PRE-CONCEPTUAL DESIGN REQUIREMENTS FOR THE MARIE FACILITY AT LANL AND THE RESULTING X-RAY FREE ELECTRON LASER BASELINE DESIGN*

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Abstract

TThe MaRIE (Matter-Radiation Interactions in Extremes) facility[1] is being proposed to advance materials science by the concurrent utilization of a diverse set of highly penetrating probes. These probes will provide the basis for developing materials that will perform predictably and on demand with currently unattainable lifetimes in extreme environments. The MaRIE facilities, the Multi-Probe Diagnostic Hall (MPDH), the Fission and Fusion Materials Facility (F^3), and the Making, Measuring, and Modeling Materials (M4) Facility will each have experimental needs for one or more high-energy x-ray beam probes, but all require a 50-keV coherent source of greater than 1e10 photons in less than 1 ps. Because of space considerations at the facility, a high-gradient design is being investigated that will use a X-band RF systems to drive a 20-GeV normal-conducting linac. Experimental requirements drive a need for multiple photon bunches over time durations greater than 1 microsecond, as well as interleaving 0.1 nC very-low-emittance bunches with 2-nC electron bunches. This paper will cover an overview of the scientific requirements for the MaRIE XFEL and the baseline XFEL design.

INTRODUCTION

The evolution of materials research drives toward new era that will focus on the ability to manipulate and control materials on scales from atomic to the continuum. MaRIE will address that frontier by providing unique capabilities in matter-radiation interactions and extreme environments to enable future materials-centric science and discovery. MaRIE will provide a comprehensive set of co-located tools to realize transformational advances in materials behavior, response, and fabrication. The MaRIE facilities, the Multi-Probe Diagnostic Hall (MPDH), the Fission and Fusion Materials Facility (F^3), and the Making, Measuring, and Modeling Materials (M4) users drive the requirement of the addition of a 50-keV XFEL. These facilities will enable dynamic probing of material on previously inaccessible time and length scales, will provide intense radiation environments, and will provide the ability to characterize and synthesize new materials. MaRIE will utilize a significantly power-enhanced LANSCE linac, coupled with a challenging 50-keV XFEL to achieve the research goals. The XFEL will be driven by a 20-GeV electron linac. This paper describes the required operational parameters of the electron linac.

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MARIE PHOTON REQUIREMENTS

Temporal Requirements

MaRIE requires intense short-pulse coherent light pulses to make sub-picosecond, high-resolution images of high-Z materials. The most stressing temporal pulse requirements are set by dynamic event measurements. These measurements will require a series of images taken over a duration of a few microseconds. The time duration to obtain an image is set by motion blur and the fastest rate of change of material structures and result in pulse lengths that must be less than 0.1 ns. Given that a typical sample being measured has a unique granular configuration, each experiment will be a stand-alone measurement and so data cannot be the superposition of images taken from a series of samples. The minimum number of images to fully characterize a dynamic measurement is on the order of 100.

Photon Energy Requirements

The two types of x-ray imaging being considered for MaRIE are radiographic imaging and diffractive imaging. Radiographic imaging is like that used in medical imaging and only requires that the attenuation be small enough to let a measurable amount of x-rays exit the sample. Diffractive imaging only uses the coherently scattered photons and is limited to lower energy photons since the amount of diffraction is inversely proportional to the photon energy, and so high resolution images with shorter detector stand-offs are easier at lower photon energies. Practically, the highest photon energy that can give the required imaging resolution is less than 80 keV. The minimum photon energy is set by the density, atomic number, and thickness of the materials of interest. The most difficult materials of interest to penetrate are the actinides, such as uranium. Figure 1 shows both the energy absorption and the coherent scattering of high-energy x-rays in two materials that reasonably span the materials of interest for MaRIE. The energy absorption gives the material heating from the x-rays, and so sets a limit on the maximum pulse intensity and number of pulses.

Intensity Requirements

The peak intensity is set by the above minimum pulse duration and photon absorption and scattering, and the number of photons to produce a high-resolution image. Calculations taking the above factors into account give a minimum $5x10^{10}$ photons/image.

