LA-UR-16-27709

Status of the Los Alamos Multi-Probe Facility for Matter-Radiation Interactions in Extremes (MaRIE)

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NAPAC16
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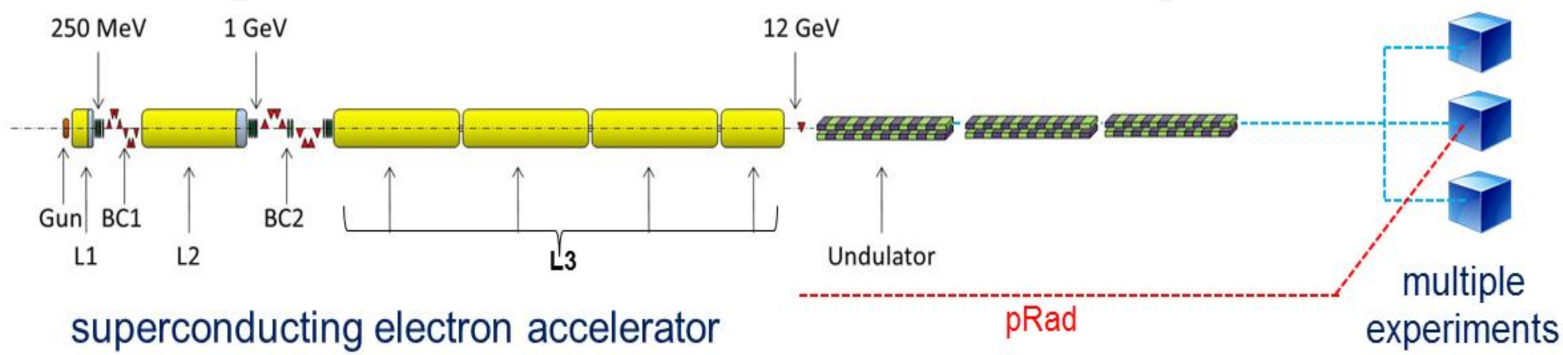
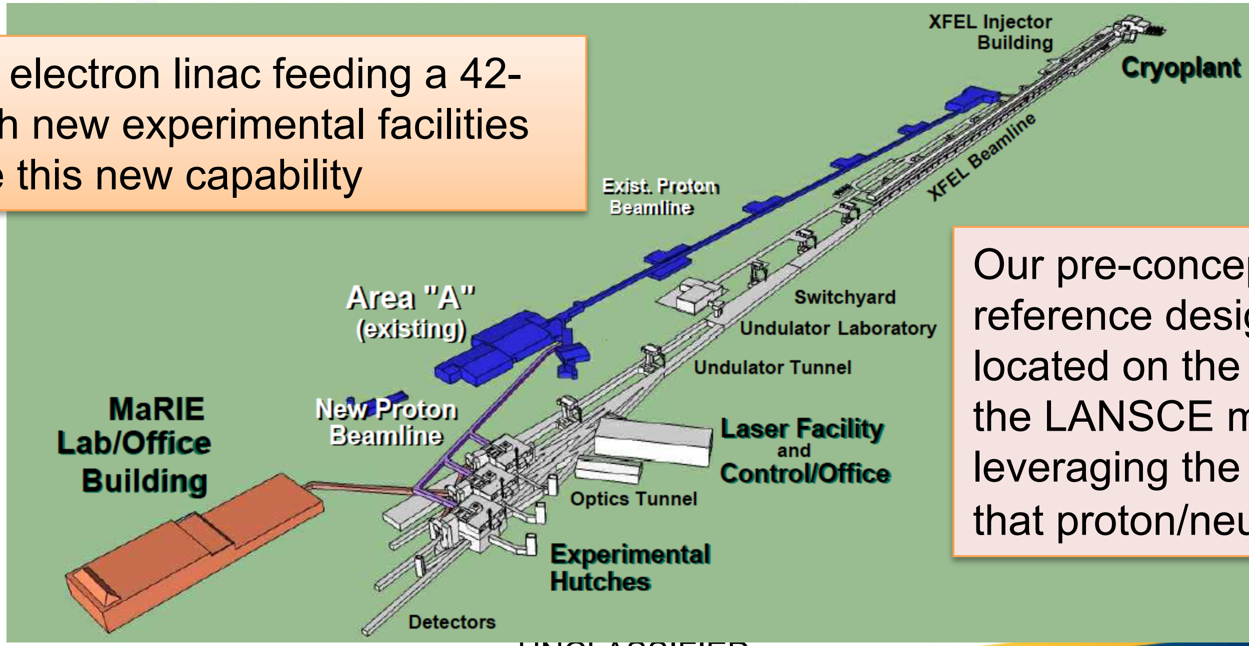
Outline

- MaRIE Overview & Requirements
- MaRIE XFEL Preconceptual Reference Design
- MaRIE Status

MaRIE at LANSCE would leverage existing proton and neutron capabilities to provide a next-generation, multi-probe facility



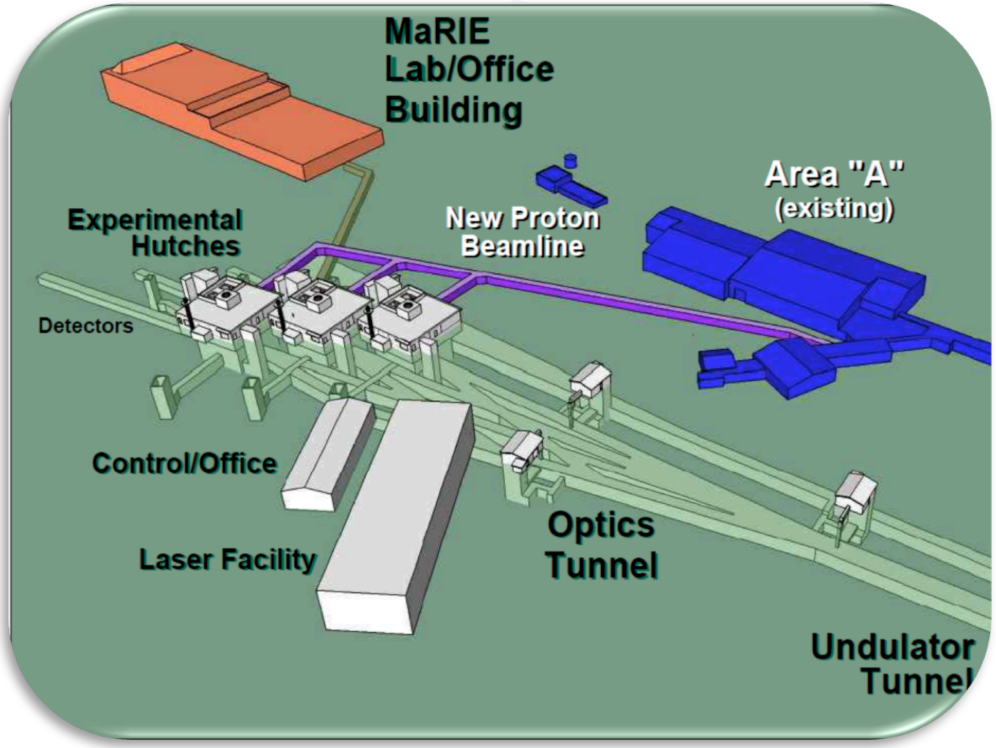
A 12-GeV SC electron linac feeding a 42-keV XFEL with new experimental facilities would provide this new capability



