# Overview of DMMSC Workshops

## State of Technology Awareness Initiative – STAI


**Rich Sheffield**

February 1, 2021

## Dynamic Mesoscale Materials Science Capability - DMMSC

LA-UR-21-20910

Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

# STAI Goal: Enhance staff awareness of worldwide activities in mesoscale materials science and related technologies

**We organize workshops to benefit present and future LANL programs by:**

- **Increasing external awareness of LANL staff and capabilities**
- **Improving existing programs and enabling new efforts by capitalizing on technology advancement occurring at vendors and institutions worldwide and setting the foundation for collaborations**
- **Reducing duplication and allowing more efficient use of limited resources for existing programs**
- **Reducing the time to respond to urgent requests from sponsors**
- **Building an extended research community that supports the DOE missions**
- **Preparing for the eventual implementation of a new mesoscale tool that can address the needs of the weapons program**

**Choice of workshop topics guided by present and future laboratory programmatic challenges**

# Advanced Probes and Data Analytics for Enabling 3-D Imaging Under Dynamic Conditions Workshop

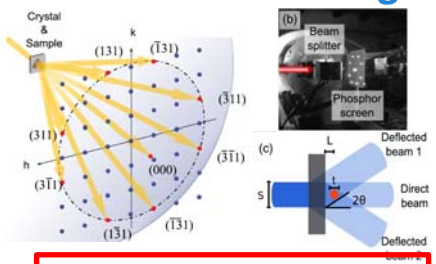
## Community Participation

- August 27-29, 2019 (Santa Fe, NM)
- Focus Sessions: Experimental Techniques, Data Analytics, Detectors and Beams
- 57 Registrants, 28 Invited talks, 6 Lightning talks
- Institutions: LANL, ANL, BNL, BYU, CMU, Cornell U, DESY, ESRF, ISU, JHU, LBNL, LLNL, NYU SoM, Northwestern U, Purdue U, SLAC, Tufts U, U Oxford, US ARL

## Challenges Addressed

- High resolution 3D imaging techniques are too slow to capture dynamics (>100s of images)
- Single pulse imaging experiments are often source limited (ie. photon-starved, or need higher energy to probe high-Z or relevant scale samples)
- Fast, high-resolution detectors don't exist
- Dynamic imaging creates huge volumes of data, and no on-the-fly data analysis tools exist

## Highlights

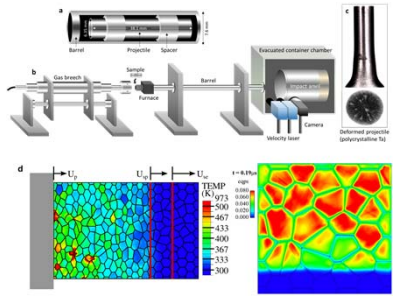



*X-Ray Multi-Projection Imaging*

Novel technique for single-pulse imaging: a crystal beamsplitter upstream of the sample creates multiple simultaneous beams.

*Villanueva-Perez et al., Optica (2018)*

*In-Situ Dynamic Loading Measurements Help Validate Mesoscale Simulations*



*Rusty Gray, DJ Luscher*

## Recommendations

- Develop multiple-beam facilities and techniques with sufficient peak intensity for single-pulse 3D imaging of dynamic events from ps - μs (at high energy for actinides)
- Implement a sustained, targeted effort for development of fast imaging detectors - with community-defined KPPs
- Support development of data analysis algorithms tailored to materials challenges - and uncertainty quantification studies
- Support collaboration to develop cross-facility easy-to-use software with data provenance

# Advanced Control Methods for Particle Accelerators

*Improving productivity and increasing availability of large-scale accelerator facilities*

## Community Participation

- August 19-21, 2019 (Santa Fe, NM)
- 26 Registrants, 21 Invited talks
- Institutions: LANL, LBNL, SLAC, CERN, ANL, RadiaSoft, UCSB, Euclid Techlabs, Google, Jlab

