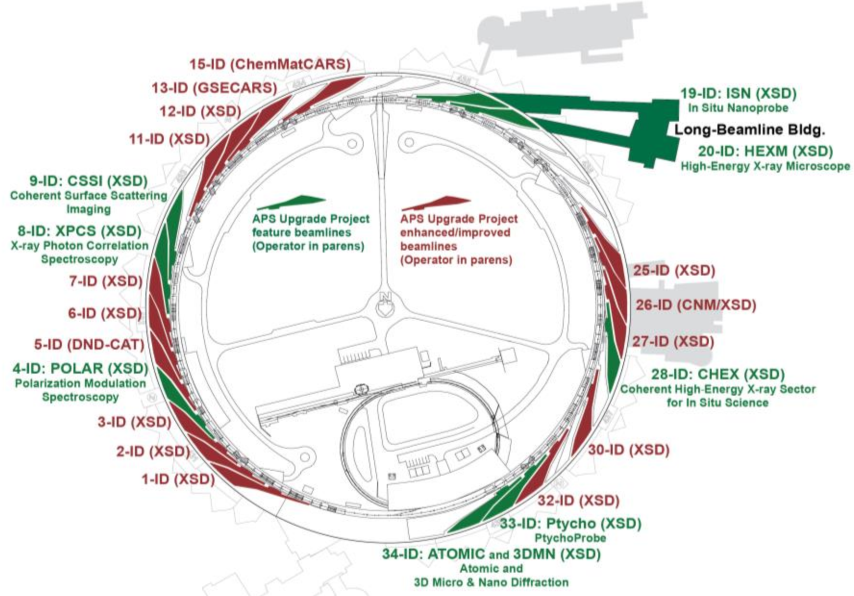
March 31, 2020

Subsequent requirements workshops were held Oct. 2021 (MEC-U partnership, long-pulse laser) and Feb. 2022 (DMSS options)

The APS-Upgrade will provide significant beam improvements that will advance our ability to study dynamic and transient phenomena of interest to NNSA.

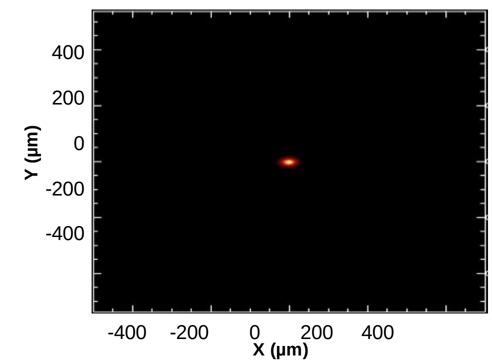
815M$ project to update and renew the facility

Re-uses 1.5B$ in existing infrastructure

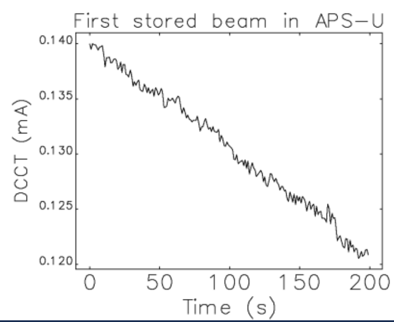


- New storage ring, **42-pm** emittance @ 6 GeV, 200 mA
- New and updated insertion devices, including superconducting undulators (SCUs)
- Combined result in **brightness increases of up to 500x**
- **9 new feature beamlines + Long Beamline Building**
- 15 enhanced and improved beamlines
- Exploit high-performance computing, AI

APS Upgrade



Today (April 20, 2024) the upgraded Advanced Photon Source (APS) took another important step forward, as the Accelerator Systems Division (ASD) team reported the first stored beam in the new storage ring.



A long beamline sector at the APS – the DMSS – would provide new capabilities for mesoscale materials science at a U.S. synchrotron.

A new sector is proposed that may contain:

- Long beamline extension with external building
- A Materials Science & Qualification Hutch
- An explosive vessel firing capability
- A pulsed power driver for complex loading
- Other dynamic drivers

Differentiating features of the beam line:

- Flexible sample environments coupled to an optimized high energy beamline
- A complementary suite of dynamic drivers to DCS
- Larger field-of-view for imaging
- Routine classified and hazardous operations
- Radioactive and Hazardous materials

APS is the brightest U.S. light source at high energies

APS has current experience building the HEXM and ISN sectors at the LBB as part of APS-U.

