

Looking Beyond LANSCE – the MaRIE facility

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May 3, 2010**

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

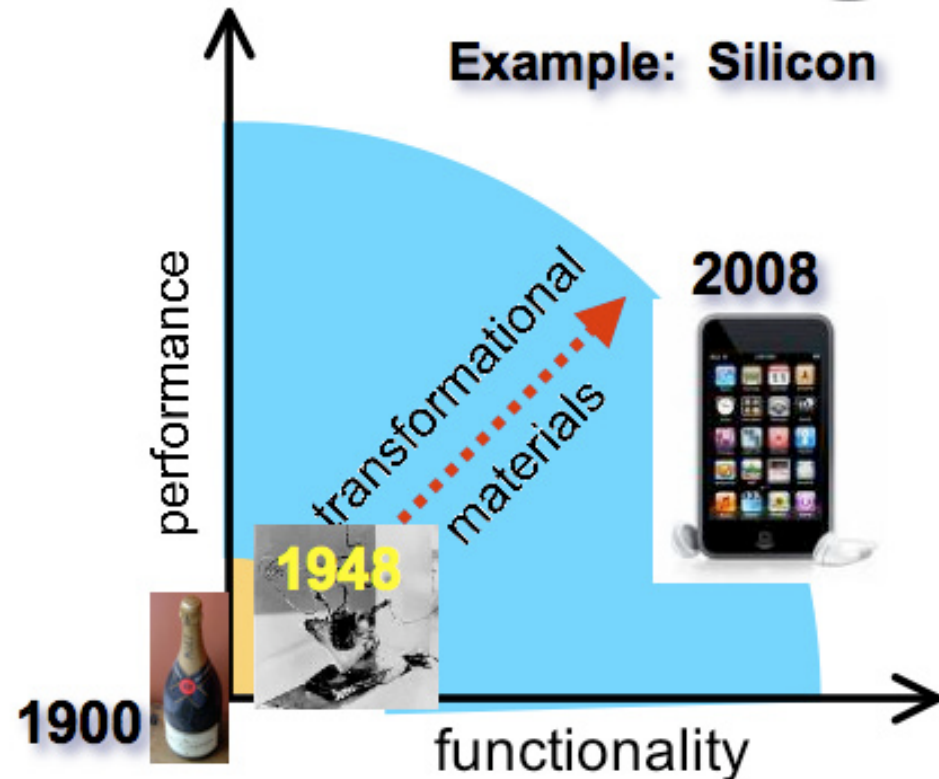
THE GOALS:

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

Macro-Mech
m



Polycrystal
mm



Single Crystal
 ∞ m

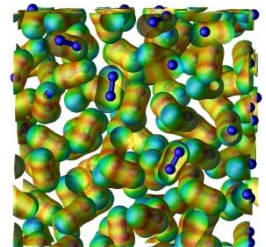
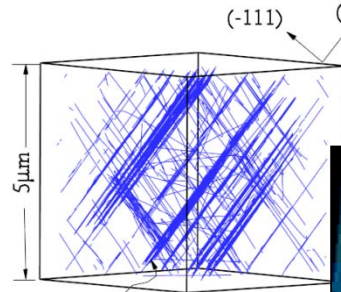
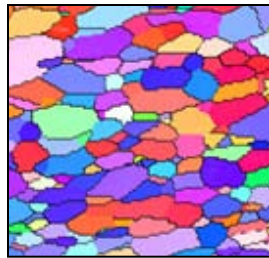
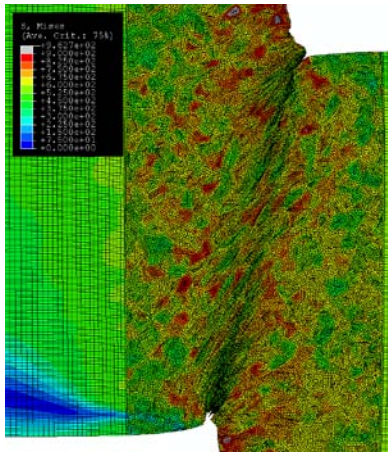