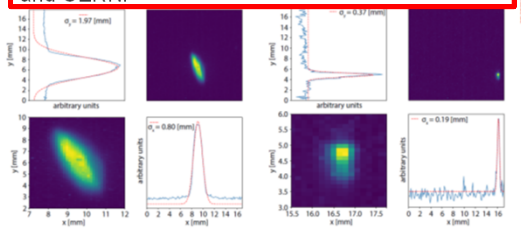
## Challenges Addressed

- Ability to quickly, minutes instead of hours, create very high quality, extremely intense beams with custom current and energy profiles
  - Algorithm development
  - Diagnostics
  - Verifying techniques
- Developing a platform for a common family of algorithms that can be shared and maintained by the community.

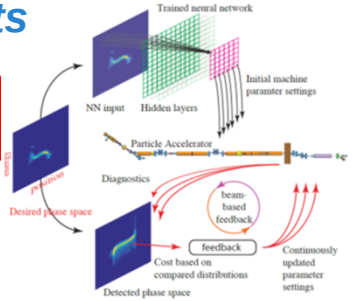
## Highlights

*Automatic optimization and tuning studies*

A direct result of this workshop was the establishment of a collaboration between LANL and CERN.



*Scheinker, A. et. al,.Physical Review Accelerators and Beams 22.8 (2019): 082802.*




*Adaptive machine learning*

Adaptive ML approach demonstration by LANL and LCLS collaboration

*A. Scheinker, PRL, 121.4, 044801, 2018.*

## Recommendations

- Need non-invasive diagnostics that can provide real time information about extremely short and intense charged particle bunches
- Study optimizer problems with unexpected and not analytically predicted configurations.
- Use neural networks to learn the mapping between various accelerator components and beam parameters such as emittance or energy spread.
- Study distribution shift systems - systems with components, e.g. magnets, that can change in time
- More collaborations among institutions

# Adaptive Sample Preparation and Target Fabrication for High-Throughput Materials Science Workshop

## Community Participation

- May 14-16, 2019 (College Station, TX)
- Jointly hosted with Texas A&M University
- 42 Registrants, 23 Invited talks
- Institutions: LANL, LLNL, NIST, SLAC, TAMU, General Atomics, UCLA, OSU, UPENN/ Hummingbird Scientific, HZDR, George Washington U
- Report available: LA-UR-19-26624

## Challenges Addressed

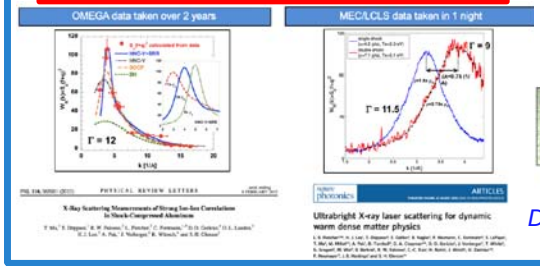
*Emergent issue for modern light sources: sample and/or target fabrication on a scale to best leverage advances in accelerators and imaging*

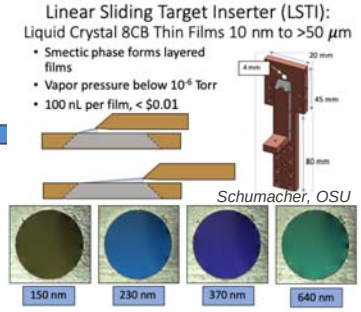
- Statistics: rapid production of single-shot samples/targets for high-throughput experiments (HEDS, dynamic materials science in extremes)
- Optimizing experiment run-time: guided optimization of sample fabrication (PSPP)

