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Title:	MaRIE: An Experimental Facility Concept Revolutionizing Materials in Extremes
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MaRIE:

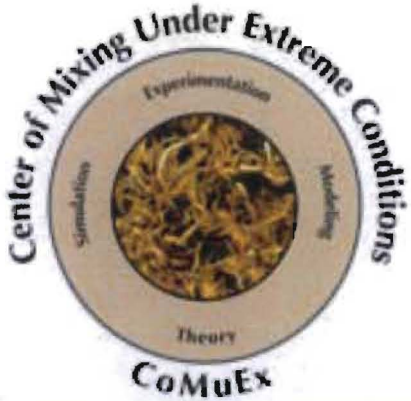
(**Ma**tter-**R**adiation **I**nteractions in **E**xtremes)

An Experimental Facility Concept Revolutionizing Materials in Extremes

An introduction presented at

"Research Needs for Material Mixing in Extremes"

Cris W. Barnes, Physics Deputy Division Leader
Los Alamos National Laboratory



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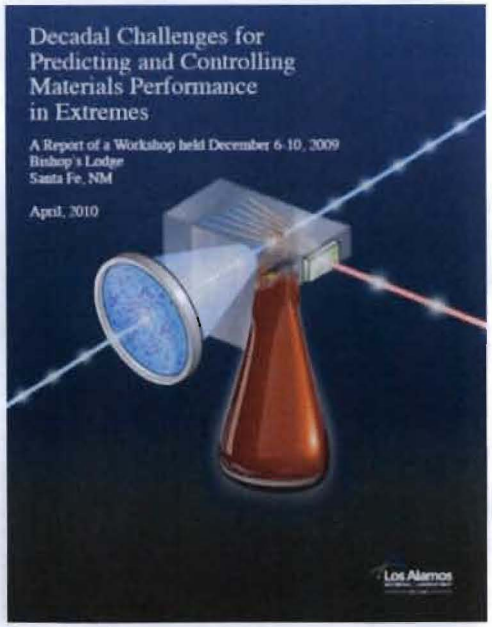
ABSTRACT

- The Matter-Radiation Interactions in Extremes (MaRIE) project intends to create an experimental facility that will revolutionize the control of materials in extremes. That control extends to extreme regimes where solid material has failed and begins to flow – the regimes of fluid dynamics and turbulent mixing. This presentation introduces the MaRIE facility concept, demonstrates examples of the science case that determine its functional requirements, and kicks-off the discussion of the decadal scientific challenges of mixing in extremes, including those MaRIE might address.

Materials research is on the brink of a new era – moving from observation to control of properties

- **Improved experimental capabilities are providing insights into these complex problems (e.g. 4th generation light sources, nanoscale synthesis and characterization, …)**
- **Simulation capabilities are providing remarkable insights at length and time scales previously inaccessible**



New capabilities will be needed to realize this vision:

In situ, dynamic measurements

simultaneous scattering & imaging

of well-controlled and characterized materials

advanced synthesis and characterization

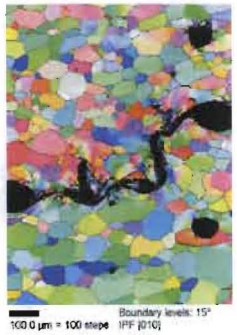
in extreme environments

dynamic loading, irradiation

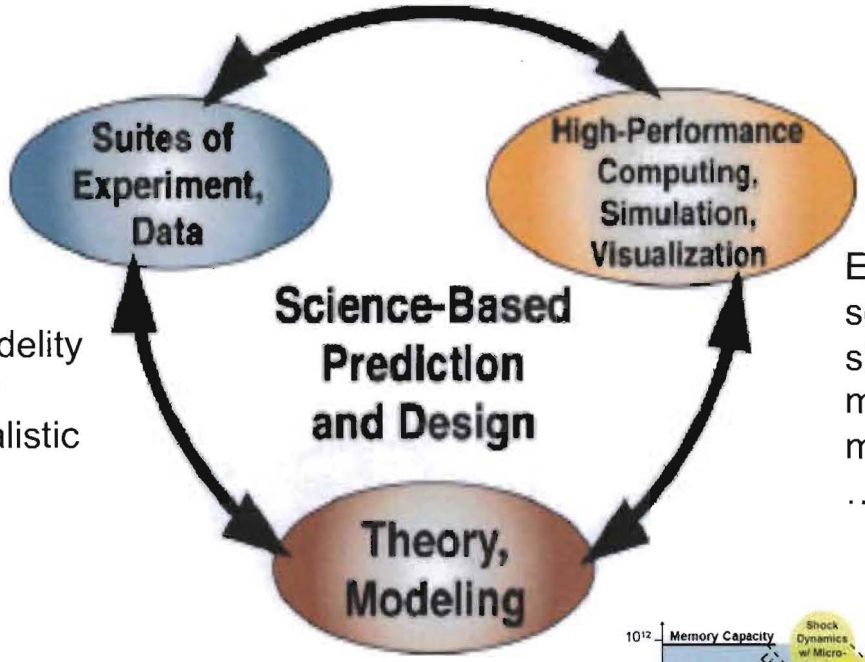
coupled with predictive modeling and simulation

materials design & discovery

Next generation simulation capabilities and experimental tools will enable discovery science at the micron frontier

