Technology risk mitigation research and development for the matter-radiation interactions in extremes (MaRIE) project

Cite as: AIP Conference Proceedings **1979**, 160003 (2018); https://doi.org/10.1063/1.5045002
Published Online: 03 July 2018

Cris W. Barnes, Juan C. Fernández, Thomas M. Hartsfield, Richard L. Sandberg, Richard L. Sheffield, John P. Tapia, and Zhehui Wang

Technology Risk Mitigation Research and Development for the Matter-Radiation Interactions in Extremes (MaRIE) Project

Cris W. Barnes[a)], Juan C. Fernández, Thomas M. Hartsfield, Richard L. Sandberg, Richard L. Sheffield, John P. Tapia, Zhehui Wang

Los Alamos National Laboratory, Los Alamos, NM 87545, USA

[a)]Corresponding author: cbarnes@lanl.gov

Abstract. NNSA does not have a capability to understand and test the response of materials and conditions necessary to determine the linkages between microstructure of materials and performance in extreme weapons-relevant environments. Required is an x-ray source, coherent to optimize imaging capability, brilliant and high repetition-rate to address all relevant time scales, and with high enough photon energy to see into and through the amount of material in the middle or mesoscale where microstructure determines materials response. The Department of Energy has determined there is a mission need for a MaRIE Project to deliver this capability. There are risks to the Project to successfully deliver all the technology needed to provide the capability for the mission need and to use those photons to control the time-dependent production and performance of materials. The present technology risk mitigation activities for the MaRIE project are: developing ultrafast high-energy x-ray detectors, combining the data from several imaging probes to obtain multi-dimensional information about the sample, and developing techniques for bulk dynamic measurements of temperature. This talk will describe these efforts and other critical technology elements requiring future investment by the project.

INTRODUCTION

The National Nuclear Security Administration (NNSA) requires the ability to understand and test how material structures, defects and interfaces determine performance in extreme environments. The MaRIE Project will contribute to the science ability for control of materials and their production for vital national security missions. To do this, MaRIE will be an x-ray source that is laser-like and brilliant with very flexible and fast pulses to see on weapons-relevant time scales (sub-nanosecond to millisecond), and with high enough photon energy to study mission critical materials. The capability will also feature advanced diagnostics needed to utilize this revolutionary x-ray source. There are risks to provide these capabilities due to the challenges of implementing the technology for all the system elements. This paper discusses initial projects in doing such technology risk mitigation.

MARIE CRITICAL TECHNOLOGY ELEMENTS

As part of the documentation supporting Department of Energy (DOE) Critical Decision (CD-)0 that there was a Mission Need for MaRIE capability, a plausible pre-conceptual reference design for a facility was developed and costed that would meet the program requirements and mission need. A risk management plan was drafted including identifying technical risks to successfully building all the system elements of the project. This led to identification of about a dozen Critical Technology Elements (CTEs) where the Technology Readiness Level (TRL) was not TRL≥7 needed at CD-2 according to the DOE Order 413.3B[1]. As part of the approved MaRIE Project, enabling research and development on these CTEs to raise their technical readiness and mitigate the technical risks to the Project is required.

Some of the technical risks are associated with the chosen alternative for the source of x-rays, whether a free-electron laser or synchrotron or other source is preferred by the Project. Other CTEs are independent of the x-ray

Shock Compression of Condensed Matter - 2017
AIP Conf. Proc. 1979, 160003-1–160003-5; https://doi.org/10.1063/1.5045002
Published by AIP Publishing. 978-0-7354-1693-2/$30.00

source alternative, and research on these has begun prior to federal decision from an analysis of alternatives. The CTEs for MaRIE are listed in Figure 1; further information can be found in reports generated as part of CD-0[2].

