STATUS OF THE LOS ALAMOS MULTI-PROBE FACILITY FOR MATTER-RADIATION INTERACTIONS IN EXTREMES*

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Abstract

The Matter-Radiation Interactions in Extremes (MaRIE) project will provide capability that will address the control of performance and production of materials at the mesoscale. MaRIE will characterize the behavior of interfaces, defects, and microstructure between the spatial scales of atomic structures and those of the engineering continuum where there is a current capability gap. The mission need is well-met with an x-ray source, coherent to optimize disordered imaging capability, brilliant and high-rep-rate to provide time-dependent information, and high enough energy to see into and through the mesoscale of materials of interest. It will be designed for time-dependence from electronic motion (picosecond) through sound waves (nanosecond) through thermal diffusion (millisecond) to manufacturing (seconds and above). The mission need, the requirements, a plausible alternative reference design of a 12-GeV linac-based 42-keV x-ray free-electron laser, and the status of the project will be described.

THE MISSION NEED

One of the main objectives of the National Nuclear Security Administration is to enable new and more rigorous science-based approaches to manufacturing and certification without the need for nuclear tests. Los Alamos has been pursuing a next-generation signature facility based on multi-probe capabilities to address this control of performance and production of weapons materials at the mesoscale for quite some time. Many of the uncertainties that remain in the assessment of weapon safety, security, and performance arise from uncertainties in material properties governed at the spatial scales between atomic structures and those of the engineering continuum (the mesoscale) [1]. The Matter-Radiation Interactions in Extremes (MaRIE) facility would provide this new capability by aiding our ability to test materials response at resolutions necessary to understand the links between materials microstructure and performance in weapons-relevant extreme environments through new and more rigorous science-based approaches to manufacturing and certification as part of science-based stewardship.

Experimental data from MaRIE would improve the understanding of interfaces, defects, and microstructure in the mesoscale and provide the ability to offer time-dependent control of processes, structures, and properties. Materials will be characterized at the mesoscale, and their dynamic behavior studied in time-dependent extreme conditions through the use of both imaging and diffractive scattering with multiple probes at multiple spatial and time scales. Exascale computing will be combined with experimental results from the MaRIE facility to enable rapid and confident deployment of new components and systems through more cost-effective and more rigorous science-based approaches.

The scientific community has identified that the challenge to accelerated discovery and use of new materials with enhanced and optimized properties is at the mesoscale, where new tools and approaches are needed to understand this regime [2]. It has become clear that in many important areas the functionality that is critical to macroscopic behavior begins not at the atomic or nanoscale but at the mesoscale, where defects, interfaces, and non-equilibrium structures dominate materials behavior [3]. Measurements are needed of scattering off the periodic structure of the material (phase, texture, orientation) as well as imaging of non-periodic structures (defects, material interfaces, and microstructures) to resolve these materials behaviors. These measurements are possible with a brilliant, high-repetition-rate, coherent X-ray source such as proposed for the MaRIE facility.

MaRIE would fill a critical gap in length scale between the integral scale addressed by hydrotest facilities such as DARHT and Scorpius and facilities for materials phenomena at smaller scale such as NIF and Z. The reference design assumes the MaRIE facility would be sited at the Los Alamos Neutron Science Center (LANSCE). The LANSCE facility has been the flagship facility for large-scale science at Los Alamos for many decades.

THE MARIE FACILITY

The proposed MaRIE facility includes a new 12-GeV electron linac driving a 42-keV X-ray free-electron laser (XFEL), coupled with the existing capabilities of the LANSCE 1-MW capable, 800-MeV proton linear accelerator (linac), a new experimental hall, and materials fabrication and characterization facilities. The LANSCE accelerator complex currently supports a broad user base including the neutron scattering community, basic science, and national security programs by providing multiple beams to several experimental areas. MaRIE builds upon LANSCE to transform the science of microstructure, interfaces, and defects of materials in extremes. This will be accomplished by providing the necessary extreme environments (pressure, temperature, radiation, etc.) coupled with multiple probes including, charged particles (protons and/or electrons), optical laser photons, coherent X-rays, and state-of-the-art diagnostics. Figure 1 shows a pre-conceptual layout of the MaRIE facility at LANSCE.