## Highlights

*High-throughput Compressed Al Ion-ion Structure Factor Measurement*

Al EOS experiments that took 3 years at OMEGA were reproduced in 5 days at LCLS




*Dynamic In-Situ Target Fabrication for Laser-based Ion Acceleration*

## Recommendations

- Engage sponsors for a long-term program to combine Materials Genome initiatives, AI/big data and science-driven advanced manufacturing to create “Materials Acceleration Platforms”
- Invest in LANL-driven collaborative university efforts in ML/AI on target fabrication for capability development
- Encourage preferential selection at user facilities for proposals using a specific target delivery protocol
- Engage LaserNETUS for organization of availability solutions for target supply

# Mesoscale Science at Extreme Conditions Workshop

*Understanding dynamic material response during fabrication and performance*

## Community Participation

- August 5-8, 2019: Classified session at LANL 8/5; open sessions in Santa Fe 8/6-8/8
- Focus Sessions: Metals, High Explosives, Manufacturing
- 85 Registrants, 35 Invited talks, 16 posters
- Institutions: LANL, SNL, Colorado School of Mines, MIT, NMSU, LSU, Purdue U, TAMU, OSU, ISU, U Iowa, UAB, UCSB, U Illinois, U Michigan, U Nebraska, U Missouri, U Tennessee, UNT
- Report available: LA-UR-19-30259

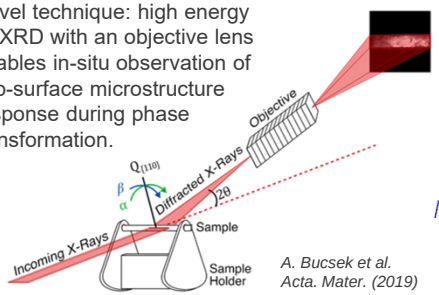
## Challenges Addressed

- Mesoscale properties drive material dynamic response – dynamic data is needed for next generation models and simulations for:
  - Phase transformation
  - Grain/defect morphology and orientation
  - Void/crack nucleation and dynamics
- Models need to bridge the gap between microstructure and continuum

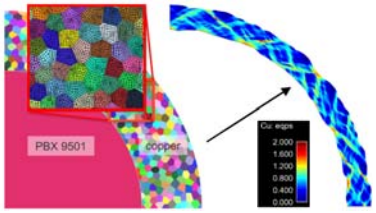
## Highlights

*Dark-field X-ray Microscopy*

Novel technique: high energy 3DXRD with an objective lens enables in-situ observation of sub-surface microstructure response during phase transformation.




*A. Bucsek et al. Acta. Mater. (2019)*




*Mesoscale Modeling of Fragmentation*

Simulation of explosive expansion using FLAG (hydrocode) with explicit grain structure; plastic strain concentrates into shear bands, leading to fragmentation.

## Recommendations

- Focus LANL funding and efforts on higher resolution techniques and facilities (DMMSC)
- Outsource to universities complementary experimental activities that can be done rapidly or with ‘table-top’ systems
- Fund collaborations with broader community, including LANL scientific workforce development

# FY 2020 Workshops were focused on improving facilities, imaging, materials performance and production

| Seminar Date | WORKSHOP TITLE | WHEN | WHERE | CONTACT |
|---|---|---|---|---|
| **February 1** | Data Science and Computation for Rapid and Dynamic Compression Experiment Workflows at User Light Sources | September 8-11, 2020 | Virtual | Christine Sweeney |
| **March 1** | Methods for Characterizing Defects in Advanced Manufacturing Processes | October 14-15, 2019 | Cornell University | John Carpenter |
| | In-situ sensing and process monitoring for NNSA relevant materials and processes. | August 25-26, 2020 | Virtual | Don Brown |
| **April 5** | Emerging Materials and Process Development for Polymer/non-metal Additive Manufacturing | August 25-26, 2020 | Virtual | John Carpenter |
| | Carbon in Extreme Conditions | October 28-30, 2019 | Santa Fe | Dana Dattelbaum |