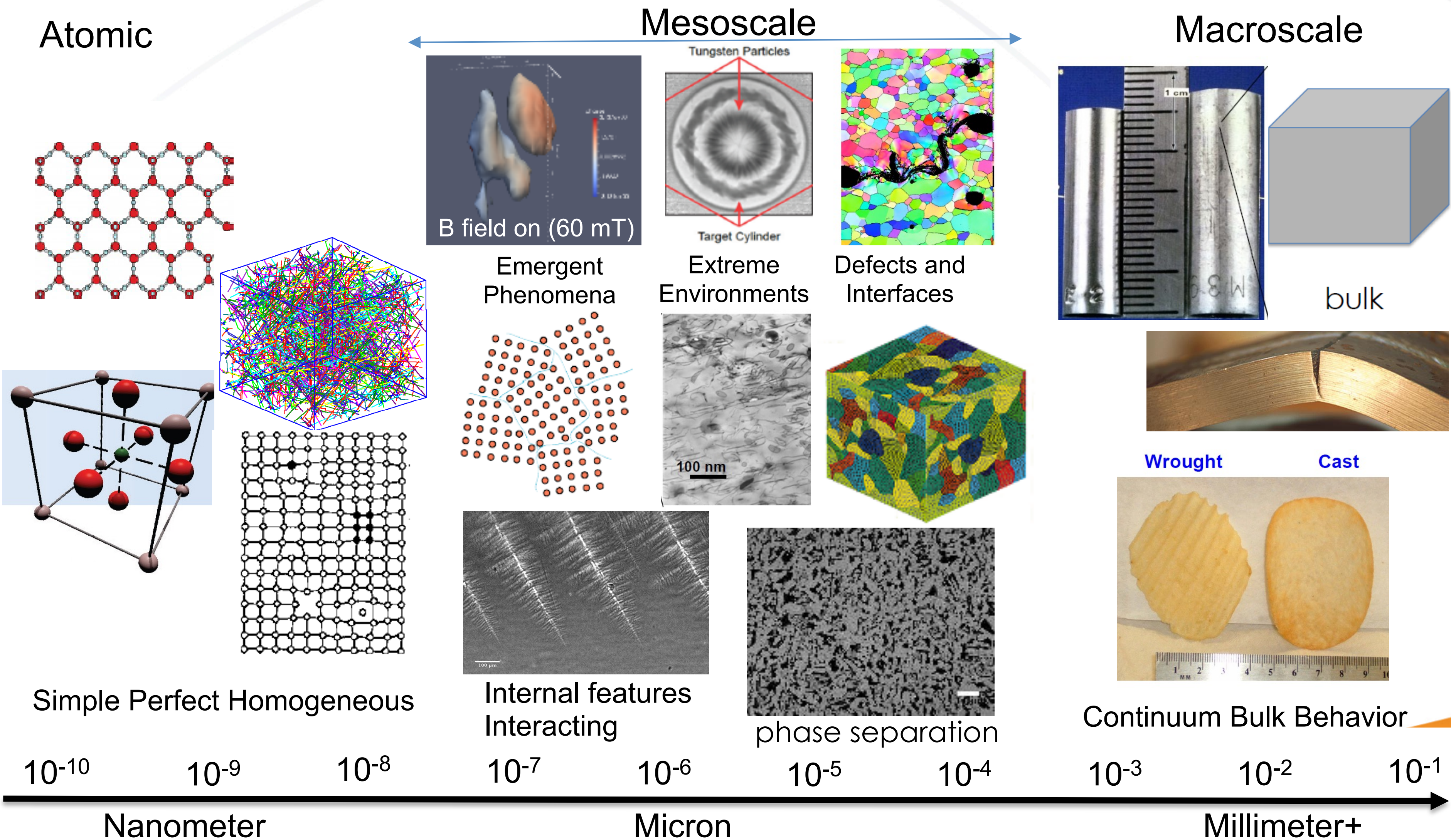
Our pre-conceptual reference design has the XFEL located on the north side of the LANSCE mesa, leveraging the capabilities of that proton/neutron facility

MaRIE would provide a transformational facility for materials research at the mesoscale.

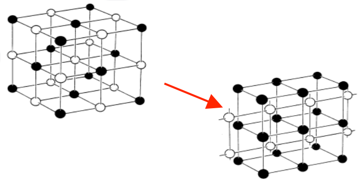
- World's highest energy x-ray scattering capability (**42-keV XFEL**)
- High repetition frequency with simultaneous charged particle dynamic imaging
- Experimental hutches for simultaneous, multi-probe measurements of in-situ transient phenomena in relevant dynamic extremes
- Comprehensive, integrated resources for materials synthesis and control, with national security infrastructure
- Materials discovery, design, and process capability



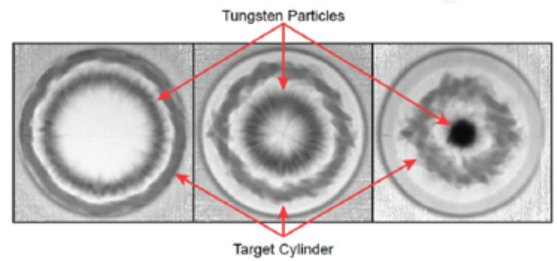
What is the mesoscale?

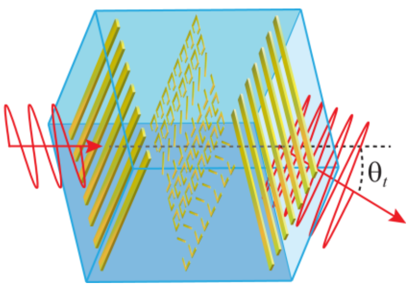


The science needs span a wide range of time scales

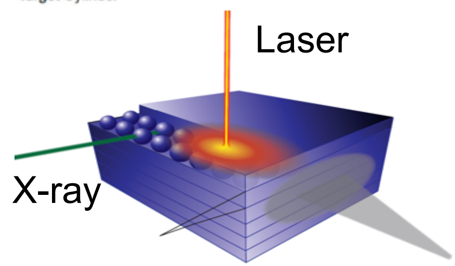


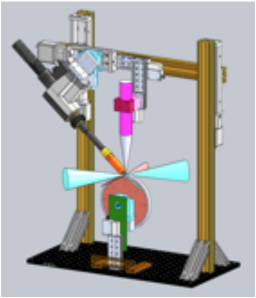
ps – 100 ns
Phase Transformations





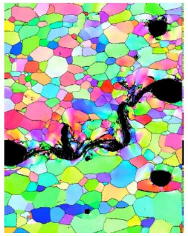
ns – 100 ns
Shock transit across grain;
Hydrodynamic instability