Molecular
Dynamics
nm



Quantum
Mechanics

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

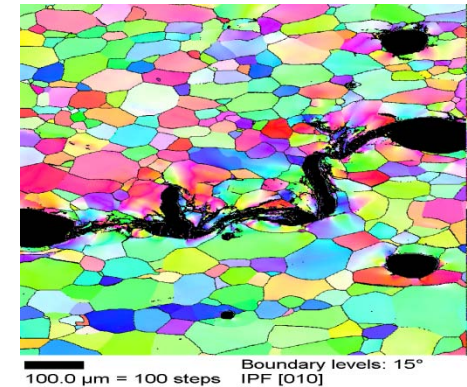


**Our future focus
at Los Alamos**

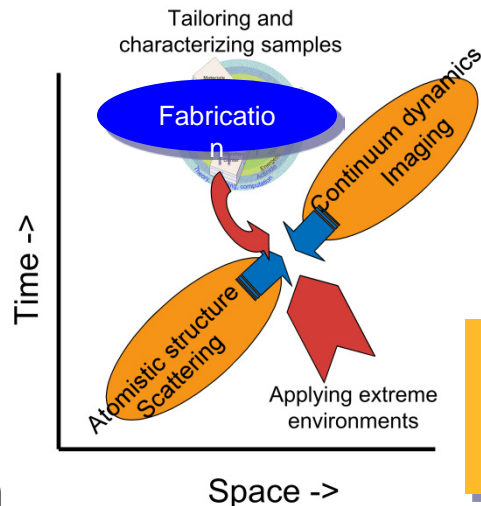
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Why the “micron frontier”?

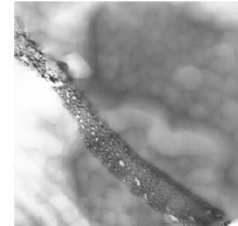
- ~ 1 μm scale (and time scale ~sound transit) represents an experimental *and* theoretical frontier, where discovery science and predictive validation meet
- Future research capabilities must allow one to bridge the atomic scale/molecular dynamics studies and continuum models/integrated tests.
 - *Defect consequences and microstructure interactions that drive materials strength and damage evolution*
 - *Translation of unit-scale emergent functionality to device realization/interface phenomena*



Shock propagation in nonhomogenous media



He bubbles on grain boundaries can cause severe embrittlement at high temperatures



One must unravel micron-scale interactions, bridging the regime between imaging and scattering – will require multiple, co-located probes

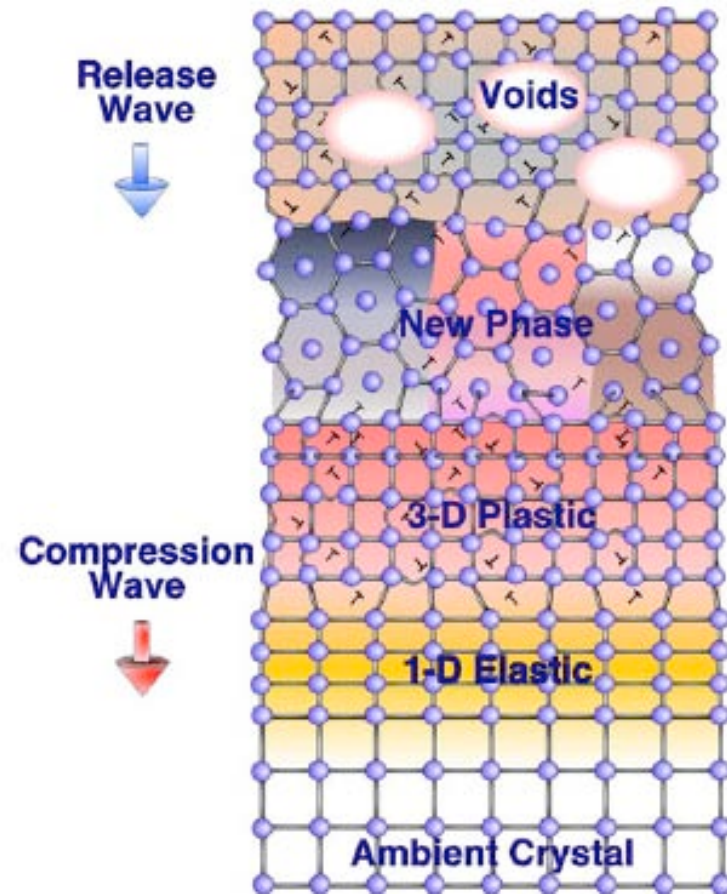
Example: Non-ideal material response to dynamic compression or shocking

Ideal response:

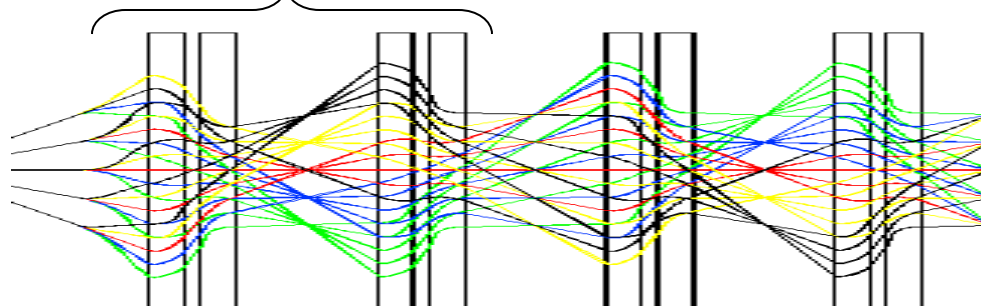
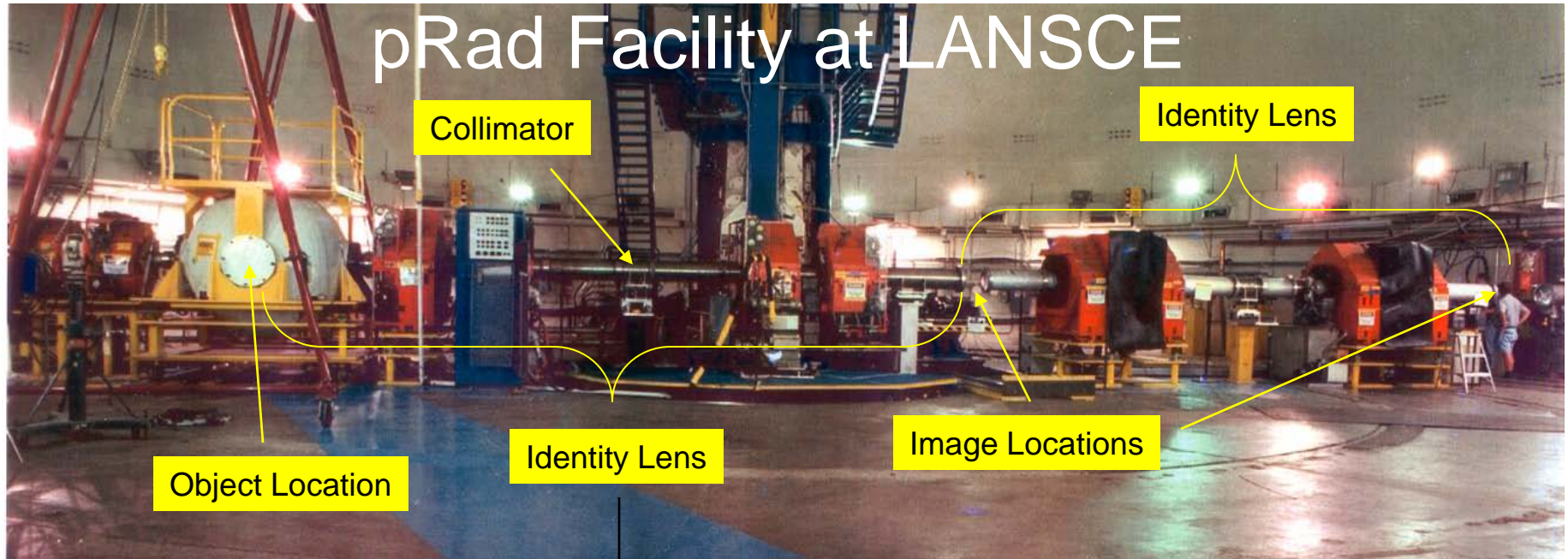
- Knowing the thermodynamic properties of the material (p_0, ρ_0) and the pressure behind the shock (p_1) or the shock velocity (u) defines the system state (Hugoniot curve)

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.