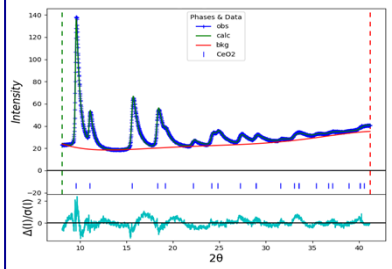
# Data Science and Computation for Rapid and Dynamic Compression Workflows at Experimental Facilities Workshop

## Community Participation

- September 8-11, 2020. 3-1/2 day Virtual Venue
- Focus Sessions: Analytics and Tools, Imaging, Machine Learning, Visualization, Workflows, Computing Facilities
- 95 registrants, 31 invited talks, 4 lightning talks
- Institutions: LANL, SNL, LLNL, LBL, ANL/APS, BNL, ORNL, PNNL, SLAC, EuXFEL, DESY, CMU, WSU, UC Davis, Santa Cruz, Minnesota, BYU, Oxford, Georgia Tech, Princeton, Michigan, Illinois, Stanford, Stony Brook, Edinburgh, Utah
- Report: LA-UR-20-27469

## Challenges Identified

- Increasing experiment data volumes and velocities
- Diverse software available but not integrated/interoperable
- Data noise, phase wraps, resolution, sparseness, artifacts
- Difficulty obtaining training and simulation data necessary for doing data science
- Lack of forward models and model shortcomings
- Lack of metadata generation and management mechanisms
- Lack of tools to drive remote experiments

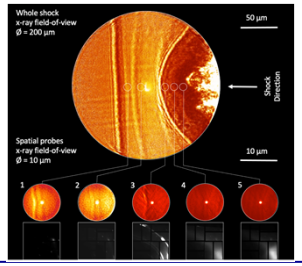



*R. B. Von Dreele.*

A profile function for pink beam diffraction used in single peak fits and in a Rietveld refinement for $CeO_2$ . Added to GSAS-II tool.

## Highlights

Research on high resolution imaging and density measurement of shock waves, defects and phase transformations.




*S. B. Brown, et al. Science Advances, vol. 5, no. 3, 2019.*

## Recommendations

- Algorithm development for analytics
- More universally applicable/accessible software tools
- Integration of multiple streams of data
- Need for metadata to access data and for tool development
- User engagement by computing facilities
- Data processing and reduction for increased data volumes
- Forward model development and combination with analytics
- Interfacility or facility-to-remote-laptop workflows

LA-UR-20-29214

*Chair: Christine Sweeney (LANL) Steering Committee: Blake Sturtevant (LANL), Christopher Biwer (LANL), Cynthia Bolme (LANL), Rachel Huber (LANL), Larissa Huston (LANL), Emma McBride (SLAC), Lowell Miyagi (U. Utah), Clemens Prescher (DESY), Kyle Ramos (LANL), Jesse Smith (ANL/APS)*

# Methods for Characterizing Defects in Advanced Manufacturing Processes

*Understanding industrial manufacturing needs*

## Community Participation

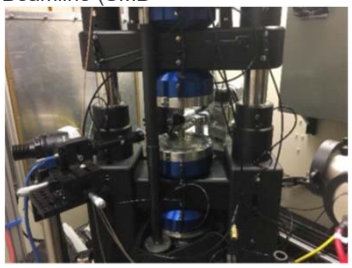
- October 14-15, 2019; Cornell University
- Focus Sessions: Metals, High Explosives, Manufacturing
- 26 Registrants, 14 Invited talks
- Institutions: LANL, CHESS, NIST, NRL, Carnegie Mellon, Diamond Light Source, GE, Renishaw, Case Western Reserve, APS, SLAC, Arcelor Mittal Colorado School of Mines, AFRL, U. of Wisconsin, VJ Technologies
- Report available: ??

