Looking Beyond LANSCE – the MaRIE facility

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Outline

• Science perspective – Grand challenge of materials and extreme matter research

• Required capabilities – experimental tools with unprecedented capabilities together with modeling and simulation

• Present and future capabilities at LANSCE and MaRIE

• Conclusions
Science perspective - Materials by design using “prediction and control” is the overarching grand challenge of materials research

THE GOALS:

Achieve Transformational Materials Performance
-Solutions require unprecedented control of defects and interfaces

Through Predictive Multi-scale Understanding
-Perform experiments with unprecedented spectral, temporal, and spatial resolution in previously un-accessed extremes

Experimental tools with unprecedented capabilities, together with modeling and simulation, are essential
Experimental tools with unprecedented capabilities are needed to validate and test the limits of modeling and simulation.

Anticipated advances in petaflop/s and exaflop/s computing – with advanced models - put us on the verge of accessing new phenomena on the micron scale.

Constitutive models
“continuum dynamics"
Finite element

Our future focus at Los Alamos

Click the picture above if a movie does not automatically play.
Why the “micron frontier”?

- ~1 µm scale (and time scale ~sound transit) represents an experimental and theoretical frontier, where discovery science and predictive validation meet.

- Future research capabilities must allow one to bridge the atomic scale/molecular dynamics studies and continuum models/integrated tests.
  - Defect consequences and microstructure interactions that drive materials strength and damage evolution.
  - Translation of unit-scale emergent functionality to device realization/interface phenomena.

One must unravel micron-scale interactions, bridging the regime between imaging and scattering – will require multiple, co-located probes.
Example: Non-ideal material response to dynamic compression or shocking

Ideal response:

- Knowing the thermodynamic properties of the material \((p_0, p_0)\) and the pressure behind the shock \((p_1)\) or the shock velocity \((u)\) defines the system state (Hugoniot curve)

Non-ideal response:

- Local nucleation and kinetics of defect structures can cause structural changes & transformations (melting, phase changes (cubic crystal to hexagonal polycrystal), cracks, and failure) resulting in material thermodynamics and EOS changes.
Proton microscopy (radiography) at LANSCE is presently an important and unique probe for measuring density in extreme dynamic systems.
Spatial, Density and Temporal Resolution of pRad at LANSCE

**Temporal Resolution**

- Camera 1 - Camera 2 - Camera 3 - Camera 4 - Camera 5 - Camera 6 - Camera 7

**Proton Flux**

- Time

**Spatial Resolution**

- 65 µm RMS with Gaussian point spread function

**Density Resolution**

\[ T = e^{-\frac{y}{\lambda}} \left( 1 - e^{-\frac{\left( \frac{\theta_p \beta}{14.1 \text{MeV}} \right)^2 X_0}{2x}} \right) \]

- 39 Radiographs per dynamic event
- 1-5% Areal Density reconstruction
Examples of present proton radiographic capabilities

**Fundamental hydrodynamics – Richmeyer-Meshkov instability**

[Image of a radiographic image with the note: Click the picture if a movie does not automatically play]
Proton radiography capabilities: EOS in dynamic materials by measuring accurate absolute density and velocity of shocks

Using $P(u_p)$ for 6061-T6 Al and jump conditions

$$\rho = \frac{\rho_0 P}{P - \rho_0 u_P^2} \quad \Rightarrow \quad \rho = 3.067 \pm 0.009 \text{ g/cm}^3 \quad (0.3\%)$$

$pRad$ absolute Density.

$$\rho = 3.07 \pm 0.03 \text{ g/cm}^3 \quad (1.1\%)$$

LASL Shock Hugoniot Data
Empirical fit
Radiographic velocity measurements
Pin velocity and radiographic density
Dynamic Materials: What can we do today at LANSCE in dynamic materials?

These studies provide excellent data at continuum scale, but don’t address causes at microstructure scale; much more is needed to develop a predictive capability!
The frontiers of extreme matter research define the future requirements for facilities, diagnostics, and probes.

**Frontier Experiments**

- **Compression Dynamics**
- **Structural Materials in Dynamic Extremes**
- **Control of Complex Materials and Chemical Processes**
- **Turbulent flows**
- **Warm Dense Matter**

**Drive Functional Requirements**

- Defect and Dislocation Dynamics; Dynamic performance of bulk material
- In-situ density, volume, macrostructure and cracks, coalescence, nucleation
- Ultrafast pump-probe; swept spectroscopy; nano-imaging
- Flow characteristics, spatial correlations
- EOS

**Which Lead to Technical Approaches**

- **Proton microscopy**: high-energy transient x-ray diffraction
- Next generation temporal control for x-rays; optical ultra-fast lasers
- High-contrast proton microscopy; phase contrast imaging
- High-intensity ultra-fast laser systems, proton microscopy

- High-energy coherent x-ray imaging; dynamic charged particle microscopy; variable strain-rate drive; multiple surface diagnostics
Our current working vision for a facility to study dynamic materials involves combining proton microscopy and coherent light sources with generating extreme environments

- High-energy (> 50 keV) photon source (for multigranular sample penetration) with high intensity (to resolve transient effects) and high repetition rate (quantitative imaging of dynamic processes)
  - XFEL light source (low duty cycle to reduce cost) – UHI Laser driven system a possible advanced alternate.
  - Can provide 3-dimensional dynamic structure information
- Proton microscopy to provide simultaneous measurements to constrain information at many scales
  - > 1GeV, with higher current (better time resolution) and high-resolution magnetic optics (for better spatial resolution)
  - Developing PRIOR collaboration for high-resolution proton microscopy is an important first step.

- Flexibility in creating material environments (pressure, strain, temperature, …)
  - Robust suite of dynamic loading and material heating techniques
- Couple probes with in-situ irradiation and controlled synthesis
  - ultra-fast/ultra-short in-situ microscopies
  - initial synthesis and post-mortem characterization

Simultaneous diffraction & dynamic density imaging
MaRIE is being designed to provide an important international user resources to solve important extreme matter challenges.

The Fission and Fusion Materials Facility will create extreme radiation fluxes. Unique in-situ diagnostics and irradiation environments beyond best planned facilities.

The Multi-probe Diagnostic Hall will provide unprecedented probes of extreme matter. X-ray scattering capability at high energy and high repetition frequency with simultaneous proton dynamic imaging.

The M4 Facility dedicated to making, measuring, and modeling materials will translate discovery to solution. Comprehensive, integrated resource for materials synthesis and control.

MaRIE will provide unprecedented international user resources.
The present MaRIE preferred alternative incorporates a new XFEL and a LANSCE proton beam power upgrade.
Conclusions

- "Bridging the micron gap" is essential for solving transformational materials grand challenges.
- MaRIE will provide unique capabilities:
  - Accessing materials irradiation/damage extremes
  - Simultaneous in situ imaging and scattering measurements
  - Incubating materials discovery and solutions through control of defects and interfaces

MaRIE is being designed to have unique co-located tools necessary to realize transformational advances in materials performance in extremes.