NNSA provides data to improve material models and weapons codes, and the underlying scientific understanding for improved predictive capabilities.

- NNSA has an unmet scientific need for predicting how changes in material microstructure impacts performance in weapons environments.
- The mission need is to “see” inside materials with sufficient resolution to quantitatively model and constrain the underlying physics phenomena controlling dynamic performance.
- A revolution in high brilliance x-ray sources and techniques is driving a corresponding transformation in dynamic materials science within NNSA.
- An intermediate-scale investment at existing light source(s) would provide data supporting NNSA missions in manufacturing science, aging assessments, materials qualification, and more rapid materials development.

Insights gained from high brilliance X-rays under conditions relevant to NNSA missions would be transformative for stockpile assessment and certification.

Back-up material

NNSA and the Tri-lab responded to a SEWD Charge (2021 NDAA) in June 2021.

"The Committee strongly encourages the NNSA to develop additional partnerships with the Office of Science to utilize the Advanced Photon Source [APS] and Linac Coherent Light Source [LCLS] x-ray light sources. The NNSA is directed to brief the Committee within 90 days of enactment of this act on its <u>plans to work with the Office of Science to incorporate additional capabilities in the planned upgrades at LCLS and APS</u> that will address NNSA <u>mission needs to interrogate the behavior of materials</u> at length and timescales necessary to study materials aging and modern manufacturing methods."

- The Tri-lab and NNSA, with DOE Office of Science responded with a briefing to SEWD and HEWD staffers.
- CD-0 package for MEC Laser was initiated Fall 2021.
- DMSS – tri-lab partnership with Argonne National Laboratory – focused workshop was held Winter 2022
- DMSS and now, M^3, studies initiated in 2023-2024.

The Office of Science is investing in APS and LCLS, dramatically improving the fundamental photon characteristics at each facility.

- LCLS is increasing brightness by 1000x in an ongoing $1B upgrade
- Fusion Energy Sciences is in CD-1 to build a new MEC end station
- Working with NNSA on possible partnership on long pulse laser

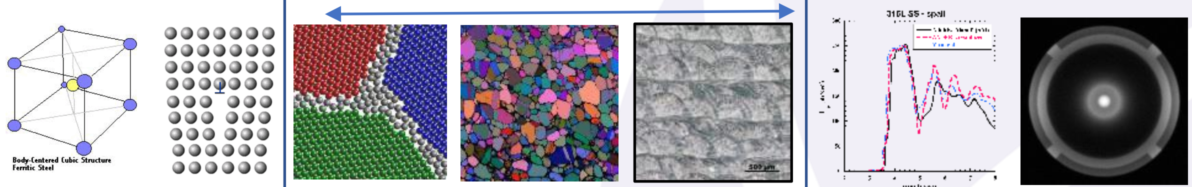
- APS-U is an $800M upgrade occurring in 2023 that will increase brightness by 50x
- Most important to NNSA dynamic experiments, the photons in a single pulse at 40 keV will increase by a factor of 4x

While NNSA is performing important work at existing facilities, it was recognized that there are still gaps, and NNSA could better partner with SC at U.S. light sources.

We must continue to certify the performance of materials in the absence of nuclear testing. Many of the scientific problems are defined by materials science at the mesoscale.

The U.S. nuclear stockpile is changing due to aging, new manufacturing practices, and stockpile modernization with new materials.

Mesoscale

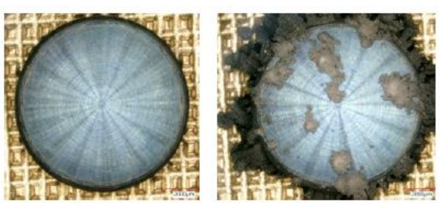


10^{-10} 10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1}

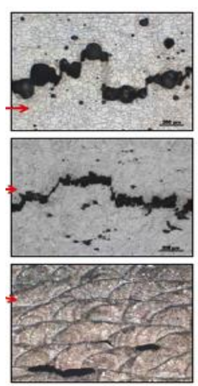
Nanometer: DCS, NIF, CINT, and Z

Identified mission need to understand how mesoscale features control performance in weapon materials

Millimeter+: Integrated hydrodynamics (U1a, DARHT, firing sites)