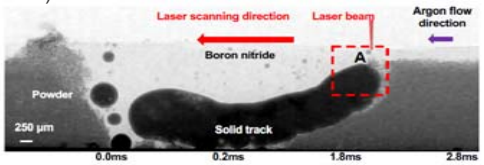
## Challenges Addressed

- Rapid qualification / certification of AM
- Identifying sub-surface defects
- Studying realistic microstructures
- Understand defect formation in metal AM
- Understand failure mechanisms in hydrogen rich and corrosive environments

## *Processing and performance of structural materials* Highlights

CHESS recently opened two new beamlines: the Forming and Shaping Technology (FAST) beamline and the Structural Materials Beamline (SMB






*Synchrotrons have penetration and give high resolution*

Radiograph showing solidified metal material after a laser pass. Variations in density due to porosity are clearly observed as the grayer portions of the solid track (Diamond Light Source)

## Recommendations

- Improving alloy modeling
- Using in-situ information to guide manufacturing
- Use machine learning to optimize AM processing
- Measuring elastic modulus wrt alloy development
- Characterize the temperature of material within a melt pool for validation of process models
- Develop methods to characterize spatial arrangement microstructural features

# In-situ Sensing And Process Monitoring For NNSA Relevant Materials And Processes

## Community Participation

- Aug. 25-26, 2020. Virtual format enabled participation from labs, industry, and academia across US.
- >100 registered, on average 45 attended each talk
- Organized by LANL (Lead: Clausen. Support: Brown, Carpenter, Crone)
- Participants from LANL, LLNL, PNNL, KCNSC, Pantex, Co. School of Mines, AFRL, NIST, Y-12, Westinghouse
- Report in preparation; will be publicly available.

## Challenges Identified

- Reduce time from discovery to implementation (Materials and Process).
- Communication between e.g. Core Mission (mission pull) and Science Base (tech. push), production and science, theorists/modelers and experimentalists.
- LANL (NNSA) specific problem, small industrial scale.
- How do we relate knobs to performance? i.e. what can we control/measure in the factory, what controls microstructure, and how does that influence properties?

## Highlights

- Several traditional (Thermocouple, pyrometry, off-gas analysis) and novel (LIBS, RUS, imaging, scattering) in-situ probes identified.
- Need to focus on what can be measure/controlled on the factory floor.
- Laser Induced Breakdown Spectroscopy (LIBS) is a promising method that can be brought to the factory floor and monitor in-situ for both qualification and compliance purposes.
- In-situ scattering probes coupled with traditional instrumentation (e.g. thermocouples, RUS) can reveal the microstructure underpinnings of macroscopic events, providing the linkage between the process (knobs) and properties.

## Recommendations

- Implementation of a “LANL week” each year to facilitate communication between Core Mission and Science, Production and Science.
- Internal (e.g. MST-8/Q) and/or External (e.g. LANL/KCNSC) sabbaticals to enhance communications.
- Future workshops focused on specific manufacturing challenges and advanced in-situ probes.
- Develop NNSA specific beamlines enabling research on materials/processes that do not fit BES mandates e.g. hazardous, sensitive, specific to mission, not publishable.

# Emerging Materials and Process Development for Polymer/non-metal Additive Manufacturing

## Community Participation

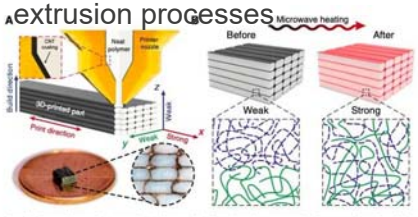
- Aug. 25-26, 2020. Virtual format enabled participation from labs, industry, and academia across US and Europe; >100 simultaneous attendees
- Co-organizers: NIST, AWE, UTEP, Phillips, LLNL
- Speakers from ARL, NIST, SNL, KCNSC, ORNL, LLNL, LANL, 3M, NIAR, UTEP, UMass-Lowell, UMich-Ann Arbor, Lincoln, Nottingham, UT-Austin, RIT, ASU, VaTech, TAMU
- Report in preparation; will be publicly available
- Recordings under review; will be publicly available

