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MATTER-RADIATION INTERACTIONS IN EXTREMES (MARIE) PROJECT OVERVIEW

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Abstract

The National Nuclear Security Administration (NNSA) has a mission need to understand and test how material structures, defects and interfaces determine performance in extreme environments. The MaRIE Project will provide the science ability for control of materials and their production for vital national security missions. To meet the mission requirements, MaRIE must be a high-brilliance, short-pulse, coherent x-ray source with a very flexible pulse train to observe phenomena at time scales relevant to advanced manufacturing processes and dynamic events, with high enough energy to study high-Z materials. This paper will cover the rationale for the machine requirements, a pre-conceptual reference design that can meet those requirements, and preliminary research needed to address the critical high risk technologies.

MARIE MISSION

MaRIE will provide critical data to advance the state-of-art in understanding materials performance in dynamic environments and to guide advanced manufacturing. Providing this capability requires two coupled key elements: state-of-art computing platforms and advanced models, and experimental facilities which can inform these models and validate the resulting calculations. These experimental facilities must be able to perform across an extremely wide range of environmental conditions, time scales, and physical resolutions. MaRIE complements the planned National Strategic Computing Initiative by providing the data to allow resolved calculations of component manufacturing processes and system response and performance in both normal and abnormal environments. Together, MaRIE and Exascale computing will enable rapid and confident development of new materials and systems through more cost-effective and more rigorous science-based approaches.

As stated in the Basic Energy Science (BES) report on Opportunities for Mesoscale Science [1], in many important areas the functionality critical to macroscopic behaviour begins to manifest itself not at the atomic or nanoscale but at the mesoscale, where defects, interfaces, and non-equilibrium structures dominate behaviour. Microstructure is important because it determines the material's macroscopic engineering properties, such as strength, elasticity, stability under heat and pressure, and how those properties evolve with time and use. The MaRIE effort will deliver the ability to study, and thus control, time-dependent processes, structures, and properties during the manufacturing process. Experimental characterization will be complemented by capabilities in synthesis and fabrication and will be integrated with advanced theory, modelling, and computation.

MaRIE will address this capability gap, which derives from our inability to see into and through optically opaque objects at the mesoscale, by using a coherent, brilliant x-ray source that has the required photon energy and repetition rate characteristics.

PROJECT STATUS

The MaRIE project has been in development since the late 2000s. In reviewing possible laboratory futures during the last contract transition, LANL determined that a National Security mission gap existed and a new science capability was needed. The Department of Energy has a formal process for the submission of major capabilities enhancements. The first step in this process is Critical-Decision 0, CD-0, that confirms a mission gap of national importance exists. However, CD-0 explicitly does not specify how the gap will be filled, such as what type of facilities or approaches are required. MaRIE had formal approval of Mission Need, CD-0, in March, 2016.

To understand the possible future budgetary impacts on DOE, a required part of the CD-0 submission is a schedule and budget estimate. A "plausible alternative" that will address most of the foreseen science gaps must be developed to define the required estimate of the project. The pre-conceptual reference design given later in this paper formed the basis of a schedule and budget estimate.

Following CD-0, the first step towards CD-1 is confirmation of Scientific Functional Requirements (SFRs) intended to address the mission gaps identified in CD-0. The Technical Functional Requirements (TFRs) follow from the SFRs and guide the Analysis of Alternatives (AoA). An independent review of the SFRs and TFRs by an external peer review committee was conducted in September, 2016. The AoA evaluates possible practical approaches to resolving the TFRs and does not assume the previously mentioned reference design will be the correct solution. The result of the AoA is a delineation of the facility requirements that will be addressed in a Conceptual Design. Presently, the DOE is convening a panel to conduct an independent AoA, which will be followed by the start of Conceptual Design. The remaining major Critical Decision gates after CD-1 are: Preliminary Design (CD-2), Final Design (CD-3), and Approval for Operations (CD-4).

SCIENTIFIC REQUIREMENTS

Careful assessment and analysis, based on the efforts of many working groups and the results of workshops [2], resulted in a set of Scientific Functional Requirements [3] that, if met, will provide the necessary measurements of

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Table 1: The envelope formed from measurement ranges for the four representative classes of materials science listed below address the science gaps identified in the mission need documents. The highlighted cells are defining requirements that can have a major impact on the facility design. The maximum macropulse length requirement of 1 ms set by requirements to observe thermal transit effects drives the design to superconducting linac technology.