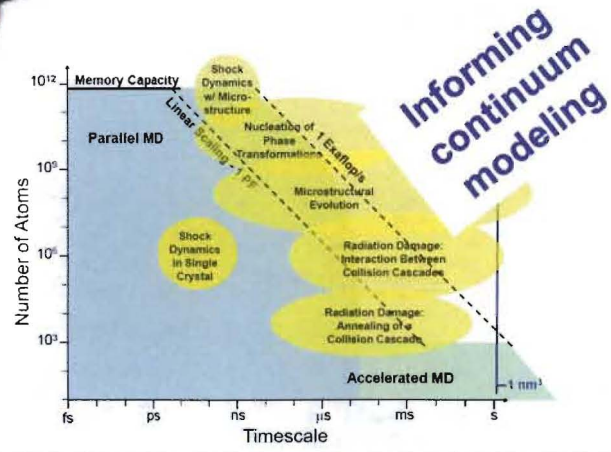


Nanoscale fabrication, high fidelity characterization, novel *in situ* diagnostics, generation of realistic extreme environments, …



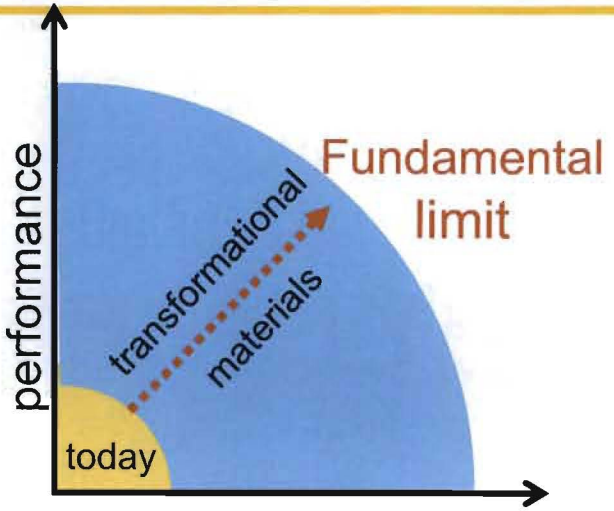
Exascale computing, multi-scale, multi-physics simulation tools, *ab initio* methods applied to larger, more complex materials, …

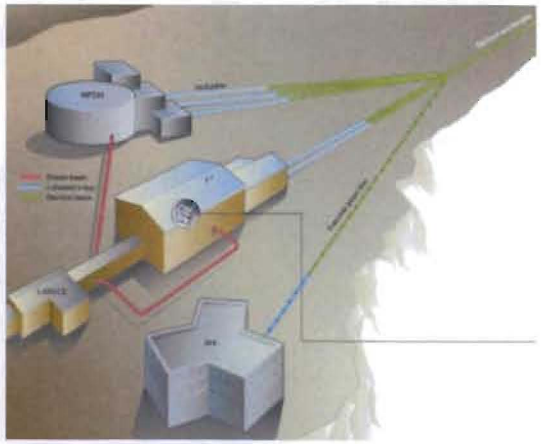
Multi-scale approaches to connect fundamental scales to bulk properties, defect generation and evolution, …



MaRIE will be the first capability with unique co-located tools necessary to revolutionize materials in extremes

- A mission need exists for prediction and control of materials in extreme environments
- MaRIE will provide simultaneous in situ, transient measurements on real materials in relevant extremes coupled to directed synthesis and characterization through predictive theory
- Building on existing capabilities at LANL, MaRIE provides unprecedented international user resources
- MaRIE facility definition is being driven by community-validated performance gaps & functional requirements





MaRIE builds on the LANSCE facility to provide unique experimental tools to meet this need

First x-ray scattering capability at high energy and high repetition frequency with simultaneous charged particle dynamic imaging [hard X-ray FEL, proton beam, high fidelity diagnostics]