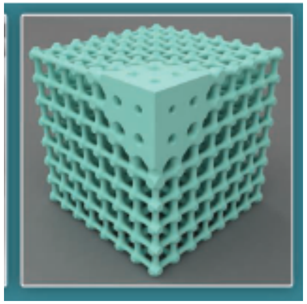
100 ns – 10 μs
Shock transit across sample

50-100 microns pRad beam



10 μs – 1 ms
Thermal pulse evolution

10 s – 10 hour
Additive manufacturing build

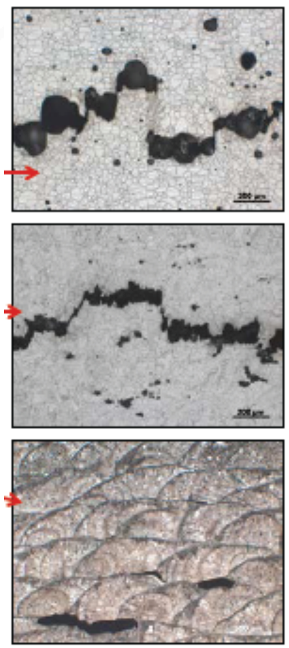


months – years
Aging effects

MaRIE will address the control of performance and production of materials for national security science at the mesoscale

MaRIE fills a critical gap in length scale between the integral scale addressed by DARHT and U1a and facilities such as NIF and Z.

Performance of additively-manufactured (AM) structural components



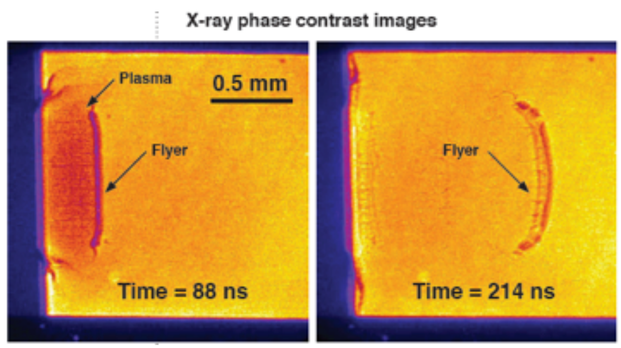
Wrought

AM Annealed

AM

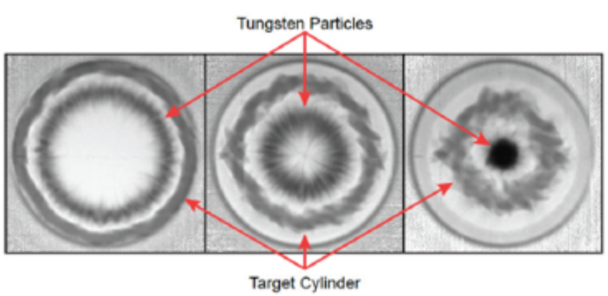
Damage in wrought vs additively-manufactured steel

High Explosive performance and safety



Functioning slapper detonators

Ejecta and Mix



Ejecta in convergent geometry

Requirements for MaRIE are set from analysis of such experiments.

--"(U) MaRIE First Campaigns," LA-CP-15-00501, June, 2015

The Scientific Functional Requirements lead to "seven" defining expectations for a MaRIE facility

- The capability to make dynamic in-situ measurements of bulk material properties of high-Z materials.
- The capability to make spatial measurements that have resolutions down to tens of nanometers.
- The capability to make movies of non-reproducible events on time scales ranging nanoseconds to many hours.
- A measurement window that makes motion blur negligible.
- The ability to measure changes in grain structure.
- The ability to make measurements using multiple probes that cover different spatial resolutions and areal densities.
- The capability to synthesize and characterize mesoscale samples before they undergo the dynamic event.

Existing hard X-ray FELs have demonstrated many of the Pre-Conceptual Reference Design characteristics

	LCLS-I	SACLA	EXFEL 2016	PAL XFEL 2016	SwissFEL 2017	LCLS-II 2019 SRF / NCRF	MaRIE 202x
X-ray energy Pulse energy photons/pulse	12.8 keV 0.93 mJ 5E11	19.5 keV 0.03 mJ 1E10	24.7 keV 1 mJ 2.5E11	20.6 keV 0.08 mJ 2.5E10	12.4 keV 1.4 mJ 7E11	5 / 25 keV 0.025 / 0.3 mJ 3E10 / 7E10	**42 keV** **0.35 mJ** **5E10**
Undulator period K_{rms}	3.0 cm 2.5	1.8 cm 0.94	4.0 cm 1.4	2.44 cm 0.94	1.5 cm 1.1	2.6 cm 0.43 / 1.5	**1.86 cm** **0.86**
Electron beam energy	16.9 GeV	8.5 GeV	17.5 GeV	10 GeV	5.8 GeV	4 / 15 GeV	**12 GeV**
Linac type Linac length	NCRF S-band 1 km	NCRF C-band 0.4 km	SRF L-band 1.7 km	NCRF S-band 0.78 km	NCRF C-band 0.46 km	SRF / NCRF 0.4 / 1 km	**SRF L-band**
Gun type Cathode	NCRF S-band Cu photo	Pulsed DC CeB_6	NCRF L-band Cs_2Te photo	NCRF S-band Cu photo	NCRF S-band Cu photo	VHF / S-band Cs_2Te / Cu	**NCRF L-band**
RF pulse Rep. rate	<1 μs 120 Hz	<1 μs 30 Hz	600 μs 10 Hz	< 1 μs 60 Hz	< 1 μs 100 Hz	CW / <1 μs 930 kHz / 120 Hz	**750 μs** **10 Hz**
# pulses/RF	1-2	1-2	2,700	1-2	1-2	N/A / 1-2	**TBD**
Bunch charge	150 pC	30 pC	250 pC	100 pC	200 pC	20 / 130 pC	**100 pC**
Bunch length	43 fs	<10 fs	50 fs	43 fs	42 fs	20 / 33 fs	**33 fs**
Norm. slice emittance	0.4 μm	0.6 μm	0.6 μm	<0.5 μm	0.2 μm	0.14 / 0.48 μm	**0.2 μm**