	Metals and Age Aware performance	**High Explosives certification and qualification**	**Turbulent Materials Mixing**	**Casting**
Spatial Resolution	<100 nm – 20 μm	< 100 nm – 20 mm	100 nm	< 1 μm – 100 μm
Field of View	100 μm – 1 mm	100 μm – 2 mm	1 mm	0.3 mm – 1 cm
# Of Frames	~ 30	~ 30	~ 30	1000 per second
Minimum Pulse Separation	< 300 ps	< 500 ps	1 ns	10 ns
Macropulse Length	5 μs	7 μs	15 μs	1 ms
Sample Thickness	> 250 μm	> 10 μm – 6 cm	1 – 10 cm	0.1 – 10 mm
Repetition Rate	< 1 Hz	< 1 Hz	10 Hz	10 Hz
Maximum Micropulse Length	< 1 ps	< 1ps	< 1 ns	< 100 ps
Lattice Measurement	0.1%	0.2%	-	0.01%
Species	Be - Pu	Typically C, H, O, N	Noble gases, Ga, Be	Actinides
Density	1%	3%	2%	1%

atomic and mesoscale phenomena to meet the mission need. Table 1 comprises four topic areas that together cover the large breadth and depth of the material science measurements that need to be addressed by MaRIE.

Following from the above requirements given in Table 1, MaRIE has to have two unique operational capabilities. First, the facility must produce high-energy x-rays to allow measuring bulk high-Z properties by maximizing elastic scattering for diffraction and minimizing absorptive heating for mesoscale measurements, and not just for thin samples, as shown in Figs. 1, 2, and 3. Note that ratio of elastic to inelastic scattering peaks between 20 to 70 keV, depending on the material. Also, the photon absorption for bulk samples, >50 grains, of higher Z materials is unacceptably high for less than 30 keV. A key design requirement, that will be central to balance of cost, risk, and performance, will be the threshold (minimum acceptable) and objective (design goal) x-ray energy.

Second, the facility must have an innovative and flexible linac pulse structure, shown in Figure 4, to make movies of phenomena on timescales ranging from electronic/ionic (sub-ps) through acoustic (ns) to shock transit (μs) to thermal (ms).

We reviewed a wide range of probe techniques that could address the expansive range of requirements given above. This preliminary analysis showed that a coherent x-ray light source is required, and an XFEL can meet the requirements for coherent brilliance, high-energy x-rays, and the very flexible temporal pulse format. Given the complexity and flexibility of linac-driven XFELs, we determined that an XFEL is the best choice for the "bounding box" schedule and cost estimate, and so was chosen for the pre-conceptual reference design.

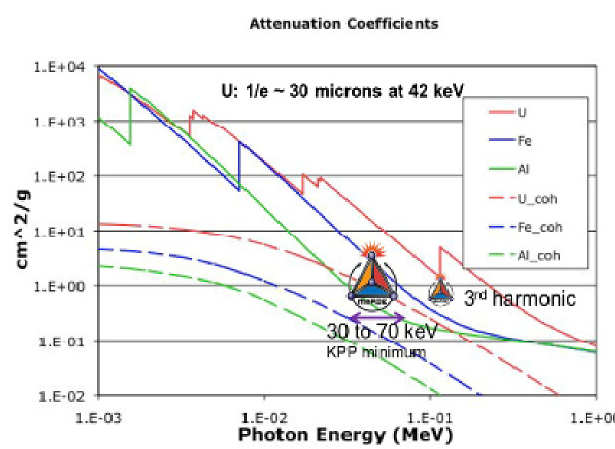

Figure 1: Plotted are inelastic (solid) and elastic (dashed) scattering [4] from 1 keV to 1 MeV for Al, Fe, and U. The Key Performance Parameters (KPP) set the operational characteristics that must be met for a determination of successful project completion. The photon energies of 30 keV to 70 keV represent a possible photon specification of the minimum acceptable operational photon energy (threshold) to the maximum planned photon energy (objective) at the fundamental XFEL photon energy.