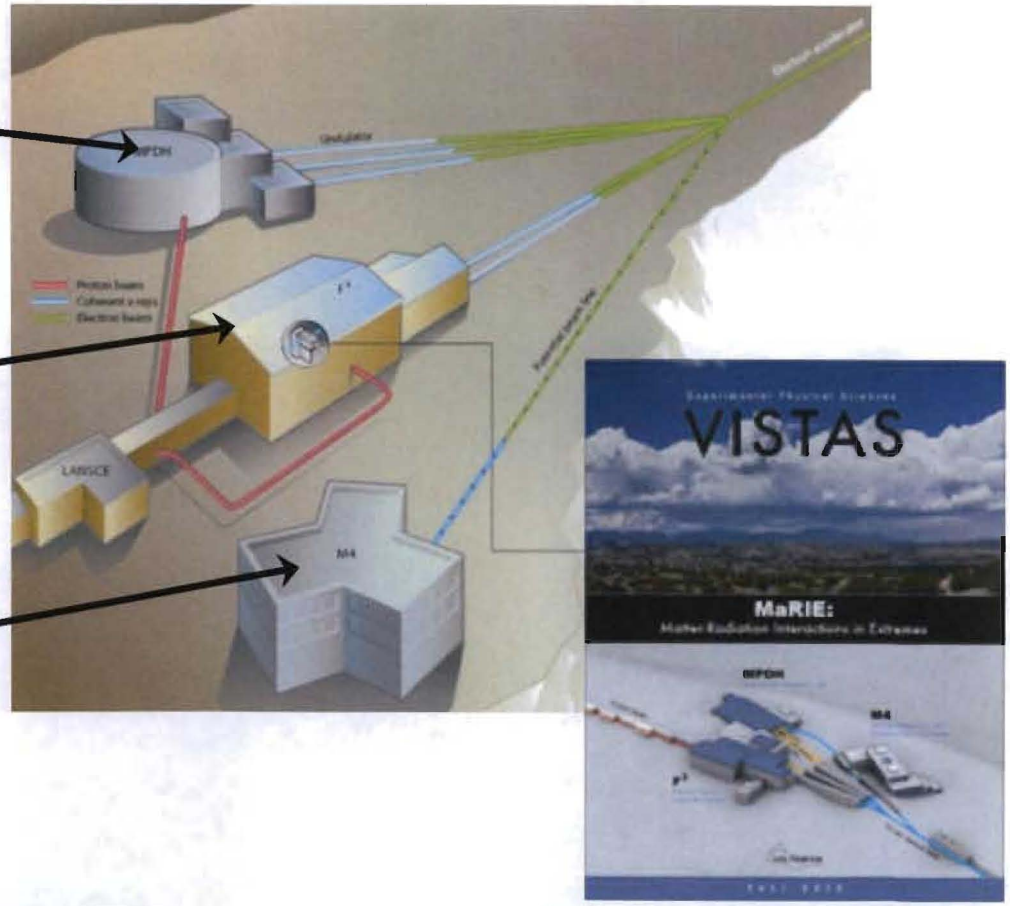
MPDH: Multi-Probe Diagnostic Hall

In-situ diagnostics and irradiation environments beyond best planned facilities

F^3: Fission and Fusion Materials Facility

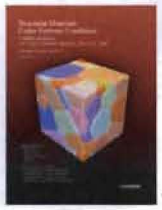
Integrated resource for materials synthesis and control, with national security infrastructure

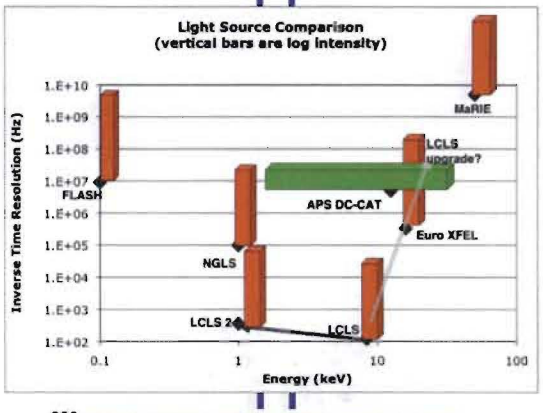
M4: Making, Measuring & Modeling Materials Facility

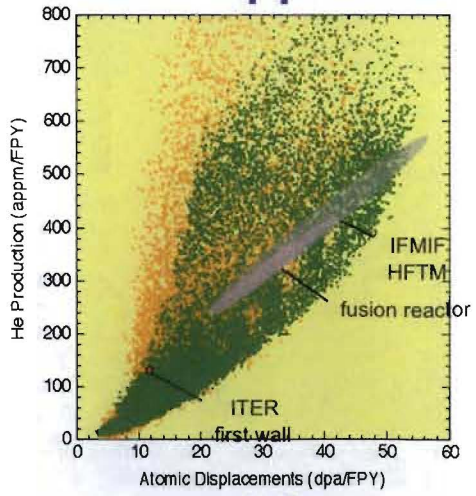


Science-driven Requirements Lead to Integrated Facility Needs Fulfilled by MaRIE

User Driven Science → Materiel Needs → **Functional Requirements** → Alternatives Analyses → **Performance Gaps** → Preferred Alternative & Roadmap → **Facility Concept**