Surface corrosion



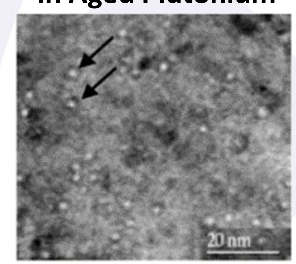
Wrought

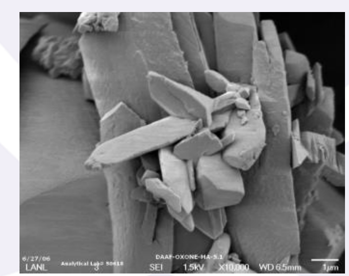
AM Annealed

AM

Damage in newly manufactured steel

Helium Bubbles in Aged Plutonium



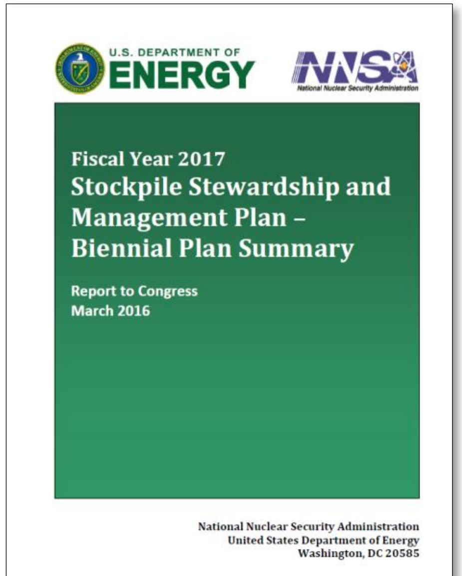


High explosives Structure-performance

NNSA's need to predict and control the microstructure of materials is also a science frontier…

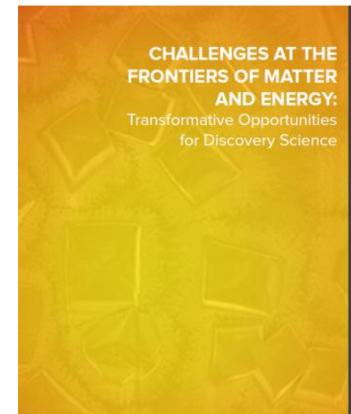
~2017

"In particular, we believe that filling the gap in our ability to **'predict and control from materials and devices to manufacturing processes'** is especially urgent."