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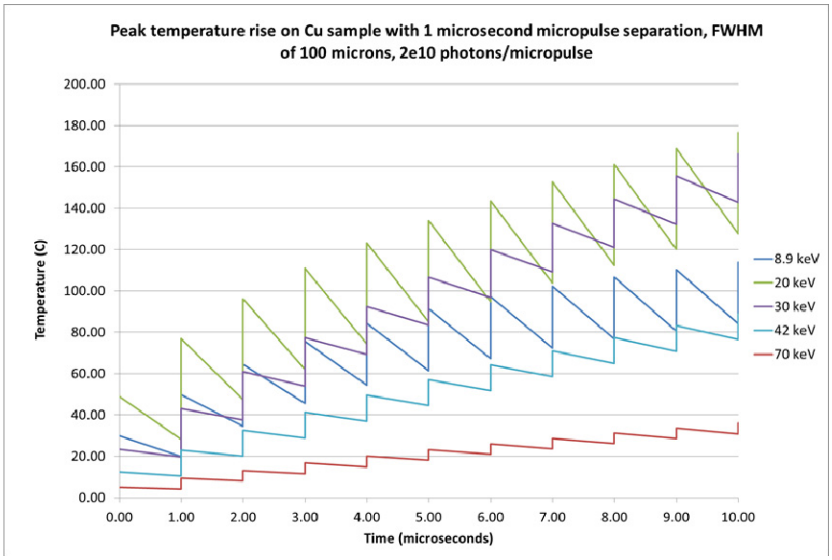

Figure 2: Graph of temperature rise for a string of closely-spaced, 1-μs pulse separation, incident x-ray pulses on copper. Pulse-to-pulse heating quickly becomes a significant effect for photon energies less than 40 keV and for the shorter pulse separations required for MaRIE measurements.

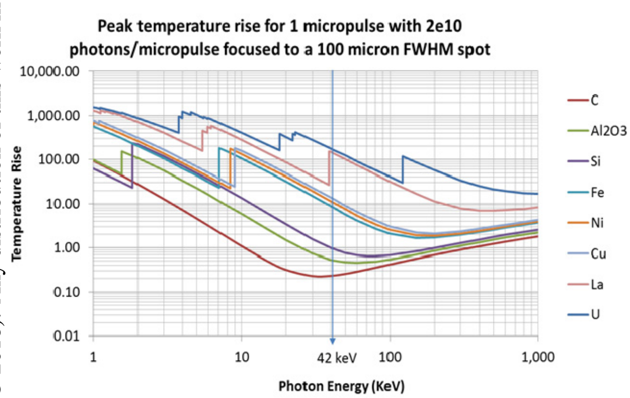

Figure 3: The plots show the fall in heating with increasing photon energy up to some minimum where the absorption flattens out and the temperature rises due to the increasing energy deposited for a fixed number of incident higher-energy photons.

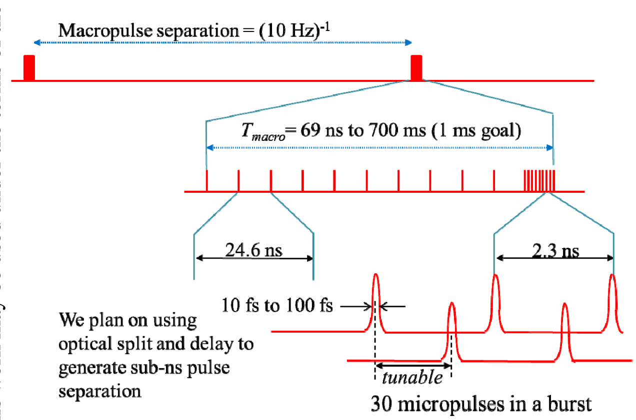

Figure 4: Pulse structure required to capture the full temporal range of dynamic events.

PRE-CONCEPTUAL REFERENCE DESIGN

The SFR-required physical properties at the temporal and spatial scales listed above can be obtained with diagnostic techniques based on radiography, Bragg scattering, and x-ray diffraction. The pre-conceptual reference design [5-8] assumes an XFEL operating at a fundamental photon energy of 42-keV. 42-keV was chosen to allow multi-pulse diffractive imaging that requires greater than 10^{10} photons/image for multi-granular high-Z samples with acceptable but not insignificant heating, as compared to 10^8 photons needed for Phase Contrast Imaging (PCI). Also, operation at a 42-keV fundamental allows for the production of sufficient 3rd harmonic photons to do PCI at the K-edge of high-Z materials, such as uranium and other actinides. The maximum macropulse length requirement of 1 ms drives the choice of superconducting linac technology.