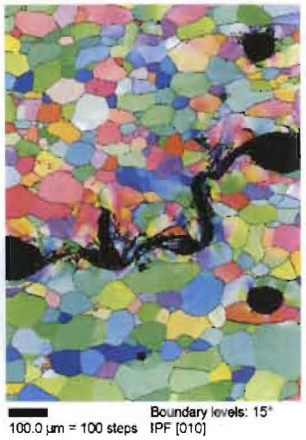
MaRIE builds upon existing $B investments at LANSCE with the addition of the:

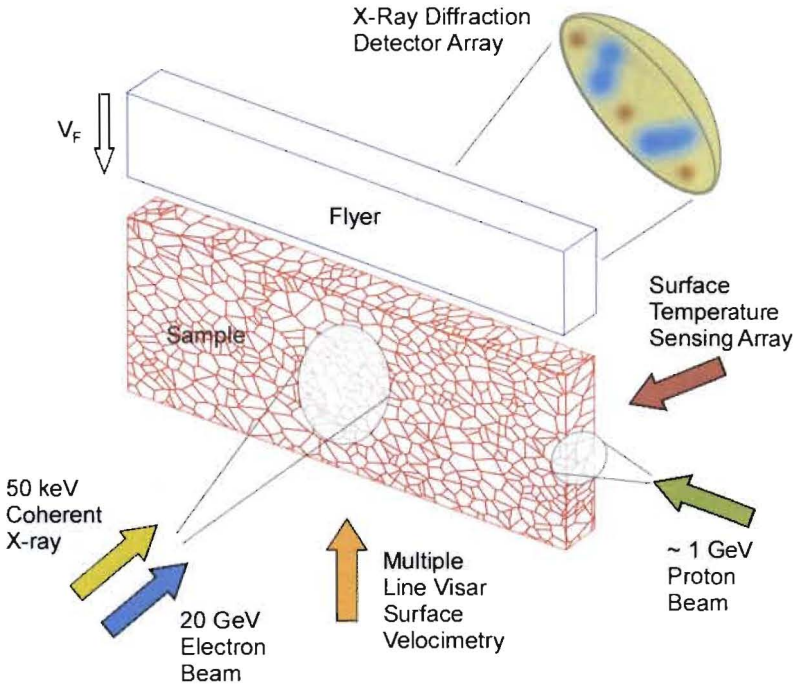
- Electron Linac with XFEL Systems
- Multi-Probe Diagnostic Hall
- Fission-Fusion Materials Facility
- Making, Measuring, & Modeling Materials Facility

MaRIE will address problems central to Department of Energy missions in energy, science, and security

- Can we predict and prevent materials damage?
- What are the consequences of materials failure for weapons performance?
- How do we accelerate the certification of materials to enable a nuclear renaissance?
- Can we discover by design materials to perform in unprecedented irradiation extremes?
- How do we predict and control microstructure for designed materials performance?
- Can we design and synthesize new materials with controlled functionality?

Understanding the role of microstructure-based heterogeneity evolution in material damage





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Meso-Scale Theory and Simulation

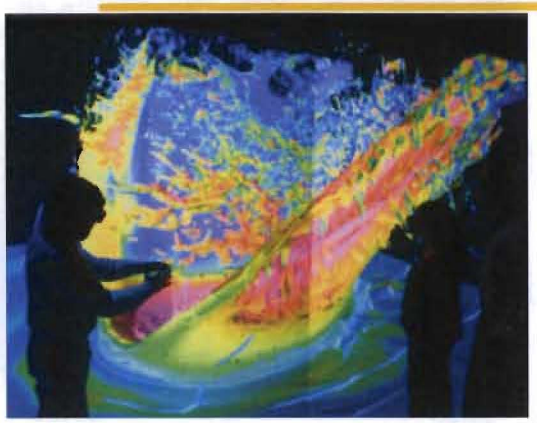
The goal :- Predict dynamic microstructure and damage evolution