	Risk independent of x-ray source	Impact
High-Energy and Ultrafast Imaging Camera	✔	Required to meet design goal of 30-frame sub-microsecond imaging rates to capture fast dynamic events with an acceptable detector efficiency for single pulse imaging at > 30 keV
Multidimensional Dynamic Imaging	✔	Required to meet design goal of single pulse quasi-3D imaging at > 1 keV otherwise only 1D imaging
Bulk Thermometry of Dynamic Materials	✔	Needed to inform material models requirement for interior temperature measurements of visible-light optically-thick samples
Development of Charged Particle Radiography for the Study of Small and Fast Physical Processes	✔	Needed for probing thick areal density samples, supporting information for quasi-3D imaging
X-ray Optics	✔	Required to meet the fluence design goal for single pulse imaging and to generate images with less than 3 ns separation
Long-Pulse Laser Technology Development	✔	Need long pulse laser bulk heater and shock driver to study material properties on the required time scales;
Start-to-End (S2E) Simulations of XFEL		Required for conceptual design
Long-Range Wakefields		Required to validate accelerator design code to TRL7 by CD-2
Bunch Compression/DeChirping		Required to validate accelerator design code to TRL7 by CD-2
Undulator and Distributed Seeding		Required to meet design goal of photons/bandwidth otherwise x10 less photons/bandwidth
Microbunching Mitigation with Laser Heater		Required to validate accelerator design code to TRL7 by CD-2
Photo-Injector Design Test		Demonstrated emittance to date is 0.2 microns; design goal of 0.15 micron is equivalent to increasing beam energy to 16 GeV ~ $200M ($360M with 1.8x)
High Voltage Converter Modulator Development		Increases reliability and reduces maintenance with an estimated savings of $1.5M/yr in present dollars

FIGURE 1. MaRIE Critical Technology Elements

CURRENT MARIE TECHNOLOGY RISK MITIGATION EFFORTS

Developing Ultrafast High-Energy X-Ray Detectors

While X-ray free-electron laser technology is rapidly developing and the risks to making high-energy brilliant photon pulses in rapid succession are reducing, the technology readiness to detect those photons effectively and efficiently remains low. Challenges[3] include: high-efficiency detection of hard X-rays (>30 keV) in a regime where Compton electron recoil becomes significant; high-dynamic range detection of sub-picosecond X-ray flashes; having many high-resolution pixels to provide quality images; and ability to frame multiple images along a single line-of-sight at GigaHertz rates consistent with acoustic and shock speeds across microstructure at the mesoscale of the materials. Such images can quickly generate massive data sets in repetitive experiments, both requiring consideration of application of big data techniques and opportunities for smarter data through compressed sensing.

Performance	Type I imager	Type II imager
X-ray energy	Up to 30 keV	42-126 keV
Frame-rate/inter-frame time	0.5 GHz/2 ns	3 GHz / 300 ps
Number of frames per burst	>= 10	10 - 30
X-ray detection efficiency	above 50%	above 80%
Pixel size/pitch	≤ 300 μm	< 300 μm
Dynamic range	10^3 X-ray photons/pixel/frame	≥ 10^4 X-ray photons/pixel/frame
Pixel format	64 x 64[1] (scalable to 1 Mpix)	1 Mpix

FIGURE 2. Simplified requirements on high-energy x-ray photon imagers for a MaRIE-like high-energy XFEL.

To meet the presently understood scientific requirements of the MaRIE project, technical requirements on the ultrafast imagers have been defined (see Figure 2).[4] The Project needs to demonstrate a Technical Readiness

Level (TRL) 4 system by CD-1 and a TRL-7 by CD-2. A **“Type I”** system meets the Project threshold requirements (30 keV photons, 2 nanosecond framing rate) and is an *evolution* from current capability. A **“Type II”** system meets objective requirements (currently 42–126 keV photons, 300 picosecond framing ration) and may take a *revolution* in detector technology. Past experience with other major light-source projects has shown success when a broad and sustained effort over a decade or more is devoted. The MaRIE Project is considering several techniques:

- Advanced silicon technology, both 3-dimensional (with multiple electrode surfaces throughout thick silicon) and high-bias;
- Multilayer/stacked thin detectors where each are highly inefficient but add up to fast efficient system;
- Higher-Z (than silicon) sensor materials then bonded to fast application-specific integrated circuits (ASICs), including truly revolutionary quantum metamaterials with nanostructured functionality;
- And indirect methods with fast X-ray scintillator materials then bonded to fast optical silicon ASICs.