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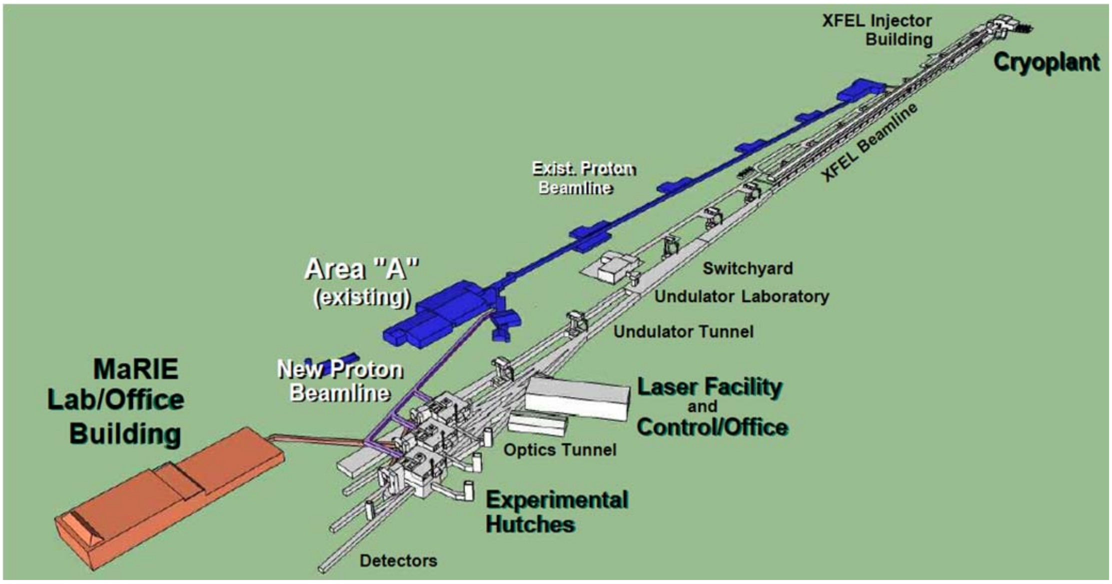

Figure 1: Pre-conceptual layout of the MaRIE facility. Note the location of the existing LANSCE proton linear accelerator (shown in blue) relative to the new MaRIE XFEL.

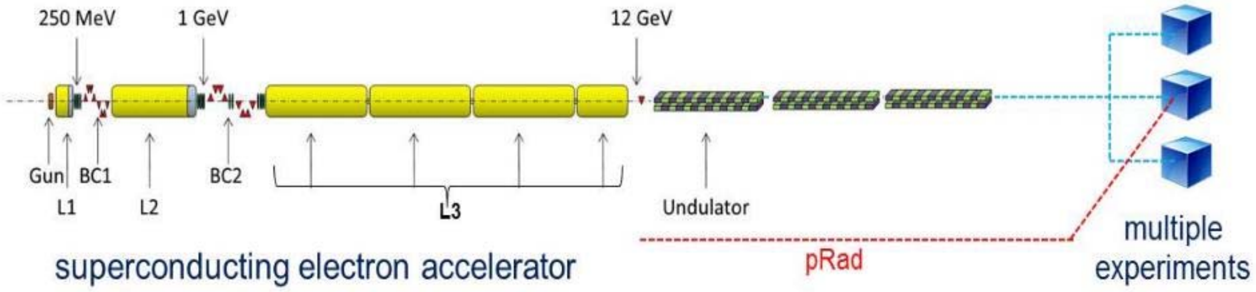

Figure 2: Schematic layout of the MaRIE X-ray Free Electron Laser.