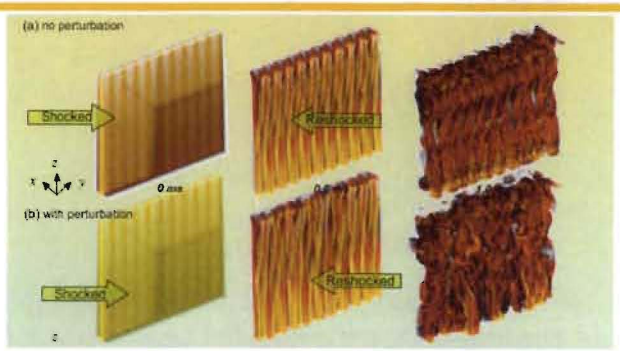
The first experiment :- Multiple, simultaneous dynamic in situ diagnostics with resolution at the scale of nucleation sites (< 1 µm; ps – ns)

The model :- Accurate sub-grain models of microstructure evolution coupled to molecular dynamics

Team includes: Curt Bronkhorst et al. (LANL, UK AWE, BYU, CalTech, Ohio State, …)

Developing predictive capability across all relevant scales for turbulent flows, including those with "strength"

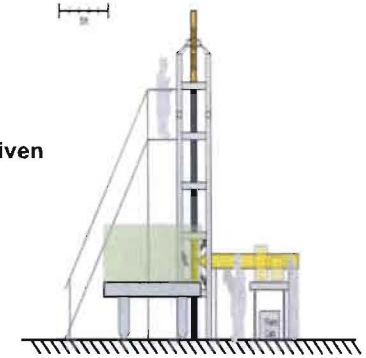


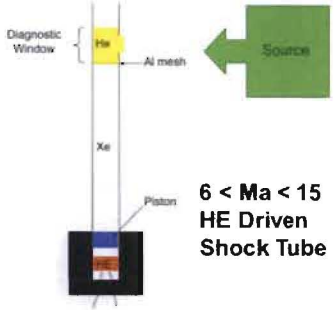


The model :-Large Eddy Simulation (RAGE)

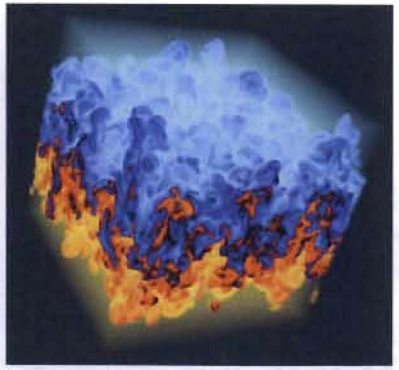
The goal :- Develop predictive capability for turbulent mix

0 < Ma < 6
Pressure Driven
Shock Tube

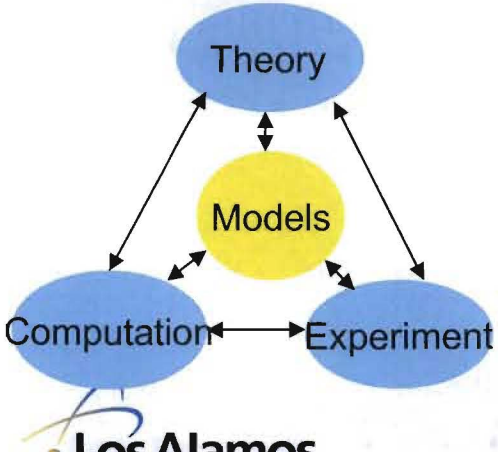




6 < Ma < 15
HE Driven
Shock Tube



The model :- Direct Numerical Simulation coupled to Reynolds-Averaged Navier Stokes turbulence model



The experiment :- Multi-scale fluid dynamics experiments with the ability to measure turbulent flows at all relevant space and time scales (μm and μsec), featuring opaque materials and/or high-velocity flows requiring high repetition measurements.

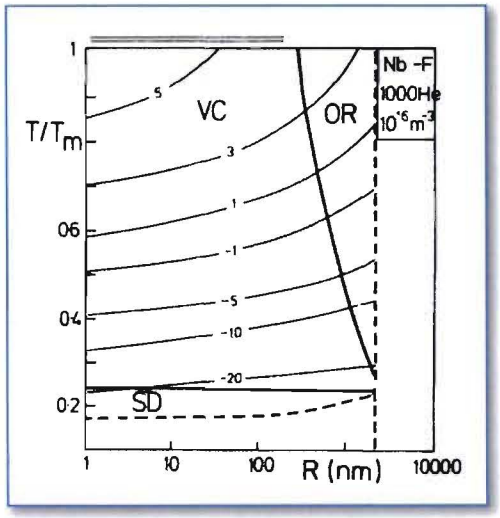
Team includes: Malcolm Andrews et al. (LANL, UK AWE, Texas, Johns Hopkins, …)