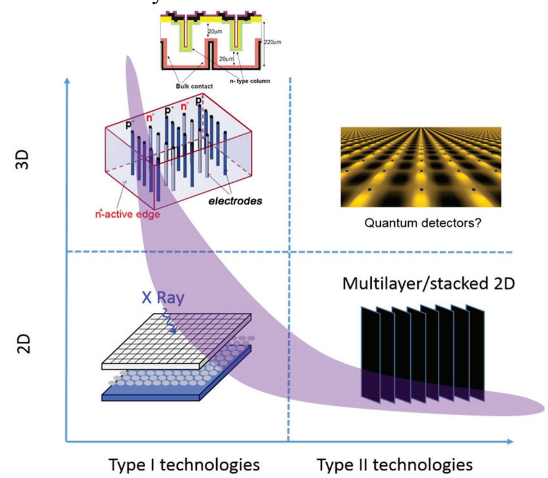

FIGURE 3. Development paths towards ultrafast high-energy X-ray imaging cameras are determined to a large extent by detector-grade sensor materials. A number of existing semiconductor and scintillator materials will allow us to explore type I technologies on the MaRIE CD schedule. Type II technologies are less certain for the time being. And some technologies are compatible with available CMOS processes (the purple shaded region).

Multidimensional Imaging

MaRIE scientific requirements desire experimental techniques that can achieve full 3D object imaging at approximately 100 nm resolution of dynamically loaded samples from limited line-of-sight diagnostics. Many proposed experiments will rely upon the *a priori* knowledge of the sample structure, grain orientation, defect distribution, or chemical speciation coupled with knowledge of how dynamic environments are being applied in order to extract the most information possible from dynamic experiments. Such prior characterization can be achieved using High-Energy Diffractive Microscopy (HEDM),[5] which can provide 3D micron-scale imaging of polycrystalline materials though it requires hours of data collection. As MaRIE will have a high degree of transverse and longitudinal coherence, HEDM might be combined with Bragg coherent diffraction imaging to increase the resolution of these 3D maps below 100 nm.[6] MaRIE capability would provide simultaneous multiple probe capability for time-dependent events. In addition to dynamic information from the coherent x-ray light source, the accelerated electrons that make the x-rays can also be used for electron radiography,[7] or in some alternative designs proton radiography may be available.

Efforts are underway to develop and robustly demonstrate 3D ‘mesoscale’ imaging of dynamically loaded material. Because at present simultaneous multiple-probe facilities are not available, samples need to be studied serially at different facilities in different experiments. Experiments at MaRIE will have ‘non-reproducible’ samples so that serial techniques will not be as applicable. At the dynamic time scales of the mesoscale, using rotational tomography takes too much time to be feasible. Maximizing the information available from the scattered coherent light is key. To make this all work, there needs to be a tight synergy between theory and modeling, experimental verification, and rapid data analysis and visualization. Theoretical and numerical efforts are currently underway to leverage and improve existing X-ray phase contrast, coherent diffraction imaging, and Bragg diffraction methodologies to maximize the achieved multi-dimensional imaging of dynamically loaded samples.[8]

Dynamic Measurements of Temperature

The goals of the MaRIE Project demand temperature measurements that are both dynamic and spatially resolved throughout the bulk of a mesoscale volume. No such technique currently exists! We are presently seeking research and development into a wide variety of dynamic techniques; this work will inform what can and what should be implemented in the MaRIE capability in pursuit of our thermometry goals.

Our first step is to implement and cross-calibrate several different existing temperature measurement systems that possess some of the qualities we desire. Understanding the peak capabilities of our current methods will not only guide their implementation at MaRIE but also guide our design and benchmarking of their successors. Last fall we held a community workshop[9] to identify promising thermometry techniques and flesh out what is the current state-of-the-art in accuracy and speed across different dynamic scales.

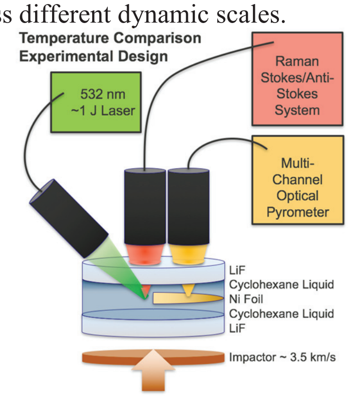

FIGURE 4. Overview of experimental design of temperature cross-calibration experiments.