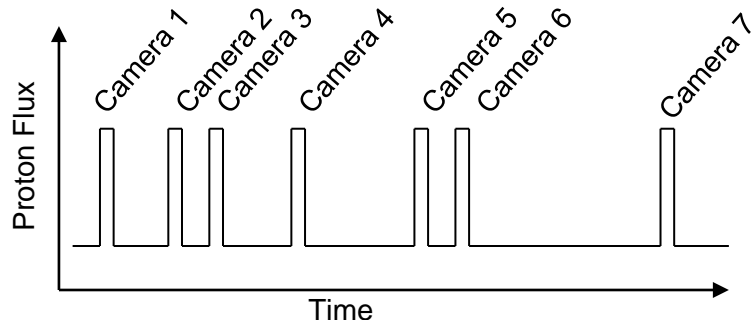


Proton microscopy (radiography) at LANSCE is presently an important and unique probe for measuring density in extreme dynamic systems

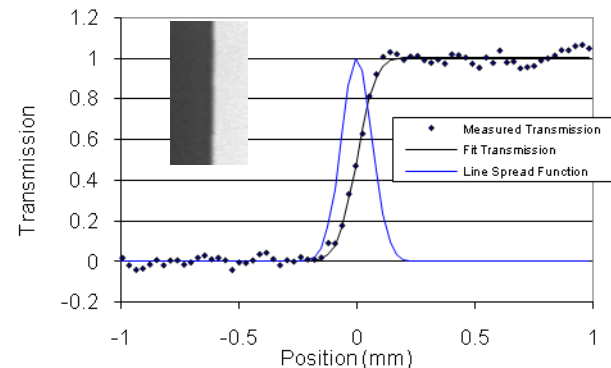


Spatial, Density and Temporal Resolution of pRad at LANSCE

Temporal Resolution



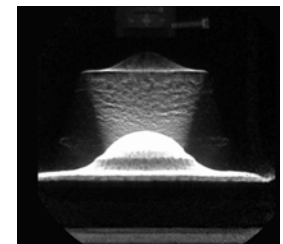
Spatial Resolution



65 μm RMS with Gaussian point spread function

Density Resolution

$$T = e^{-x/\lambda} \left(1 - e^{-\left(\frac{\theta_c p \beta}{14.1 \text{ MeV}} \right)^2 \frac{x_o}{2x}} \right)$$