PRE-CONCEPTUAL REFERENCE DESIGN

The pre-conceptual layout of the MaRIE XFEL is shown schematically in Fig. 2 above. The source of electrons for the XFEL is provided by a 12-GeV superconducting linac operating at an RF frequency of 1.3 GHz. Both normal-conducting and superconducting (SC) linacs were considered. Only a SC linac can effectively meet the long macropulse requirements needed to achieve the spatial and temporal resolutions needed for the broad range of experiments to be performed. The photoinjector design is based on the PITZ photoinjector with a modified solenoid configuration [4] to improve the output beam emittance needed to generate the required 5 x 10^{10} photons at 42 keV in each 33-fs pulse with a very narrow 5 x 10^{-4} bandwidth. The pre-conceptual linac layout assumes the use of International Linear Collider (ILC) [5] type 1.3-GHz multi-cell/multi-cavity cryomodules, and 3.9-GHz DESY FLASH [6] cavities and cryomodules to accelerate and linearize the beam phase space, respectively. The undulator design is similar to the SwissFEL U15 design [7]. The output energy of the electron gun is 5 MeV. The injector system accelerates the beam up to 250 MeV before the first bunch compressor (BC1) in the present layout but may be revised to a higher energy to improve beam performance. A summary of key accelerator/XFEL performance parameters is presented in Table 1 below.

Technical Challenges

Achieving a small beam emittance and maintaining it throughout the linac and XFEL is critical for high-efficiency lasing in the undulator to meet photon flux and coherence requirements for MaRIE. Coherent synchrotron radiation (CSR) can be a limiting factor however, preliminary studies of a double-chicane compressor (see Fig. 3) seems to mitigate the effects of CSR for our design. Figure 4 shows projected emittances before and after BC1 [8, 9]. The dominant technical challenge to maintaining the required beam quality appears to be the micro-bunch instability (μBI). Several methods to suppress μBI are being investigated including use of a laser heater to heat the pre-compressed bunch, reducing the residual beam dispersion, or micro-bunching the beam with a laser modulator and eliminating the second bunch compressor (BC2, Fig. 2). Some form of distributed seeding will be required to improve the spectral contrast and narrow the bandwidth of the XFEL output beam. Figure 5 shows a layout of the MaRIE XFEL undulator and the proposed locations of the three spectral filters for distributed seeding [10]. Simulation results using Genesis are also shown in Fig. 5. Note the increase in photon flux as a function of position along the undulator. All of these effects including wake fields and incoherent synchrotron radiation on electron beam quality will be studied.

Technical Risk Reduction

Several technical gaps have been identified [11] that will need to be addressed through a multi-year plan to reduce technical risks. For the XFEL/Linac, risk reduction will be expected to focus on photoinjector performance, achieving and maintaining small electron beam emittance, minimizing wake-field effects, and achieving and maintaining the required beam energy spread; requirements include 5 x 10^{10}, 42-keV photons within 2 x 10^{-4} bandwidth for single-shot coherent diffractive X-ray imaging; <300-ps x-ray pulse separation. Risk reduction activities are also needed for MaRIE detectors – high resolution (sub-µm) requires very small pixel size (or high magnification); sub-ns framing times, fast on-board storage, high quantum efficiency, high dynamic range, and low noise. MaRIE radiography/imaging requirements need improvements in contrast for thin systems (~ 1 g/cm^2 vs. 10 g/cm^2); improved temporal resolution/improved imaging resolution; requirements: 10-ns gating, 10-ns inter-frame time, scintillator decay ~ 4 ns; new detector materials are also needed.

Table 1: Accelerator/XFEL Key Performance Parameters

Electron Beam Requirements				**Photon Requirements**	
Energy	12 GeV	**bunches per macropulse**	10 to 100	**Energy**	4 to 42 KeV
RF frequency	1.3 GHz	**RMS slice energy spread**	≤ 0.015%	**# per bunch**	> 2 x 10^{10}
Linac type	Superconducting	**Macropulse energy variation**	≤ 0.02%	**% Transverse coherence**	70%
SC cavity gradient	31.5 MV/m	**Pulse energy variation within a macropulse**	≤ 0.01%	**Pulse length**	≤ 100 fs
Beamline angle	2.0 degrees, max. @ 12 GeV	**Min. bunch separation**	2.3 ns	**Bandwidth**	5 x 10^{-4}
Macropulse duration	0.1 ms, max.	**Dropped bunch rate**	1x10^{-3}	**Divergence**	≤ 1 µrad
Electron source	Photoinjector	**Norm. slice emittance**	≤ 0.2 micron, rms	**Polarization**	linear
Bunch charge	0.2 nC, max.	**Max. repetition rate**	10 Hz	**Tunability**	1%/ms

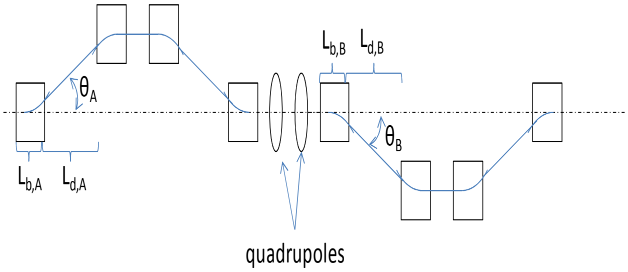

Figure 3: Schematic layout of the proposed double-chicane bunch compressor for MaRIE to mitigate CSR.