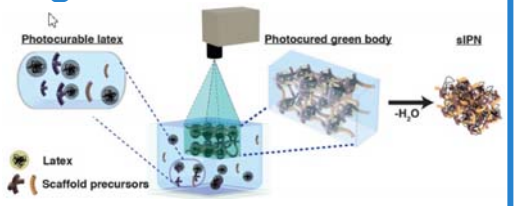
## Challenges Addressed

- **Feedstock development:** what pressing material gaps to fill in near- and long-term?
- **Process monitoring, characterization, and modeling:** what approaches enable accelerated process improvement and rapid qualification?
- **Qualification and standards:** how will standards adapt to evolving technologies? What tools are useful for material screening and analyzing PSPP relationships?

## Highlights

Reducing directional effects in ADF materials using a carbon nanotubes activated using localized microwave heating after using traditional additive manufacturing extrusion processes




Overcoming the traditional tradeoff of printability/viscosity with increasing molecular weight by encapsulating the polymer in an aqueous scaffold

## Recommendations

- **Workshop** linking data science and production qualification with AM technology for polymers in NNSA. Focus on class B components and methods for rapid qualification including common qualification frameworks that enable increased responsiveness at PAs. Include LLNL, SNL, LANL, KCNSC
- **Follow-up workshop lead by LANL/KCNSC** focused on multifunctional feedstock and component needs for global security applications. Needs to incorporate university partnerships, industrial collaborators, and classified discussions.


Topical areas covered:

- Carbon coagulation kinetics, including both modeling and in situ measurements
- Equation of state: HE and shock-driven chemistry
- Equation of state: ICF applications
- Integrated modeling of ICF experiments

# FY2021 Proposed Workshops focus on improving facilities, imaging, materials performance and production

| WORKSHOP TITLE | WHEN | WHERE | CONTACT |
|---|---|---|---|
| Ultrafast imaging and tracking instrumentation, methods and applications 2021 | Sept. 2021 | SLAC | Jeph Wang |
| 16th SCINT conference | Sept. 20-24, 2021 | Santa Fe | Jeph Wang |
| Novel accelerator-based technologies for addressing materials dynamics at the mesoscale | ~Aug 26-27, 2021 | virtual | Nathan Moody |
| Data Science Methods for Materials Advances | March, 2021 | virtual | Joanne Wendelberger |
| 3D microstructural information from limited or single 2 D measurements (attached to 5th International Congress on 3D Materials Science) | June 29-July 2, 2021 | DC | Reeju Pokharel |
| Manufacturing and qualification for HE | ~ August, 2021 | DC area | Kyle Ramos |
| High Energy X-Ray Diffraction and Imaging Applied to Manufacturing and Aging | March, 2021 | virtual | Don Brown |
| AM Polymers for mission critical systems | TBD | TBD | John Carpenter |
| Design for Manufacture, Pu Aging and Chemistry | 3rd qtr | LANL | Dana Dattelbaum, Anthony Fredenburg |

Updated: 1/13/20

# STAI workshops focus on advancing dynamic mesoscale material science and so addresses LANL mission gaps

- **Supports LANL staff awareness of latest techniques for understanding production processes and performance of weapon relevant materials**
- **Promotes internal and external awareness of LANL interest in mesoscale science, light source utilization, and XFELs, with a side benefit of advertising for future recruitment**
- **Builds a research community that supports national security missions**
- **Provides platform to initiate collaborations, for example:**
  - EXFEL: materials science experiments and controls
  - Detectors: hard-energy x-rays and GHz rates
  - LCLS: materials science experiments and XFEL performance

# State of Technology Awareness Initiative (STAI) supports DMMSC through workshops

- **STAI provides planning assistance, funds, and logistical support for DMMSC-related workshops**
- **A link for past workshop reports can be found on the DMMSC homepage**
- **If you know of a relevant DMMSC/mission critical technical gap to base a workshop, contact sheff@lanl.gov**