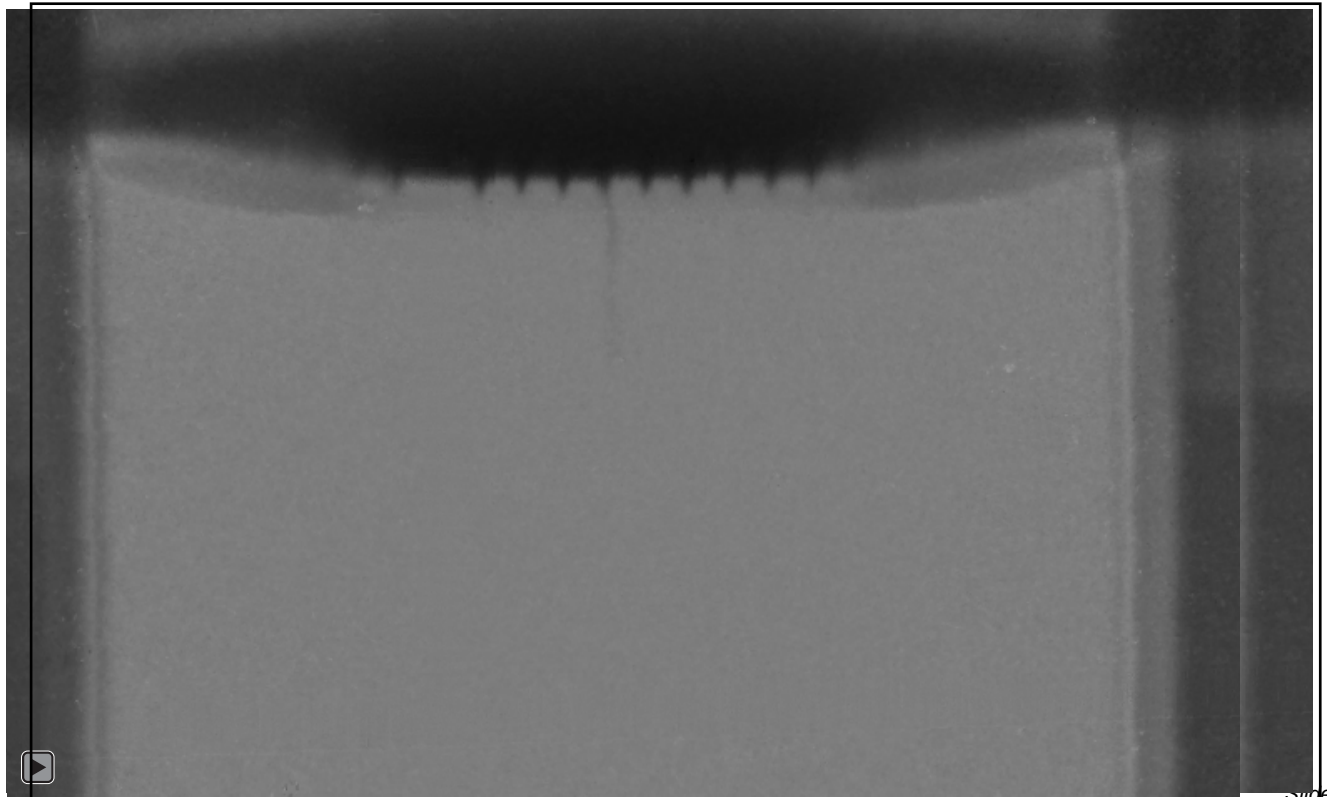
1-5% Areal Density reconstruction

39 Radiographs per dynamic event

Examples of present proton radiographic capabilities

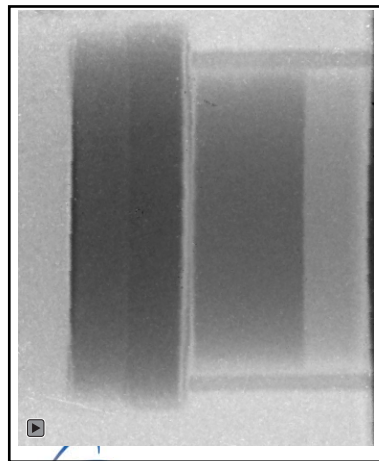
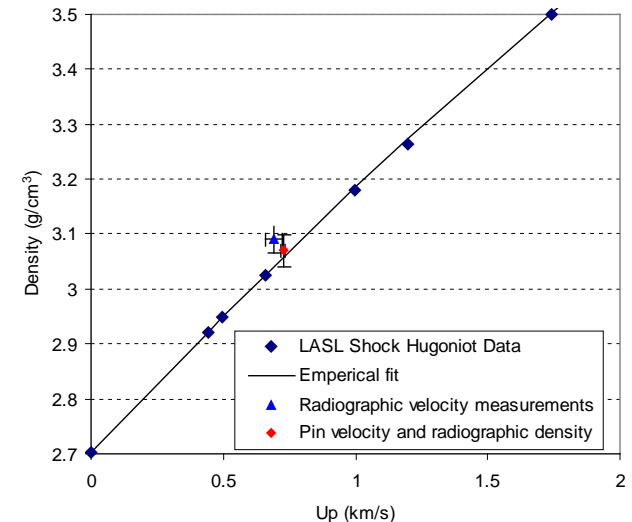
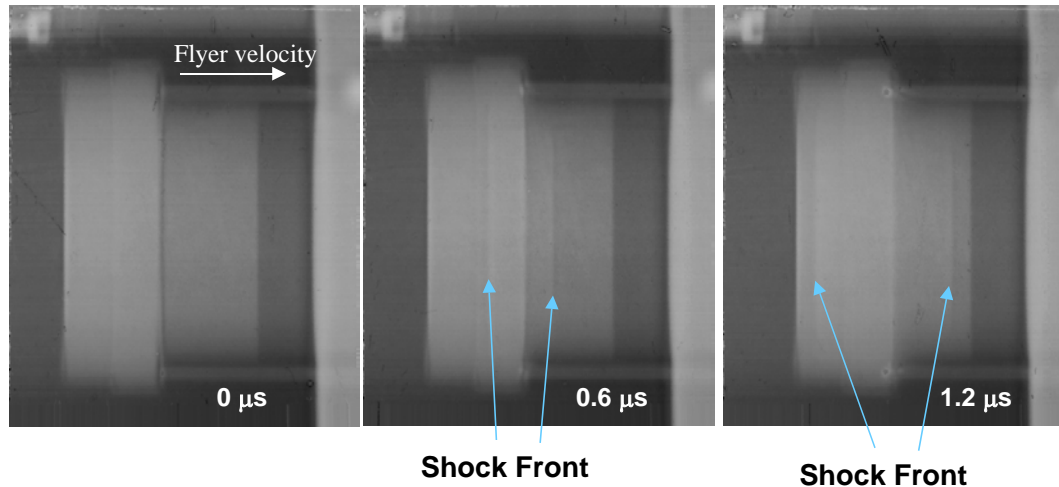
Fundamental hydrodynamics – Richmeyer-Meshkov instability