One of the workshop recommendations was that the best current method of dynamic temperature measurements—multi-wavelength optical pyrometry—still requires verification of absolute accuracy in dynamic conditions. Raman Stokes/anti-Stokes spectroscopy methods provide just such an absolutely accurate measurement in bulk, but are limited to very specific experimental materials and conditions. We've commissioned a broad collaboration of experts in both pyrometry and Raman spectroscopy to carry out a study using both techniques to produce an identical—and, if possible, simultaneous—dynamic temperature measurement. The study will shock a cyclohexane liquid, upon the bulk of which a Raman temperature measurement will be performed. A thin nickel foil suspended in the liquid will quickly equilibrate to the liquid temperature and provide a radiant surface for the pyrometric measurement. These results provide independent validation of the accuracy of the optical pyrometry techniques that will likely be the benchmark for and possibly the progenitor of future MaRIE thermometry.

Another technique that can measure bulk rather than just surface temperature is neutron resonance spectroscopy (NRS), as first demonstrated for shock-loaded materials at the LANSCE accelerator neutron source.[10] NRS uses the traversal of a polychromatic neutron beam through the bulk of the material of interest and its subsequent energy-resolved detection. The neutrons with kinetic energy corresponding to a nuclear resonance in the material (typically several to ten's of eV in a heavy metal) are scattered and removed from the beam after its traversal. These resonances not only uniquely identify the material, but are also Doppler-broadened because of the thermal motion of the atoms in the material. A measurement of the Doppler broadening can be used to deduce the temperature. The development of an NRS thermometry diagnostic suitable for MaRIE requires the development of a compact and intense source of neutrons. Dramatic increases in neutron flux have been demonstrated using high-quality intense short-pulse optical lasers,[11] which have led to consideration of such bright neutron sources for interesting applications[12,13] including NRS on MaRIE. Unfortunately, the transit time at the sample for the difference in arrival of fastest to slowest neutrons in the incident neutron spectrum moderated to cover the nuclear resonance is hundreds of nanoseconds which makes this a slow method for the mesoscale. One can shorten this transit time by placing the moderated source closer to the sample, which is possible to do with an optical laser system, and by going to higher energy resonances. The system choice becomes a question of relative cross-section, source flux, background, and detector efficiency while optimizing the time response.

Meanwhile, with the termination of the Trident Laser Laboratory, a different facility for studying such neutron sources was needed. Initial tests at the Texas Petawatt Facility, with similar high-contrast quality, showed for similar intensity (same pulse energy, ¼ the pulse duration, but with twice the f-number) similar fluxes of neutrons could be produced.

ACKNOWLEDGMENTS

The MaRIE Technology Risk Mitigation research and development is the work of a large number of collaborators. We especially recognize Garrett Kenyon, Benjamin Liu, Ghanshyam Pilania, John Smedley, Jinkyoung Yoo, Renyuan Zhu, John Barber, Saryu Fensin, Reeju Pokharel, Nokalai Yampolsy, Brendt Wohlberg, Anna Llobet, John Lang, Peter Goodwin, Shawn McGrane, Lynn Veesser, Bob Corrow, Brian Catta, Larry Rodriguez, Patrick Medina, Cort Gautier, Miguel Santiago, Sylvia Ann Junghans, Andrea Favalli, Metodi Iliev, and the staff at the Texas Petawatt Facility. We are extremely grateful for the leadership provided by the late David Holtkamp. We also thank Staci Brown of NA-113 and Dana Dattelbaum of the Dynamic Materials Properties Campaign at Los Alamos for support.

REFERENCES

[1] *Management of Major Capital Acquisition Projects*. DOE Order 413.3B, (U.S. Department of Energy, Washington, DC, 2016)

[2] Alex H. Lacerda and Cris W. Barnes, LA-UR-16-20803 (2016); Cris W. Barnes, LA-UR-17-24477 (2017).