From Quanta to the Continuum: Opportunities for Mesoscale Science

Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science

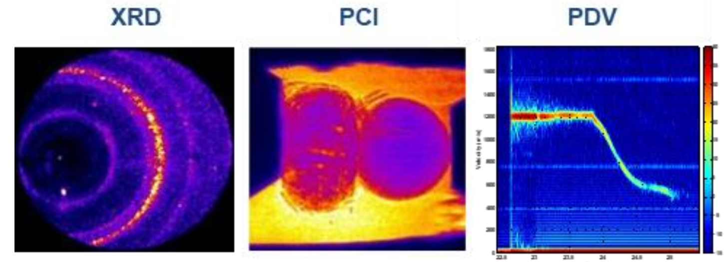


science.energy.gov/bes/news-and-resources/reports/basic-research-needs/

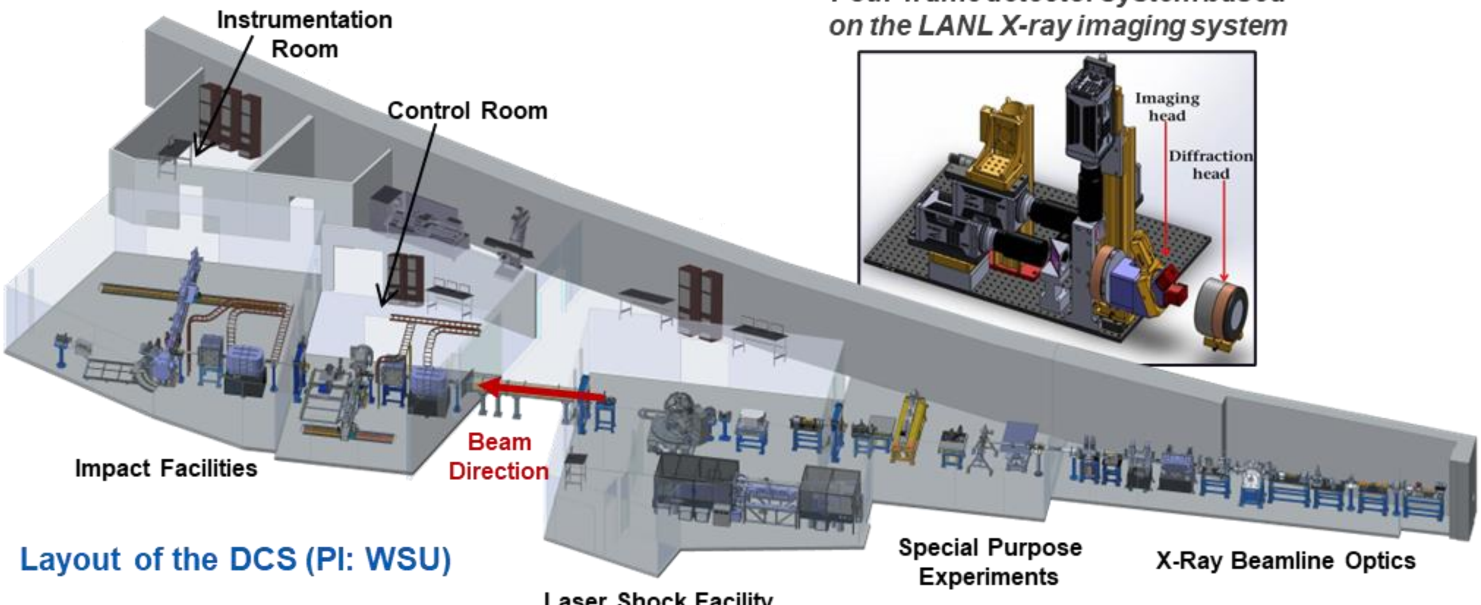
…that motivates new capabilities and will demand co-design for success

NNSA has been growing its efforts at U.S. and international light sources over the last decade to address NNSA missions

DCS is designed to optimally link dynamic compression platforms to a dedicated synchrotron beam line. Focus on time-resolved, in-situ diffraction, imaging, and continuum measurements – response across length and time scales!



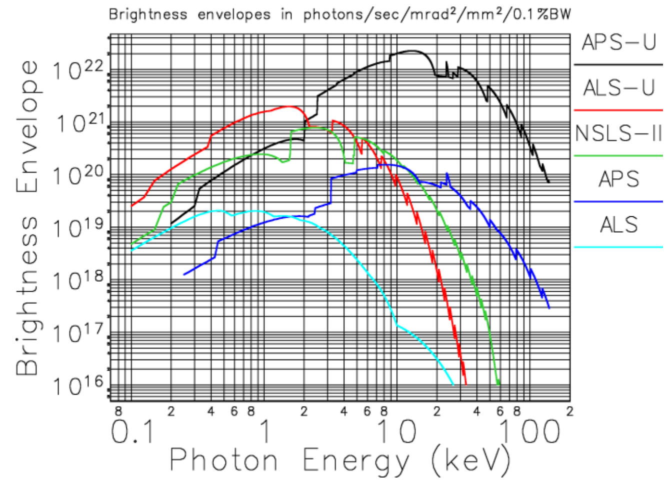
Four-frame detector system based on the LANL X-ray imaging system



Layout of the DCS (PI: WSU)

Why APS for DMSS?

- **The APS is the brightest DOE light source for energies above 20 keV; APS-U will increase the brightness over 500x in this energy range.**
- **Its energy, brilliance, micro-focused beams and bunch timing structure make it unique and ideal for dynamic experiments of interest to NNSA.**
- **The upgrade includes a new, low emittance storage ring at 6 GeV (200 mA), new and updated insertion devices and superconducting undulators (SCUs), and 9 new feature beamlines.**
- **The future bunch structures planned to follow the APS upgrade include a 48-bunch mode with 80 ps FWHM (76.7 ns spacing) and 324-bunch mode with 80 ps FWHM (11.4 ns spacing). Notably, the number of electrons per bunch in 324-bunch mode will double with the upgrade.**
- **APS and NNSA have also recently partnered to establish classified operations and data handling, and its site plan allows for SNM and high explosives.**



APS Upgrade