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automatically play*



Slide 9

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

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

pRad absolute Density.
 $\rho = 3.07 \pm 0.03 \text{ g/cm}^3 \text{ (1.1\%)}$

PHYSICAL REVIEW B 77, 220101(R) (2008)

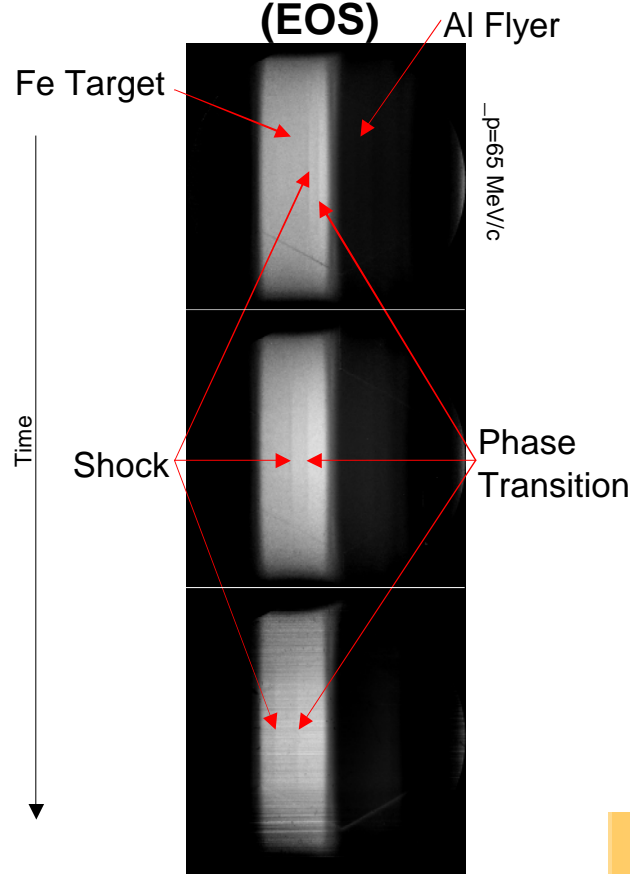


Proton radiography and accurate density measurements: A window into shock wave processes

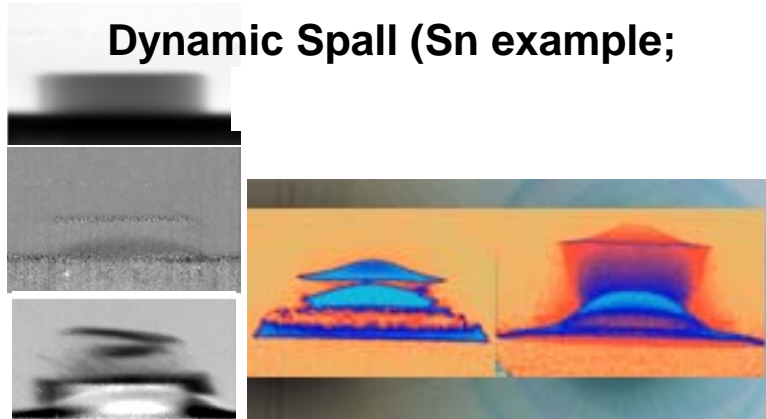
P. A. Rigg,* C. L. Schwartz, R. S. Hixson, G. E. Hogan, K. K. Kwiatkowski, F. G. Mariani, M. Marr-Lyon, F. E. Merrill, C. L. Morris, P. Rightly, A. Saunders, and D. Tupa
 Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
 (Received 4 February 2008; published 5 June 2008)

Dynamic Materials: What can we do today at LANSCE in dynamic materials?