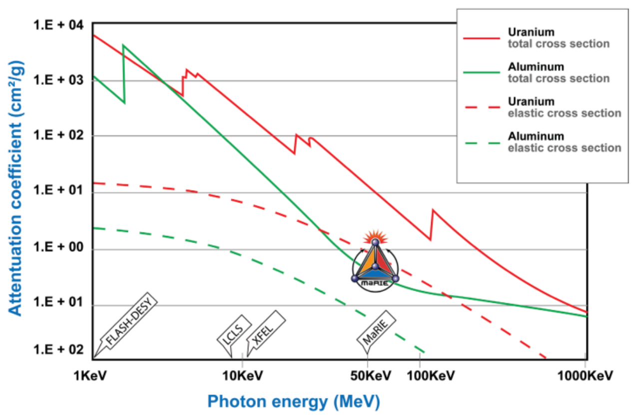

Figure 1: Photon absorption and coherent scattering coefficients for uranium and aluminium. Photon adsorption leads to sample heating, and the elastically scattered fraction gives scattering information.

Physical Limitations of Site

Since an XFEL is very sensitive to the electron beam quality and beam quality is negatively impacted by bends, an accelerator design that fits on the mesa with limited bend imposes design limitations. The originally proposed site at LANL had the XFEL aimed at the target areas for the LANSCE linac, but had only approximately 600 m of length available for the linac and the associated XFEL hardware. Complications incurred by interferences between the XFLE end stations and the existing LANSCE end stations has led to a new layout that runs alongside and just north of the existing LANSCE linac.

Requirements Summary

Through a series of workshops the light source requirements for the MaRIE MPDH, F^3, and Making, M4 were developed. these requirements are summarized in Table 1. The requirements and the major effects that sets the parameters are:

- Photon energy - set by gr/cm^2 (the areal density) of sample and atomic number
- Photon number for an image - typically set by signal to noise in detector and size of detector
- Time scale for an image - fundamentally breaks down to transient phenomena, less than ps, and semi-steady state phenomena, seconds to months
- Bandwidth - set by resolution requirements in diffraction and/or imaging
- Beam divergence - set by photon number loss due to stand-off of source/detector or resolution loss in diffraction
- Source transverse size/transverse coherence - the source spot size will set the transverse spatial resolution, if transversely coherent then this limitation is not applicable so transverse coherence can be traded off with source spot size and photon number
- Number of images/repetition rate/duration – images needed for single shot experiments/image rep rate/ duration of experiment on sample
- Repetition rate - how often full images are required
- Longitudinal coherence – 3D imaging
- X-ray Polarization - required for some measurements
- Tunability – time required to change the photon energy a fixed percentage

REFERENCE XFEL DESIGN

The baseline reference design, shown in Figure 2 [2] is based on either directly measured or modest extensions of measured performance of the highly successful LCLS XFEL. [3]

Our FEL simulations show an expected photon production rate of ~ 5x10^{10} X-rays from a 20-GeV electron beam with the following parameters: 100 pC, 30 fsec, 3.4 kA, 0.015% energy spread, and a 0.30 mm-mrad emittance. The x-ray spectral bandwidth is less than 10^{-3}.

Table 2 lists the baseline reference design as well as the stretch goals for the XFEL linac structure. The 20-GeV electron beam may be used for high-resolution radiography, and so the radiographic electron beam requirements have been added. Although the radiographic emittance requirements are not difficult to attain, ~1000 mm-mrad, the number of electrons required for an image is much more than that required for the XFEL. The wakefields from these higher charge bunches might impact the performance of the XFEL. Before proceeding into final design for the XFEL, the following performance extensions should be demonstrated: Interleaving of 0.1 nC pulses with 1 nC pulses, detailed source-to-end simulations of the baseline 2.8 GHz design, including tolerance/error studies, the generation of 1.5 microsecond long RF pulses, and establishing break-down stand-off limits in S-band structures.