The reference design is based on an L-band 12-GeV superconducting linac similar in design to the European XFEL [9], schematically shown in Figure 6. Time-independent GENESIS simulations, Figure 5, indicate that greater than 2×10^{10}, 42-keV photons within 0.01% bandwidth can be obtained using the expected electron beam parameters. We have also included a 150 m tunnel contingency to go to 15 GeV in the future that would give ~2x times the number of photons, or allow for higher photon energies. The Photon Facility Functional Requirements, given in Table 2, follow directly from the imaging requirements to achieve the SFRs, and provides the Facility Functional Requirements basis for the pre-conceptual reference design. Detailed information on the design is given in reference [5-8]. The electron beam requirements for the XFEL proper, electron driver linac, and electron radiography imaging are given in Tables 3, 4 and 5, respectively.

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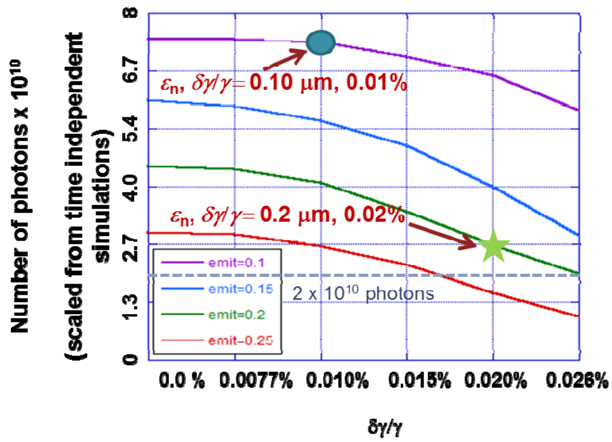

Figure 5: The blue circle shows the design goal for the electron beam of 0.1 μm emittance at 0.01% energy spread. For contingency, the XFEL calculations use the green star parameters, a factor of two higher emittance and energy spread.

Table 2: The Photon Characteristics Required to Meet the Imaging Requirements

Photon FFRs	
Design energy (keV)	5 to 42 (42 to 126 at 3rd harmonic)
Coherent Photons per image	$2x10^{10}$ ($1x10^{8}$ at 3rd)
Energy Bandwidth (ΔE/E)	$2x10^{-4}$ to $<10^{-5}$
Divergence	< 10 μrad
Pulse length	≤ 100 fs

Table 3: The XFEL Electron Beam Requirements

XFEL electron beam FFRs			
Pulse charge	0.2 nC	Normalized rms slice emittance	≤ 0.2 μm
Slice energy spread	≤ 0.02%	Micropulses per macropulse	30
Macropulse repetition rate	10 Hz	Minimum micro-pulse separation	2.3 ns

Table 4: Electron Beam Accelerator Requirements

Electron beam FFRs			
Energy	12 GeV	Electron source	Photo-injector
Linac fund. frequency	1.3 GHz	Max. macropulse duration	1 ms
Linac type	Super-conducting	Macropulse to macropulse energy variation	≤ 0.02%
SC L-band cavity gradient	31.5 MV/m	Pulse energy variation within a macropulse	≤ 0.01%
Maximum beamline angle	2.0 degrees @ 12 GeV	12 GeV FWHM micropulse length	33 fs

Table 5: Electron Radiography Requirements

eRad electron beam FFRs			
Pulse charge	1 nC	Normalized emittance	<1000 microns
Microbunch energy spread	≤ 0.02%	Macropulse repetition rate	10 shots per day
Micropulses per macropulse	10	Min micropulse separation	23 ns