MaRIE: An international user facility for matter in extremes

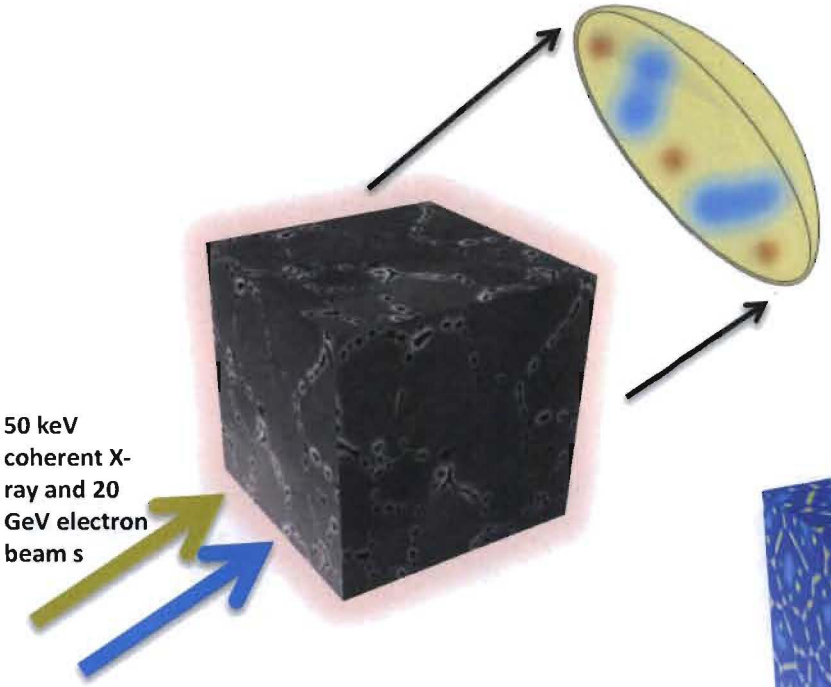
- We seek the broadest picture for future research opportunities.
- The next 3 plenaries illustrate a variety of our "national security science" interests and challenges. They build a pyramid: from fundamentals, thru intermediate scale, to large-scale mixing.
- Afterwards. panel breakouts will address the "charge" by:
  - identifying priority research directions,
  - capability opportunities , and
  - projected capability needs.

BACKUP SLIDES

Understanding creep via transient measurements of cavity growth under fast neutron irradiation



The goal :- Predicted and measured cavity growth mechanism maps of creep under extreme irradiation conditions



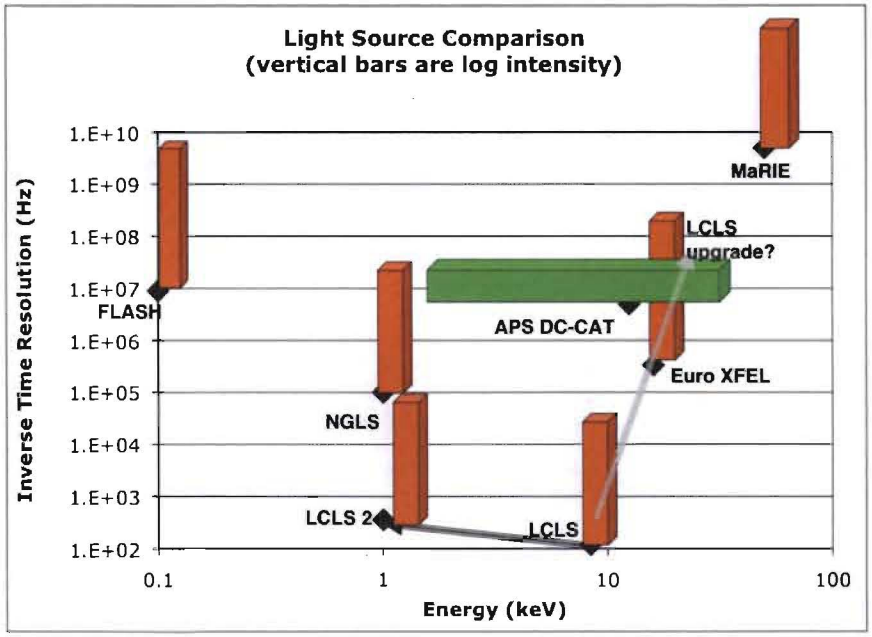
The first experiment :- Transient imaging and scattering measurements of *mesoscale* objects with *nm spatial resolution* in an extreme radiation environment