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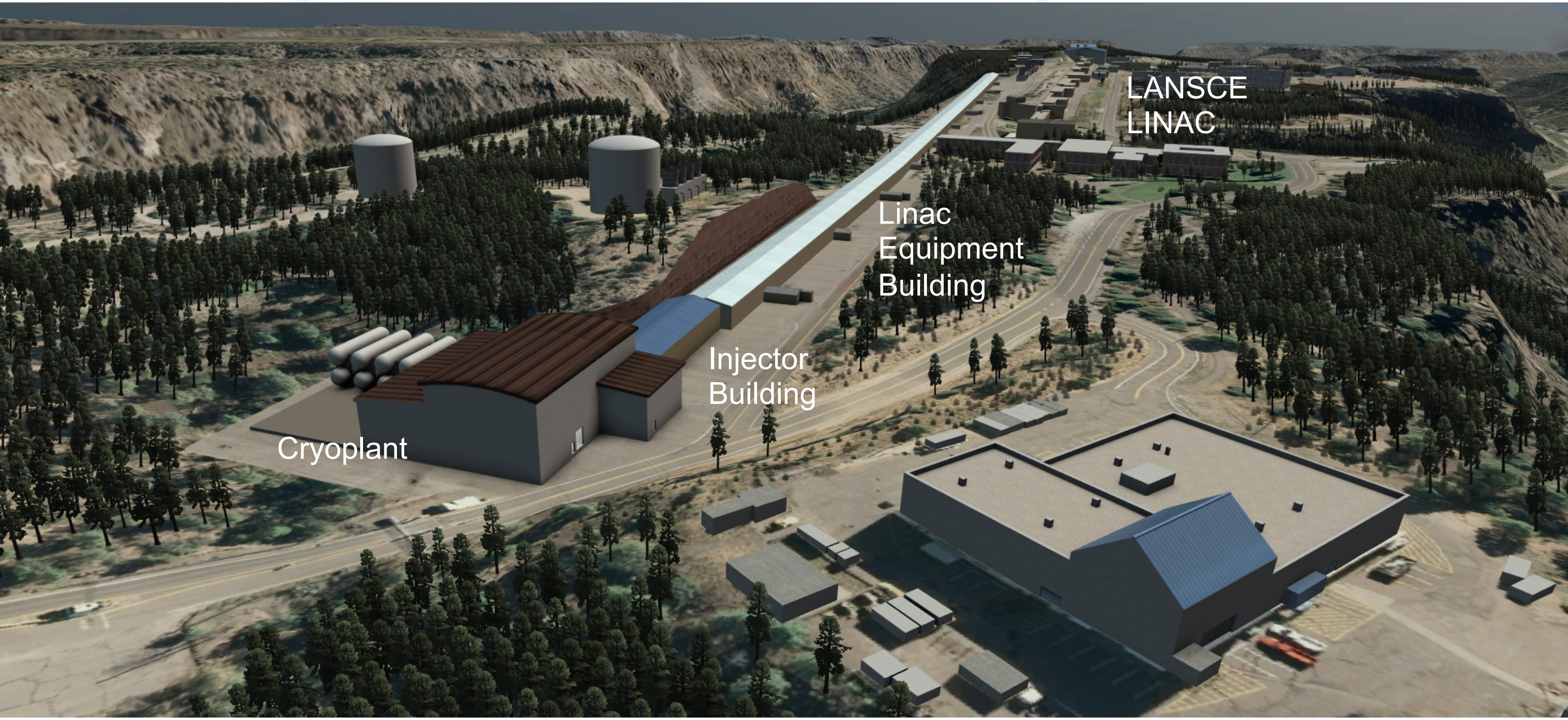
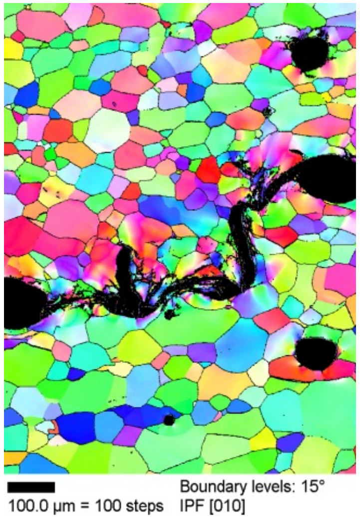
Artist Rendition of MaRIE Conventional Facilities

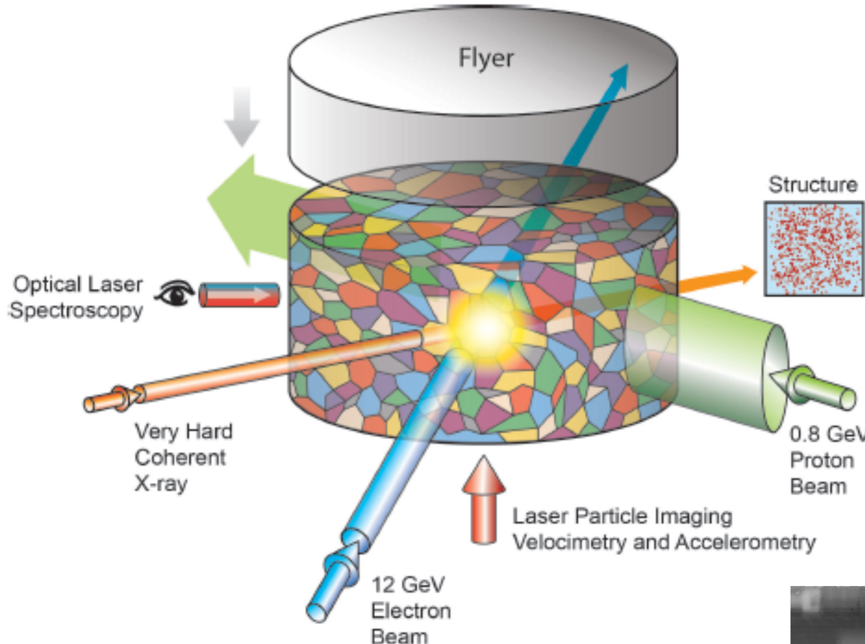


Challenging experiments are planned to observe the *dynamic microstructure* and *phase evolution* in materials down to the sub-granular level while connecting to the macroscale



The goal

Predict dynamic microstructure and damage evolution.



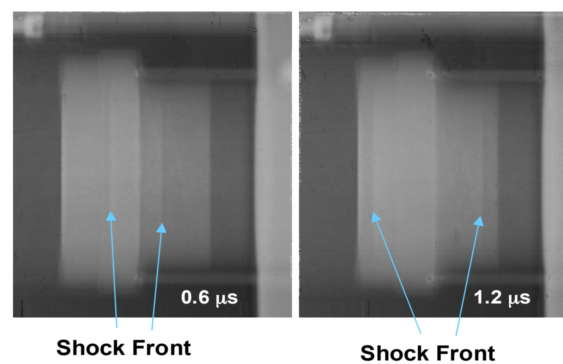
Requirements:
Sub-μm spacial resolution
100’s – 1000’s-μm samples
Sub-ns time resolution,
~30 frames in
1−10-μs duration

The model:

Accurate sub-grain models of microstructure evolution coupled to molecular dynamics.

The first experiment

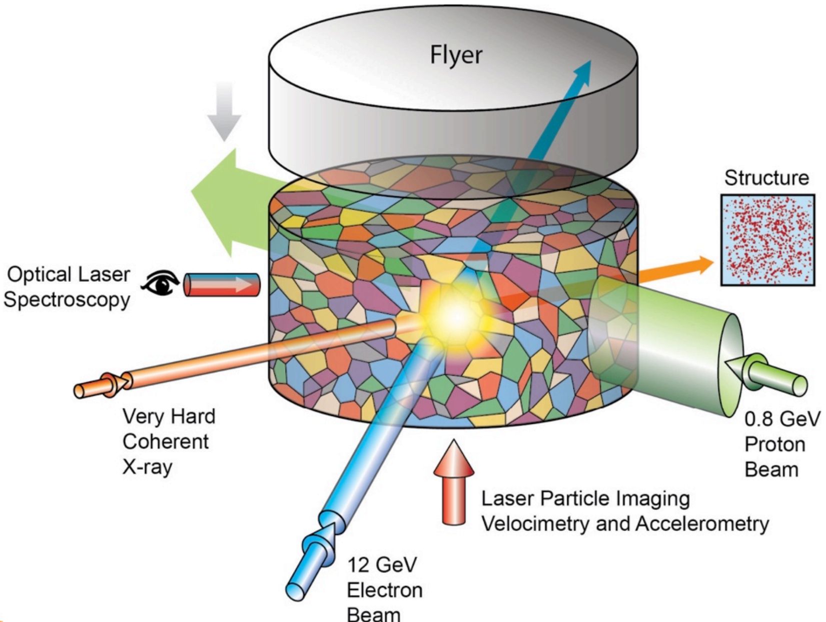
Multiple, simultaneous dynamic *in situ* diagnostics with resolution at the scale of nucleation sites (< 1 μm; ps – ns)