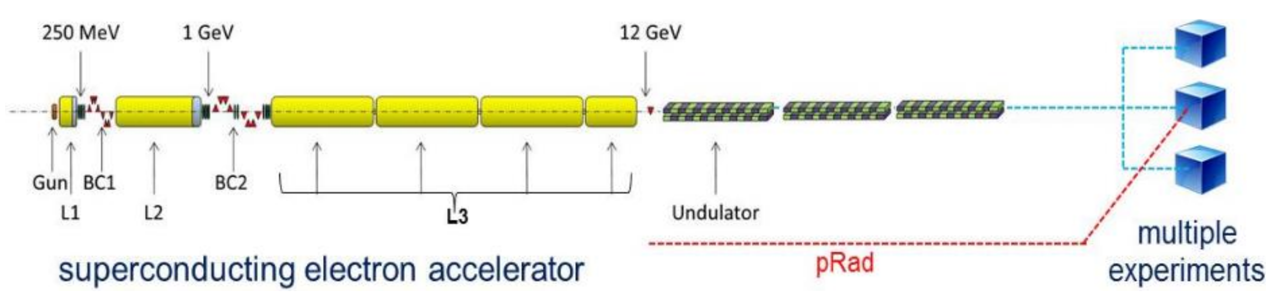

Figure 6: Pre-conceptual XFEL reference design schematic. For example, the first three major accelerator systems specified in this reference design document are: L-Band Photoinjector – Cu cathode, up to 0.2 nC, 10 ps FWHM (3 ps rms) out of gun, 1.1 ms RF macropulse, single 10 MW klystron drive, rms phase and amplitude jitter less than 0.03 degree and 0.03%. this is followed by cryomodule 1 that is based on ILC and DESY XFEL, and is: 9 cavities per cryomodule capacity, 9 cells per cavity, single 1.3 GHz multi-beam klystron (MBK) drive, RMS phase and amplitude jitter less than 0.03 degree and 0.03%, respectively, maximum cavity gradient of 31.5 MV/m, 200 kW/cavity, 18 cavities fed from a single klystron, $Q_{ext} = 3.9x10^{6}$. this is followed by cryomodule 2, again based on ILC and DESY XFEL, 1.3 GHz (2 cavities), 3.9 GHz (6 cavities; 3rd-harmonic for linearization), 1.3 GHz cavity pair parameters and power as in CM1; 3.9 GHz single klystron drive, fields maintained to less than 0.03 degree and 0.03%, cavity gradient 20 MV/m, 3 kW/cavity, Q_{ext} for the 3.9 GHz cavities = $1.2x10^{7}$; final output energy = 250 MeV when setting up for bunch compression in BC1. Also shown are x-ray-only end-stations and simultaneous, with x-ray pulses, electron and proton radiographic capabilities at an x-ray end station.

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TECHNOLOGY RISK MITIGATION PLAN

The Technology Risk Mitigation Plan (TRM) is aimed at bringing the facility technologies to a technical maturity level necessary for completion of a Conceptual Design with a well-bounded cost and schedule estimate, as required by the DOE CD process. TRM also reduces risk to project success by better defining scope and requirements of programmatic equipment. For inclusion in Conceptual Design, the components and/or proposed systems had to have at least been operated in laboratory environment.

The present TRM plan [10] can be split into two categories: technologies unique to an XFEL and technologies independent of the x-ray source type. Should an XFEL be chosen as the preferred alternative then the following technology gaps must be addressed to confirm the production of $5x10^{10}$ photons at 42-keV with $2x10^{-4}$ bandwidth, and a micropulse spacing of 300 ps, as needed to base Conceptual Design:

- The photoinjector emittance must be demonstrated by a combination of relevant measurements at other facilities and then on a test stand at LANL.
- Electron beam energy spread has a major effect on XFEL performance. Energy spread source models for wakefields, Coherent Synchrotron Radiation, and microbunch instability, must be validated for inclusion in the simulation models. These models and dechirper energy correction must be demonstrated through relevant measurements at other facilities.
- Distributed seeding offers a path to attaining the required XFEL bandwidth and so relevant demonstrations at other facilities is required.
- Conceptual design requires a robust start-to-end modeling and simulation. Thus a key TRM activity is to incorporate the models from the above demonstrations and verify the codes.
- High Voltage Converter Modulator development can have a large impact on initial system cost and significantly lower operation and maintenance costs.
- TRM is also planned for on-going activities that are independent of the x-ray source, such as: High-Energy and Ultrafast Imaging Cameras, Multidimensional Dynamic Imaging techniques, Bulk Thermometry of Dynamic Materials, Development of Charged Particle Radiography for the Study of Small and Fast Physical Processes, X-ray Optics, and Long-Pulse Laser Technology Development [11].

All of the preceding TRM technologies are required to attain the full facility benefit and several will have a major impact on the facility layout.

CONCLUSION

The Project is progressing with initial funding. We are looking to fund research to identify and reduce technical risk, decrease cost, and expand performance. We are exploring opportunities for collaborative R&D that would be relevant to MaRIE risk mitigation and conceptual design that builds on the expertise and resources at existing facilities worldwide.

In summary, the proposed MaRIE facility would offer new complementary capabilities to those at existing experimental facilities. The MaRIE capabilities will provide the tools scientists need to develop and manufacture next-generation materials that will perform predictably and with controlled functionality in extreme environments, and enable the discovery and design of advanced materials needed to meet 21st-century national security and energy security challenges.

ACKNOWLEDGMENT

The development of the MaRIE Project and the work presented in this paper is the result of the strong effort of the MaRIE team, with contributions from a large number of colleagues from across LANL, other DOE laboratories, universities, and industry.

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