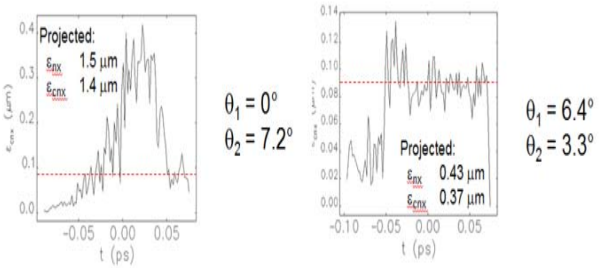

Figure 4: Projected emittances before (left) and after (right) BC1. Note the nearly factor of 4 reduction.

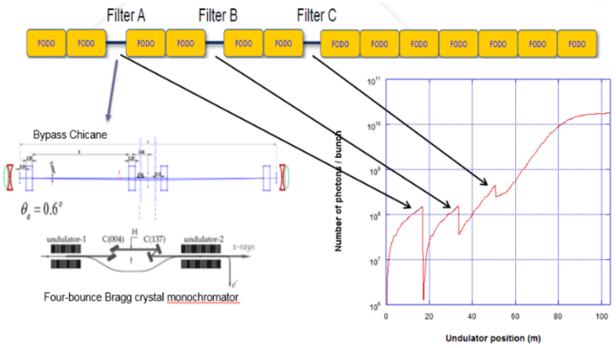

Figure 5: Proposed approach for distributed seeding to increase photon flux while maintaining the desired 5x10^{-4} bandwidth. Genesis simulation results are also shown.

MARIE EXPERIMENTAL REQUIREMENTS

As mentioned earlier, long-term mission and science challenges for materials science that can be met by data obtained using the capabilities of the proposed MaRIE facility have been identified by engagement with the scientific community and through a series of workshops. These challenges motivate the science need and define a series of experiments that establish performance requirements for the MaRIE facility. These experiments include studying dynamic materials performance such as multiphase high explosive evolution, dynamic performance of plutonium and surrogate metal alloys, and turbulent material mixing in variable density flows. Experiments to inform process-aware manufacturing such as aging of materials, controlled functionality of new materials, and advanced and additive manufacturing are also planned. The spatial and temporal measurements to resolve these phenomena require a broad range of operating parameters for the MaRIE XFEL. Figure 6 summarizes the range of MaRIE operating parameters. It should be noted that optical splitting will be used to generate sub-ns pulse separation.

Time resolved measurements into and through the mesoscale require X-rays that are coherent, brilliant and of high repetition rate, and of sufficiently high energy. Materials to be studied range from beryllium to plutonium and sample thicknesses from approximately 10 microns to 10 cm [12].

The 42-keV photon energy and flux of the MaRIE XFEL are chosen to be a trade-off between maximizing elastic scattering for diffraction measurements, minimizing absorptive heating in the sample, and the maximum areal density of the expected samples to be measured. High resolution requires a minimum number of coherently-scattered photons per sub-ps pulse. Using known attenuation coefficients for the materials of interest, this sets the required incident number of photons on a sample to be ~5 x 10^{10} per pulse.

The present plan is for the MaRIE facility to leverage the existing LANSCE proton/neutron capabilities by combining the 42-keV XFEL operating at a high repetition rate with simultaneous charged-particle dynamic imaging. The use of multiple probes allows each probe beam to cover a different parameter range for material or process interrogation. By providing flexible multi-probe pulse structures, including high repetition rates, measurements can be tailored to interrogate the full evolution of a process from unperturbed sample measurement through the beginning of void formation, to phase change of the material, to final deconstruction of the sample. The XFEL beam allows the highest spatial resolution over the smallest framing time for diffractive imaging. Electron radiography is being considered and would allow interrogation at intermediate time scales and spatial resolution, ~25-50 ns and ~1-10 µm, respectively. Proton radiography would be used for either early or late-time, and larger-scale imaging.