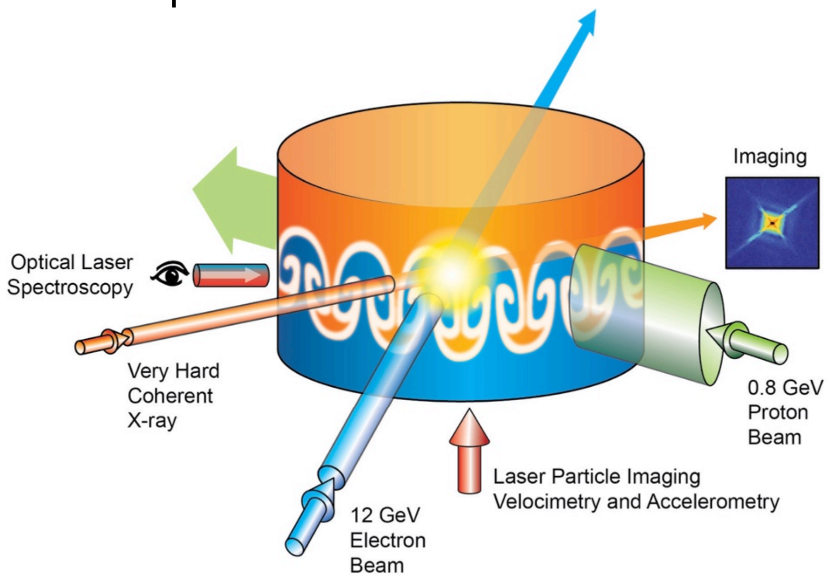
MaRIE will allow us to break apart the problem.

We are working to provide specific quantified examples of the need for multiple probes driven by the science

- **Phase response under failure (Bronkhorst)**
  - Broad field-of-view to determine shock location, rarefaction waves, gross grain motion
  - Narrow x-ray field-of-view to measure phase and grain plastic response



- **Ejecta evolution from Richtmyer-Meshkov jetting (Bolme)**
  - Broad field-of-view to determine bulk fluid motion and vorticity
  - Narrow x-ray field-of-view to scatter off ejecta and determine phase and structure evolution



Spatial and temporal resolutions for MaRIE mesoscale experiments are defined by analysis of the possible measurement techniques

	Metals Manufacture and Age aware performance	HE certification and qualification	Turbulent Materials Mixing	Welding and Additive Manufacturing
Spatial resolution	<100 nm - 20 µm	100 nm - 20 µm	500 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	up to 30	up to 30	up to 30	1000 per second
min pulse sep	< 300 psec	< 500 psec	30 nsec	10 nsec
macropulse length	10 µsec	100 µsec	15 µsec	1 msec
sample thickness	> 250 µm	> 10 µm – 6 cm	1 – 10 cm	0.1 to 10 mm
Repetition rate	<1 Hz	< 1 Hz	10 Hz	10 Hz
species	Be - Pu	Typically C, H, O, N	Noble gases, Ga, Be	Be - Pu

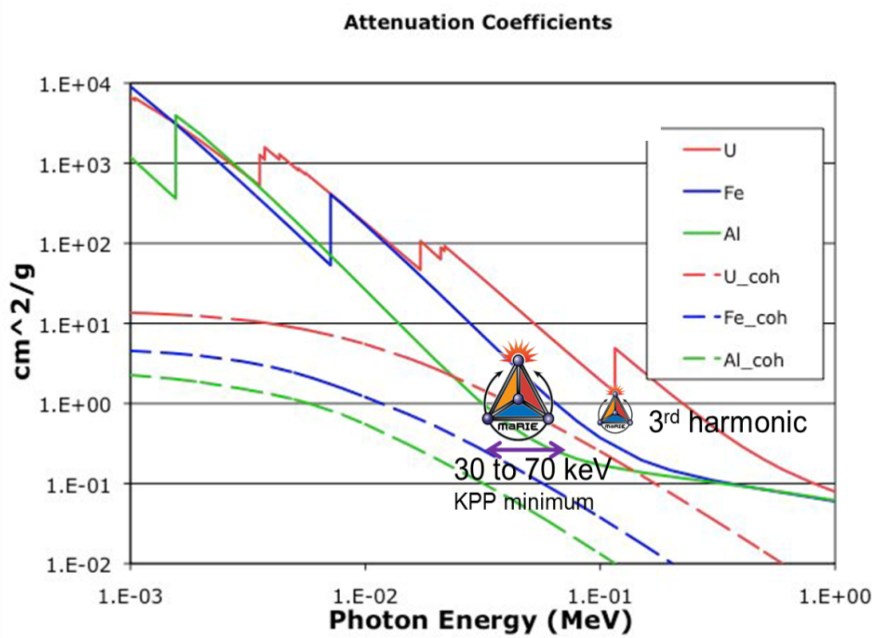
We believe that only a superconducting linac can cost effectively meet the long macropulse requirements driven by the SFRs

Possible probe beams each cover a different parameter range in time and space for sample interrogation

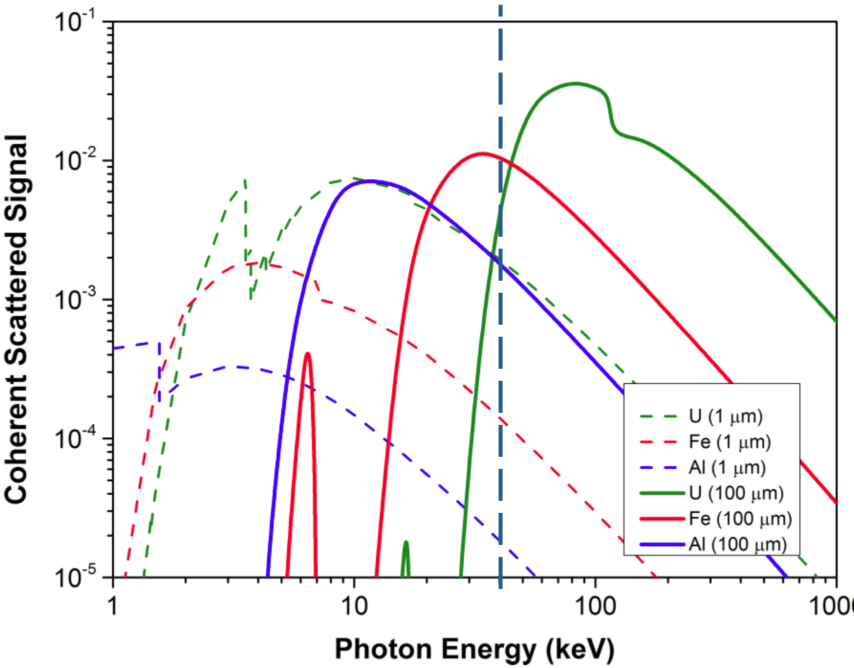
- XFEL has sub-ps pulse lengths, sub-ns pulse spacing, sub-micron resolution, but is limited in sample thickness at 42 keV to < 0.1 mm for high-Z materials
- eRad has ~10 ps pulse lengths, ~20 ns pulse spacing or pulse length, $\leq$1 μm resolution, penetrate $\leq$ 2 mm high-Z materials
- pRad has 50 ns pulse lengths, 100 ns pulse spacing, >10 μm resolution, penetrate >1 cm high-Z materials