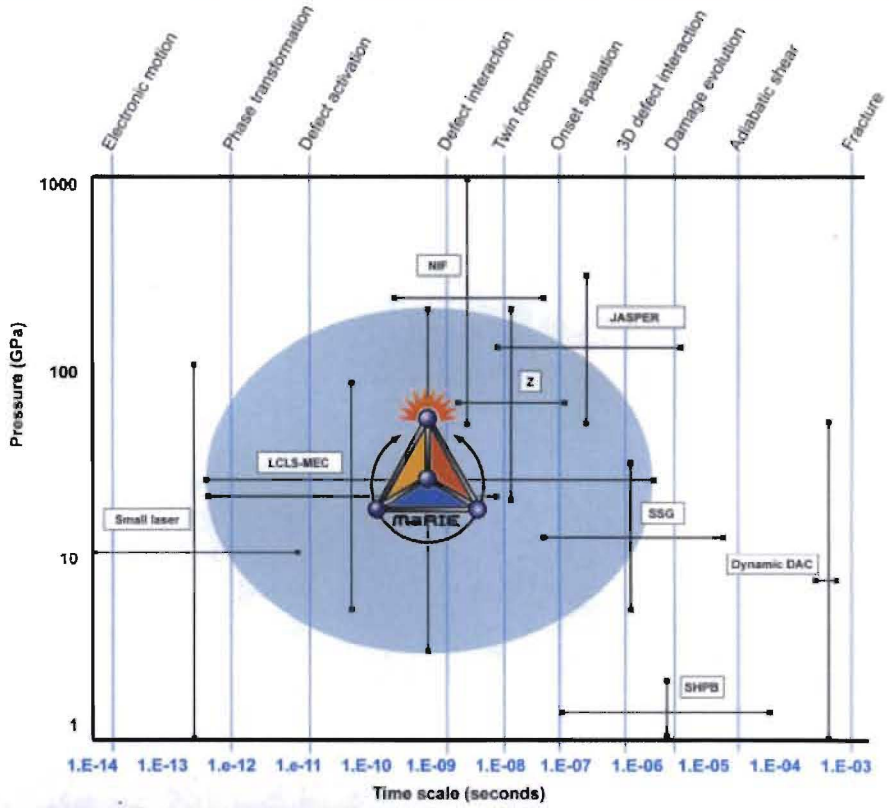
The model :- Phase field simulation of heterogeneous nucleation of gas bubbles

Team includes: Marius Stan et al. (LANL, ANL, Wisconsin, INL, CEA …)

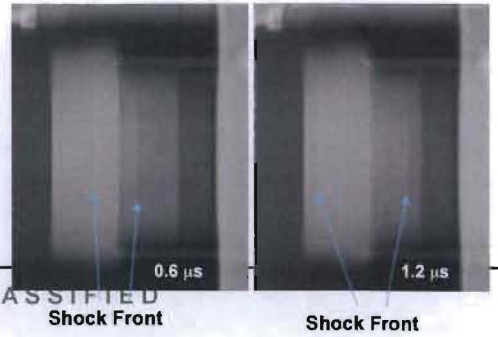
Through Multi-Probe Diagnostic Hall, MaRIE provides unique scattering and imaging capabilities to bridge the micron gap in extreme environments

A high-energy-photon (50-100 keV) XFEL allows multigranular sample penetration and multipulse dynamics without significant sample perturbation