The proposed experimental hall includes three experimental hutches. The main central hutch would include multiple probes, extreme environments produced using high-explosives-driven gas guns and flyer plates, high magnetic fields and high-power laser systems, and a single end station. The probe beams would be used for radiographic or diffraction imaging. The remaining two experimental hutches would be used to study complex materials design through the integration of advanced synthesis, including single-crystal growth, in situ characterization, and theory validation. These hutches would only have X-ray probes and up to two end stations each. One X-ray end station would allow for in-situ measurements during materials synthesis and additive manufacturing. Experimental facilities equipment would initially be based on existing hardware already in use at LANL and at other light sources such as SLAC and ANL, with planned improvements through on-going R&D.

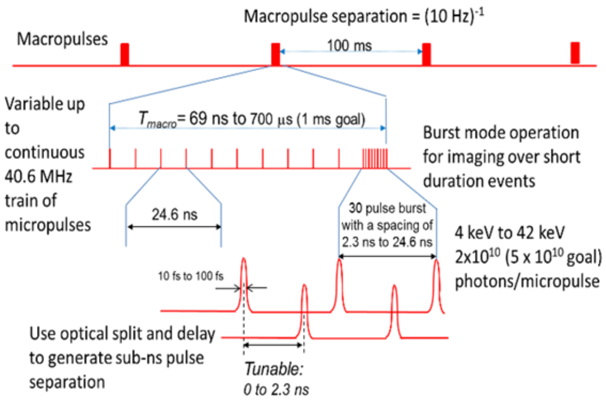

Figure 6: MaRIE electron linac pulse requirements. Note the broad range of pulse length and timing flexibility required.

SUMMARY

The new MaRIE facility would be used to discover and design the advanced materials needed to meet 21st-century national security and energy-security challenges to develop next-generation materials that will perform predictably in extreme environments. We are continuing to follow present US Department of Energy (DOE), National Nuclear Security Agency (NNSA) guidance regarding submission of a large construction project.

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REFERENCES

[1] C. Barnes, "MaRIE – A Proposal for Matter-Radiation Interactions in Extremes Capability," MaRIE Project Document, December 7, 2015.

[2] See, for example, the Workshop Reports at http://www.lanl.gov/science-innovation/science-facilities/marie/workshop-reports.php including: "Decadal Challenges for Predicting and Controlling Materials Performance in Extremes," Los Alamos National Laboratory, LA-UR-10-02959, 2010.

[3] "From Quanta to the Continuum: Opportunities for Mesoscale Science," A Report for the Basic Energy Sciences Advisory Committee by the Mesoscale Science Subcommittee, September 2012.

[4] S. Russell *et al.,* "MaRIE XFEL Pre-Conceptual Reference Design Injector," Los Alamos National Laboratory, LA-UR-15-21963, 2010.

[5] FNAL "Cryomodule Design," `https://ilc.fnal.gov/accelerators/cryomodule.html`

[6] FNAL "3.9 GHz Cavity Program," `https://ilc.fnal.gov/accelerators/3.9Ghz.html`

[7] T. Schmidt *et al.,* "SwissFEL U15 Prototype Design and Frist Results," in *Proc. FEL2012*, Nara, Japan, August 26-31, 2012, pp. 666-669, 2012.

[8] J.W. Lewellen, "Progress on the MaRIE 1.0 Linac Baseline Design," LA-UR-13-25445, 2013.

[9] J.W. Lewellen *et al*., "Status of the MaRIE X-FEL Accelerator Design," in *Proc. 2015 Int'l Part. Accel. Conf.*, Richmond, VA, USA, May 2015.

[10] D. C. Nguyen et al. "Distributed Seeding for Narrow-Linewidth Hard X-Ray Free-Electron Laser," in *Proc. FEL2015*, Daejeon, Korea, August 23-28, 2015, pp. 301-304, 2015.

[11] "MaRIE Technology Maturation Plan," MaRIE Project Document, TMP-0003, November 2015.

[12] "MaRIE 1.0: A Flagship Facility for Predicting and Controling Materials in Dynamic Extremes," LANL publication, LA-UR-12-00500, 2012.