	spatial resolution	Framing time	sample thickness# Z=13	sample thickness# Z=26	sample thickness# Z=92
prad*	> 20 μm	50 nsec	15 cm / 0.8 GeV	3 cm / 0.8 GeV	1 cm / 0.8 GeV
erad*	> 1 μm	> 25 nsec	6 cm / 12 GeV	5 mm / 12 GeV	1 mm / 12 GeV
X ray	> 0.1 μm	< 100 psec	>10 μm/ 8 keV 2 cm/ 42 keV	500 μm/42 KeV 4 mm/122 KeV	200 μm/42 KeV 2 mm/122 KeV

The 42-keV photon energy and flux are a trade-off between maximizing elastic scattering for diffraction, minimizing absorptive heating, and sample thickness



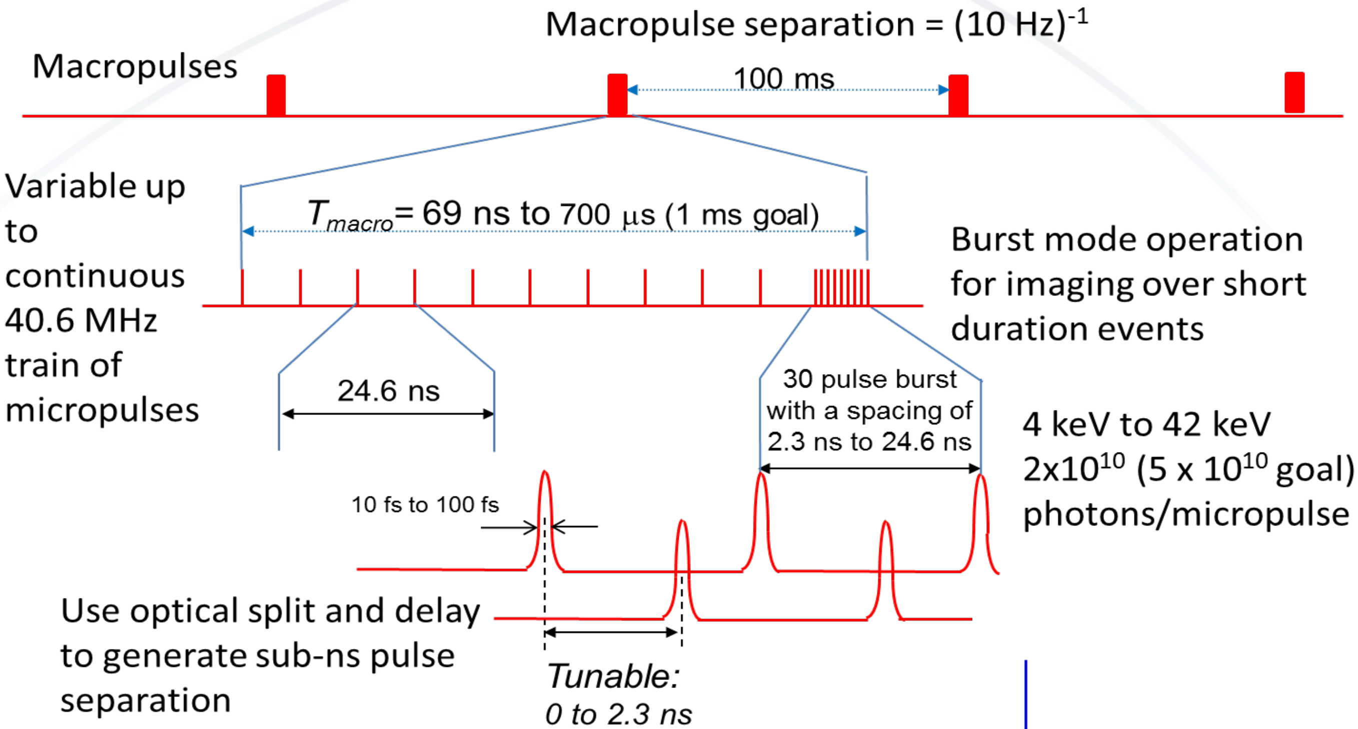
High resolution requires a minimum number of coherently scattered photons per sub-ps pulse. This sets the incident number of photons on a sample of ~2x10^{10}.

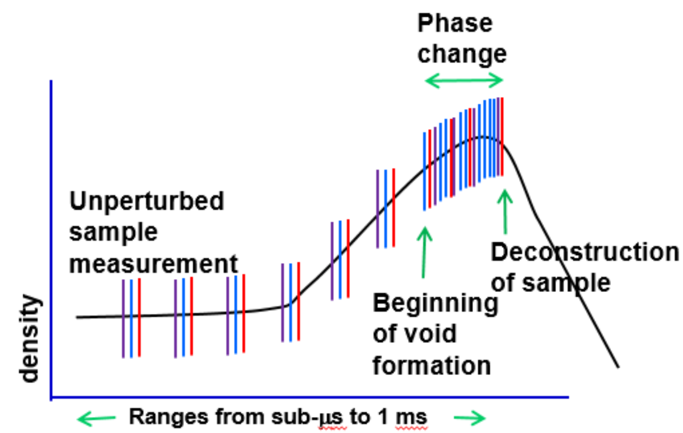


The fraction of incident photons coherently scattered just once, the coherent scattering signal, as a function of incident photon energy for various materials at thicknesses of 1 μm (dashed lines) and 100 μm (solid lines)