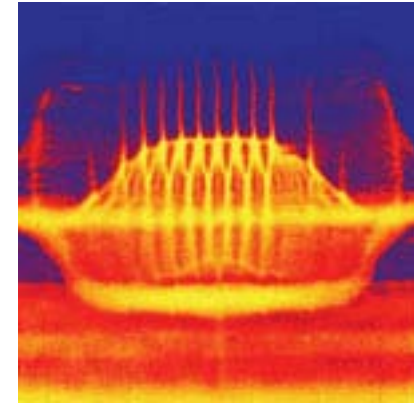
Internal Phase Transition (EOS)



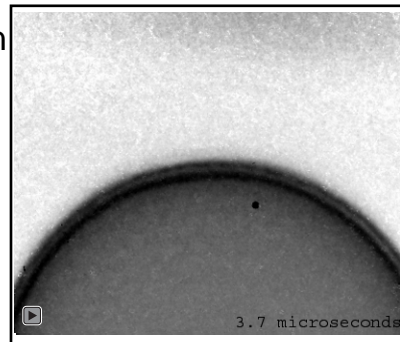
Dynamic Spall (Sn example;



Hydro Instability

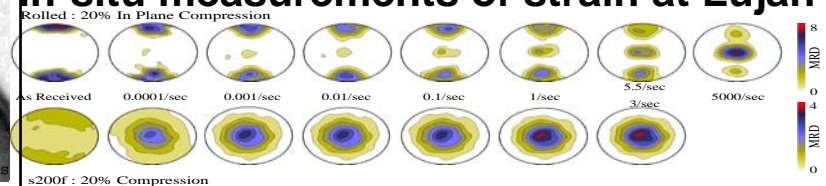


Dynamic Material Failure



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a movie does not play
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In-situ measurements of strain at Lujan



***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

High-energy coherent x-ray imaging; **dynamic charged particle microscopy**; variable strain-rate drive; multiple surface diagnostics

Proton microscopy; high-energy transient x-ray diffraction

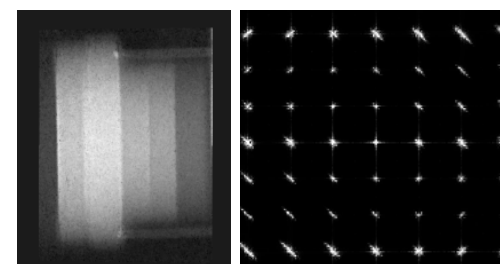
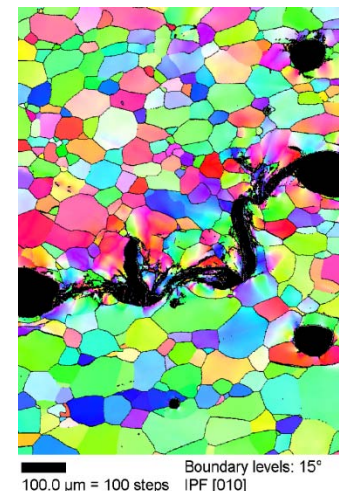
Next generation temporal control for x-rays; optical ultra-fast lasers

High-contrast proton microscopy; phase contrast imaging

High-intensity ultra-fast laser systems, **proton microscopy**

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

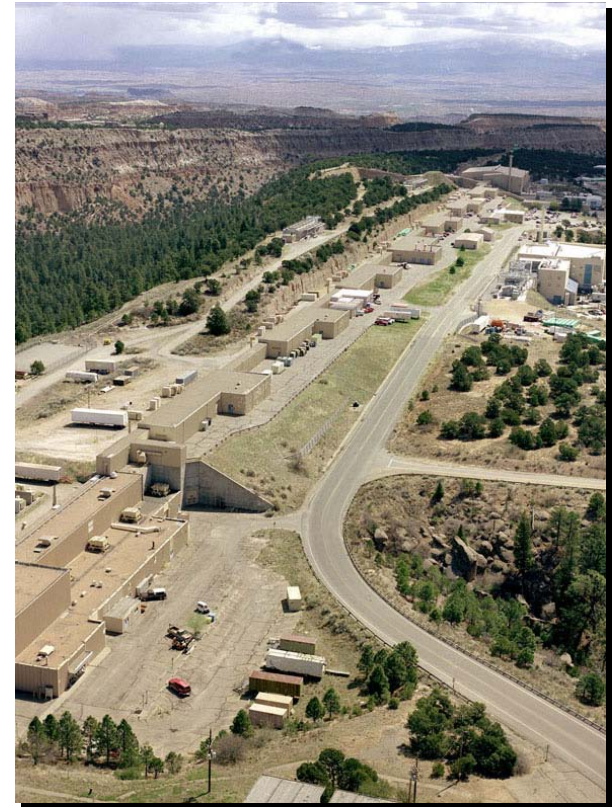
Unique in-situ diagnostics and irradiation environments beyond best planned facilities

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





Conclusions

The transition from “observation & validation” to “prediction & control” is a central mission challenge AND the frontier of materials research

- **“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