[3] Zhehui Wang, LA-UR-12-20464 (2012); Z. Wang, C. L. Morris, J. S. Kapustinsky, K. Kwiatkowski, and S.-N. Luo, Rev. Sci. Instrum. **83** (2012) 10E510.

[4] Peter Denes, Sol Gruner, Mike Stevens, and Zhehui Wang, LA-UR-17-22085 (2017).

[5] U. Lienert, S. F. Li, C. M. Hefferan, J. Lind, R. M. Suter, J. V Bernier, N. R. Barton, M. C. Brandes, M. J. Mills, M. P. Miller, B. Jakobsen, and W. Pantleon, JOM J. Miner. Met. Mater. Soc., **63:7** (2011) 70–77.

[6] I. Robinson and R. Harder, Nat. Mater., **8:4** (2009) 291–298; Mathew Cherukara. Reeju Pokharel, Timothy O'Leary, Jon Baldwin, Evan Maxey, Wonmsuk Cha, Joerg Maser, Ross Harder, Saryu Fensin, and Richard Sandberg, submitted to Nano Letters (2017).

[7] F. E. Merrill, J Fabritius, F. G. Mariam, D. Poulson, R. Simpson, P. Walstrom, and C. Wilde, AIP Conference Proceedings 1793, 060004 (2017); doi: 10.1063/1.4971560

[8] J. L. Barber, C. W. Barnes, R. L. Sandberg, and R. L. Sheffield, Phys. Rev. B, **89** (May 2014) 184105; B.A. Pound, J.L. Barber, K. Nguyen, M.C. Tyson, R.L. Sandberg, Phys. Rev. B, **96** (Aug 2017) 054104. [9] Alex Lacerda, Al Migliori, Juan C. Fernandez, David Holtkamp, Lynn Veeser, Sven Vogel, Laura Smilowitz, George Rodriguez, Shawn McGrane, Dmitry Yarotski, LA-UR-17-22239 (2017).

[10] V. W. Yuan, J. David Bowman, D. J. Funk, G. L. Morgan, R. L. Rabie, C. E. Ragan, J. P. Quintana, and H. L. Stacy, Phys. Rev. Letters **94** (2005) 125504.

[11] M. Roth, D. Jung, K. Falk, N. Guler, O. Deppert, M. Devlin, A. Favalli, J. Fernandez, D. Gautier, M. Geissel, R. Haight, C. E. Hamilton, B. M. Hegelich, R. P. Johnson, F. Merrill, G. Schaumann, K. Schoenberg, M. Schollmeier, T. Shimada, T. Taddeucci, J. L. Tybo, F. Wagner, S. A. Wender, C. H. Wilde, and G. A. Wurden, Phys. Rev. Letters **110** (2013) 044802.

[12] N. Guler, P. Volegov, A. Favalli, F. E. Merrill, K. Falk, D. Jung, J. L. Tybo, C. H. Wilde, S. Croft, C. Danly, O. Deppert, M. Devlin, J. Fernandez, D. C. Gautier, M. Geissel, R. Haight, C. E. Hamilton, B. M. Hegelich, D. Henzlova, R. P. Johnson, G. Schaumann, K. Schoenberg, M. Schollmeier, T. Shimada, M. T. Swinhoe, T. Taddeucci, S. A. Wender, G. A. Wurden, and M. Roth, J. Appl. Physics **120** (2016) 154901.

[13] J. C. Fernández, D. C. Gautier, C. Huang, S. Palaniyappan, B. J. Albright, W. Bang, G. Dyer, A. Favalli, J. F. Hunter, J. Mendez, M. Roth, M. Swinhoe, P. A. Bradley, O. Deppert, M. Espy, K. Falk, N. Guler, C. Hamilton, B. M. Hegelich, D. Henzlova, K. D. Ianakiev, M. Iliev, R. P. Johnson, A. Kleinschmidt, A. S. Losko, E. McCary, M. Mocko, R. O. Nelson, R. Roycroft, M. A. Santiago Cordoba , V. A. Schanz, G. Schaumann, D. W. Schmidt, A. Sefkow, T. Shimada, T. N. Taddeucci, A.Tebartz, S. C. Vogel, E. Vold, G. A. Wurden, and L. Yin, Phys. Plasmas **24** (2017) 056702.