J. L. Barber *et al.,* Phys. Rev. B **89** (2014) 184105

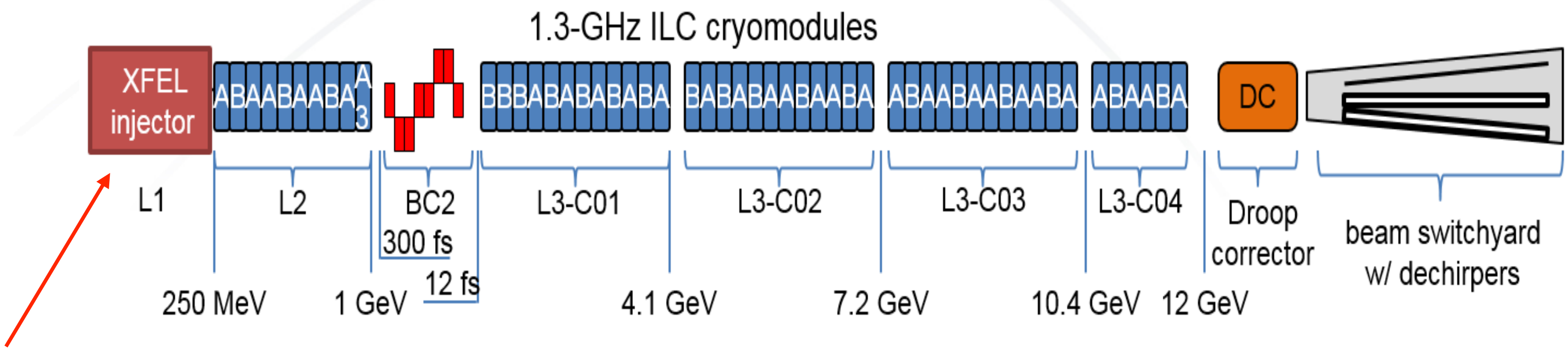
The MaRIE pulse format needs to be very flexible

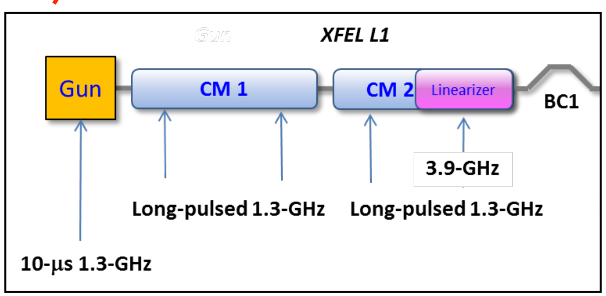




700-μsec macropulse requires a superconducting accelerator

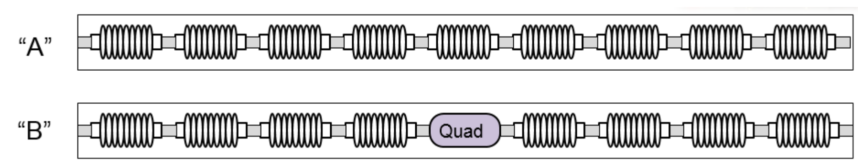
An XFEL pre-conceptual reference design that meets the MaRIE performance requirements has been developed as part of the CD-0 process





A — 9-cavity ILC cryomodule, “A”-type

B — 8-cavity ILC cryomodule, with quad / corrector / BPM, “B”-type



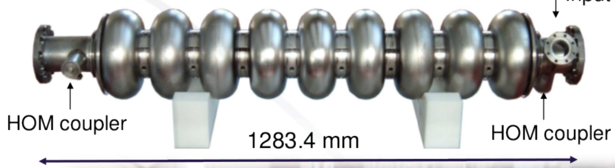
	1.3-GHz cavities	3.9-GHz cavities
L1 (X-FEL)	11	9
L1 (eRad)	11	9
L2	78	9
L3	360	0
Total	460	27

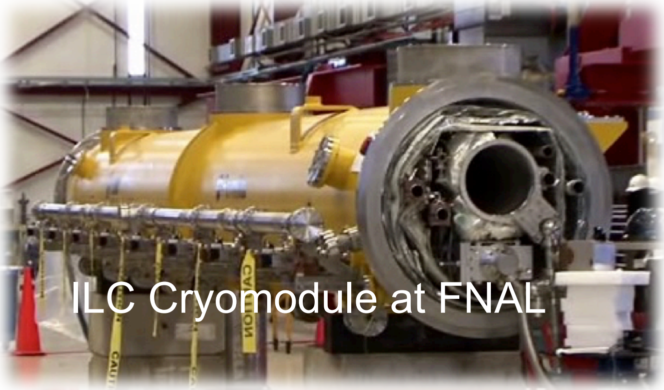
Performance Parameters derived from the measurements quantify the accelerator/XFEL requirements

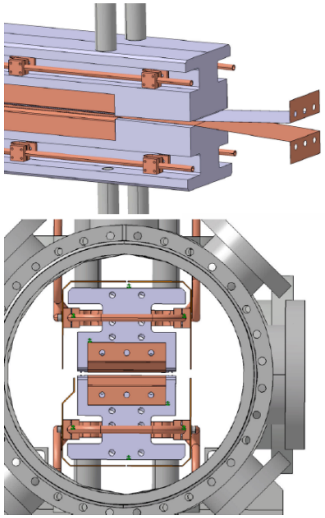
Electron Beam Requirements				Photon Requirements	
Energy	12 GeV	# of bunches per macropulse	10 to 100	Energy	4 to 42 KeV
Linac fundamental frequency	1.3 GHz	RMS slice energy spread	$\leq$ 0.015%	# per bunch	$5x10^{10}$
Linac type	Superconducting	Macropulse to macropulse energy variation	$\leq$ 0.02%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

MaRIE pre-conceptual reference design is based on current technology.

- Accelerating cavities and cryomodules based on 1.3-GHz ILC and DESY XFEL designs
- FLASH 3.9-GHz cryomodules to linearize the beam phase space
- Undulator design based on SwissFEL U15



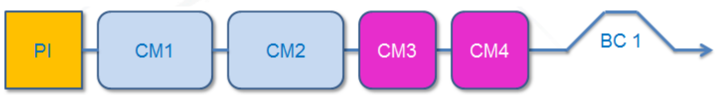




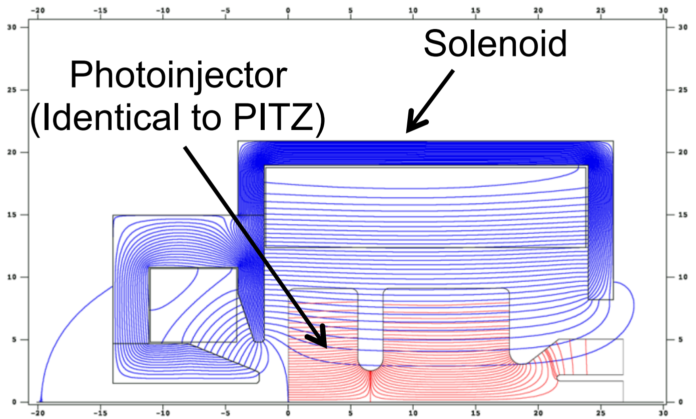
Courtesy of T. Schmidt

	Symbol	Value
Undulator period	λ_u	18.6 mm
Undulator magnetic field	B_0	0.7 T
rms (peak) undulator parameter	K_{rms} (K_{peak})	0.86 (1.22)
FEL resonance wavelength	λ_0	0.2934 Å
FEL (Pierce) parameter	ρ	0.0005
Calculated 3D gain length	L_G	2.6 m
Calculated 3D saturated power	P_S	9 GW
FEL pulse energy at saturation	W_p	0.3 mJ

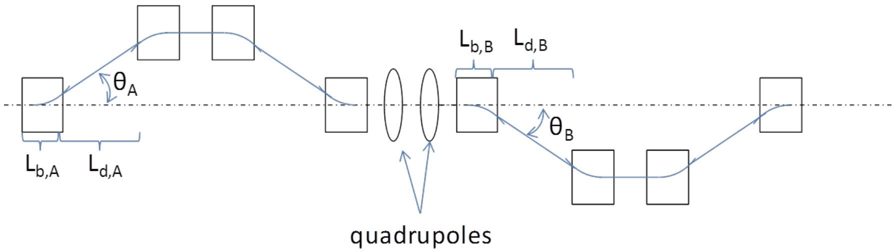
The MaRIE XFEL injector pre-conceptual design incorporates several innovations to meet performance requirements.