Table 1: The light source requirements given in this table are the requested performance parameters and may exceed the capabilities of the planned light source, but do serve as the ultimate performance goals. Also, the FFF facility has a radiographic requirement for imaging nuclear reactor fuel pins. Due to the high Z and approximately 1 cm thickness of a fuel pin, up to 400 keV photons are required. However since these are radiographs and do not rely on diffraction, coherence is not required. So a short undulator section, as compared to the XFEL undulator, can be used to generate these photons from the 20-GeV electron beam.

	MPDH	FFF		M4	
Design energy is normally top of range (keV)	5-50	~10 to >50	10 to 400	0.1 to 1.5	10 to 50
Photons per image	10^{11}	10^{11}	10^{9}	10^{9}	10^{11}
Time scale for single image	<1 ps	>1 s	0.001 s	10-500 fs	50 fs
Energy Bandwidth (ΔE/E)	10^{-4} to $<10^{-5}$	10^{-4}	3×10^{-3}	10^{-4}	10^{-4}
Multiple pulse rep. rate/duration	120 Hz/day; 10 shots/day	0.01 Hz/mo.	1 Hz/month 1 kHz / 5 sec 0.02 Hz / day	1 KHz/day	10 Hz/day; 1 Hz over several days
Polarization	Linear	linear	no	Linear/circular	linear
Tunability in energy (ΔE/E per unit time)	2%/pulse	fixed	5% in 2 µs	10%/s	Factor of 5 over a day
Expected typical spot diameter(s) at target (microns)	1 to 100	100	1 to 10000	0.1 to 10	0.1 to 10

Table 2: The reference design column consists of a self-consistent set of operational parameters for the XFEL electron accelerator. The advanced design column gives the desired maximum performance for each cell individually and is independent of the other rows. The engineering issues in green cells are based on straight-forward extensions of performance obtained at existing facilities. The engineering issues in yellow cells have not been demonstrated, but should be resolvable with more development. The red cells are beyond state-of-art and will be challenging to reach. White cells are calculated or defined from the other parameters.

Linac	Baseline	Advanced
Energy	20 GeV	20 GeV
Linac frequency	3 GHz	11 GHz
Linac type	RT Cu	RT Cu
Cavity gradient	35 MV/m	70 MV/m
Maximum beamline q	4 degrees	0.2 degrees
Bunch compressor 1	6 m	6 m
Bunch compressor 2	22 m	200 m
RF pulse duration	1.5 ms	1.5 ms
RF pulse rise time	0.1 ms	0.1 ms
RF peak power	80 MW	70 MW
RF Repetition rate	60 Hz	120 Hz

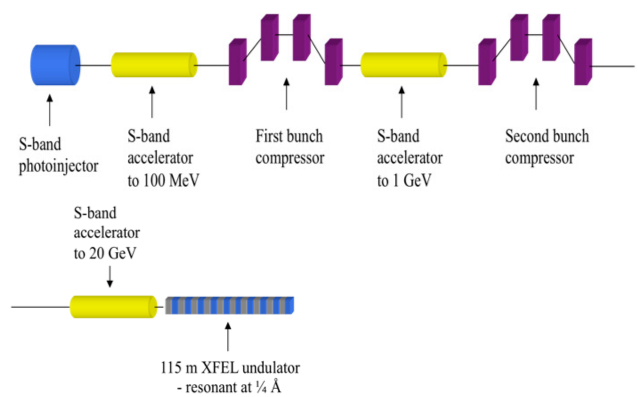

Figure 2: Preliminary layout of 50-keV XFEL 20-GeV electron linac.

SUMMARY

The science need for a 50- keV coherent light source to be part of the MaRIE signature facility is firmly based on user diagnostic probe requirements. The probe requirements and the subsequent alternatives analysis forms a good basis for proceeding with a MaRIE signature facility that incorporates an XFEL.

REFERENCES

[1] http://marie.lanl.gov/
[2] P. Emma el al, Nature Photonics 4 (2010) 641.