- **Photoinjector (PI)**
  - 1.3-GHz, normal conducting.
  - Long pulse (100 μs) operation, 60 MV/m gradient at cathode.
- **Cryomodules 1 & 2 (CM1 & CM2)**
  - 1.3-GHz superconducting.
  - Capture beam from PI, accelerate and introduce energy slew for BC1.
- **Cryomodules 3 & 4 (CM3 & CM4)**
  - 3.9-GHz superconducting.
  - Linearize beam energy slew for BC1.
- **Bunch compressor 1 (BC1)**
  - ~ 20x compression at ~ 250 MeV.



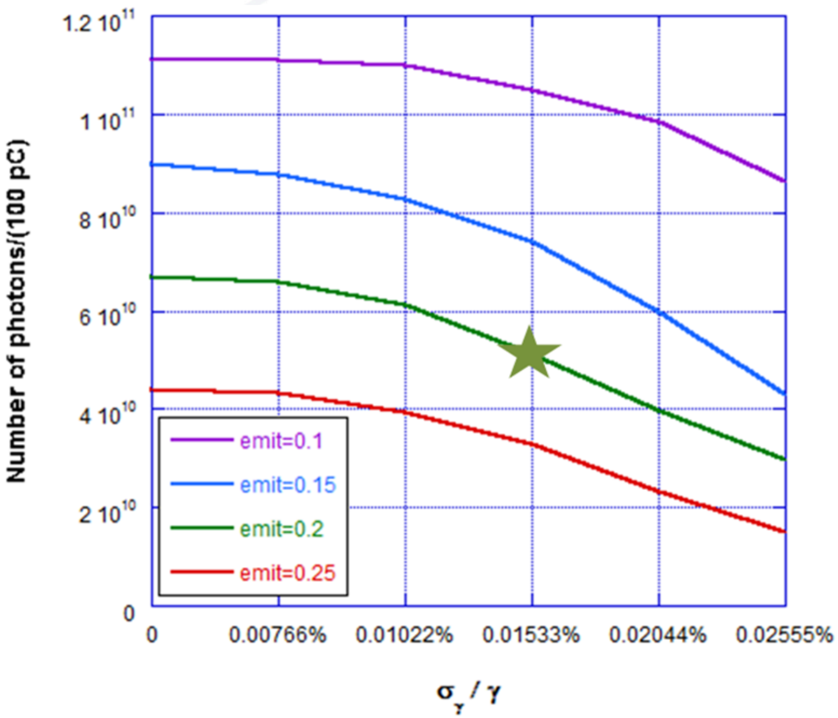
The MaRIE photoinjector design is based on the PITZ photoinjector with a modified solenoid configuration.

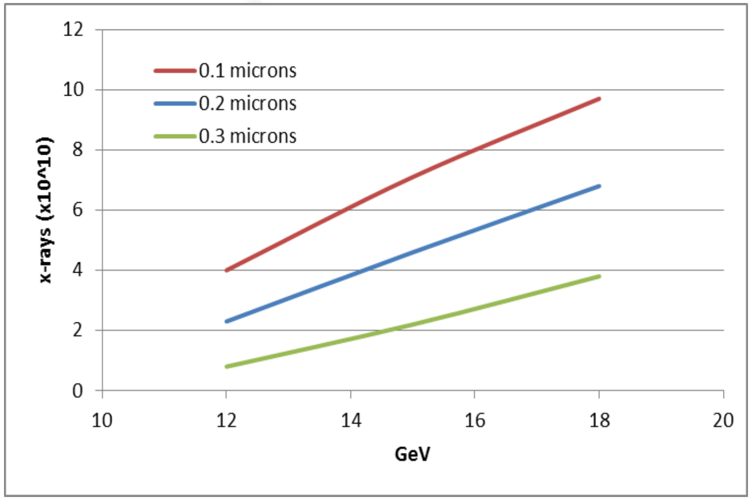


Double reversed-chicane helps reduce time-dependent dispersion from CSR wake.

Pre-conceptual design assumes 100 pC because we need a small emittance and small energy spread

Time-Independent GENESIS Simulation Results





We can gain photons by going to higher electron beam energy

Beam parameters: **100 pC, 30 fsec, 3.4 kA**
0.015% energy spread
0.20 μm emittance

Photon requirements: 5×10^{10} 42-keV photons
0.02% bandwidth

We have 150-m tunnel contingency to go to 15 GeV in the future; worth ~2x photons.

Significant technical challenges remain to meet the MaRIE performance goals.

- **Microbunch Instability** – dominant challenge; made harder because of our tight energy-spread limit; suppression ideas include laser heater to pre-compress bunch, use residual dispersion (LBNL), “microbunch” the beam and eliminate BC2 (e-SASE)
- **CSR** – novel bunch compressor design; propose demo at BNL
- **Wakefields** – important for MaRIE XFEL, not as important for other XFELs; long-range wakefields may limit the bunch spacing due to poor compressor or induced energy spread; propose measurement at FNAL
- **Emittance** – we need the brightest electron injector ever; plans for injector test facility at LANL
- **Distributed Seeding** – new concept; propose demo at SLAC
- **Droop Corrector** – short Cu linac (3 m) to compensate during shortest macropulse lengths; needed due to variable pulse format
- **Dechirper** – old concept; relatively low risk; propose demo at BNL

In summary, MaRIE will be a revolutionary capability:

- The brilliance of an XFEL
- Transformative imaging techniques with coherence – "ordered light for disordered systems"
- ★ Designed for time-dependence from electronic motion (picosecond) through sound waves (nanosecond) through shock transit across samples (microseconds) through thermal diffusion (millisecond) to manufacturing (seconds and above)
- ★ High-energy to not destroy mesoscale samples with that brilliance and give that time-dependence (and perhaps provide larger reciprocal space resolution)
- ★ Not just x-ray facility, but designed for multiple simultaneous probes
- Designed with strong connection to the needs of scientific predictive capability from theory, modeling, and computation
- Providing comprehensive materials discovery capability to collaborative teams
- Enabling science-based qualification and certification, leading to the "revolution in manufacturing science"

MaRIE Status

- Project presently in the pre-conceptual planning phase
- We have a pre-conceptual accelerator/XFEL reference design
- Cost & Schedule estimate is based largely on current technology
- Following US Dept. of Energy, National Nuclear Security Agency (NNSA) guidance regarding submission of a large construction project
- Following DOE Order 413.3B requirements and process
- Beginning to initiate discussions with potential partner labs.

Acknowledgements

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