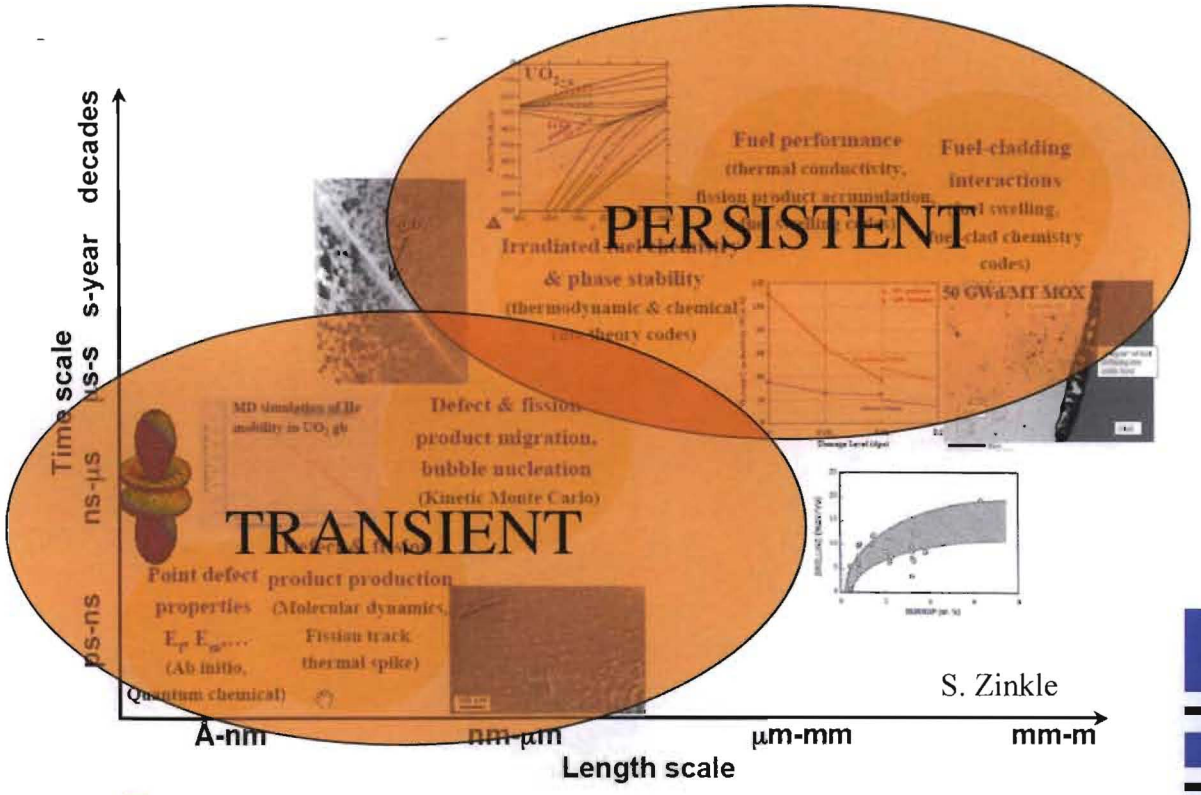


Meanwhile, proton microscopy can provide absolute density & velocities through the sample volume

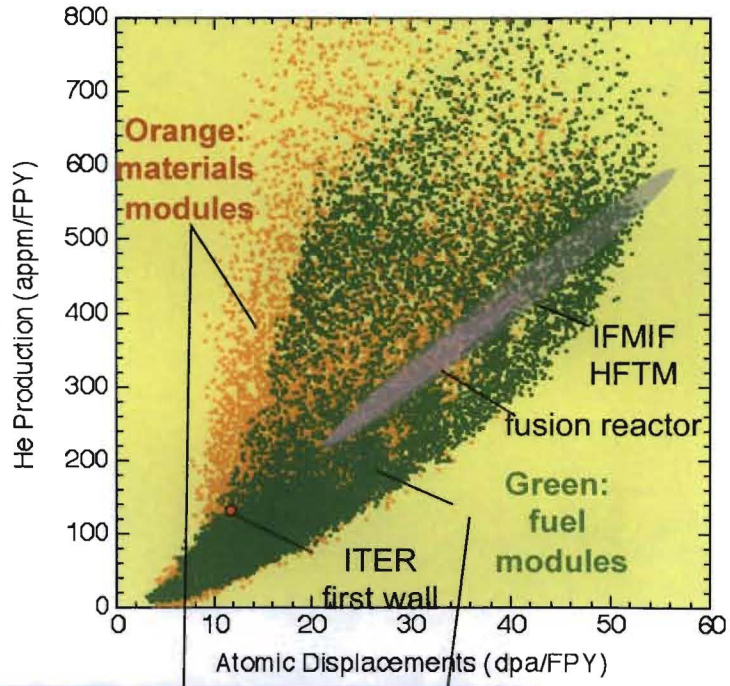


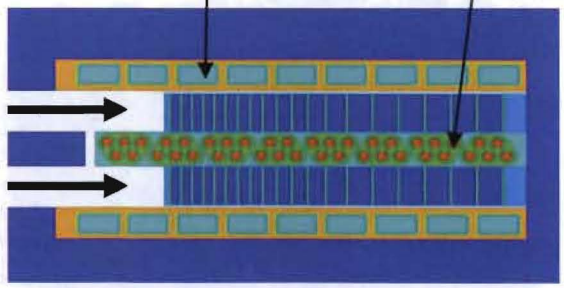
Through Fission Fusion Materials Facility, MaRIE creates extreme radiation fluxes and advances the frontiers of radiation damage science through in situ measurements

The same x-rays (protons) enable in-situ (near in-situ) measurements…



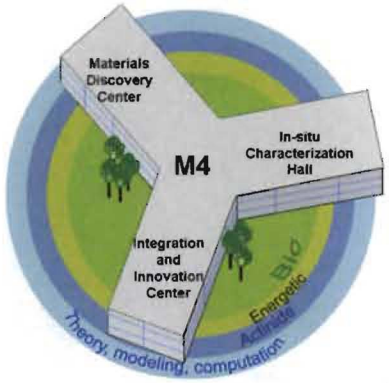
…in relevant environments

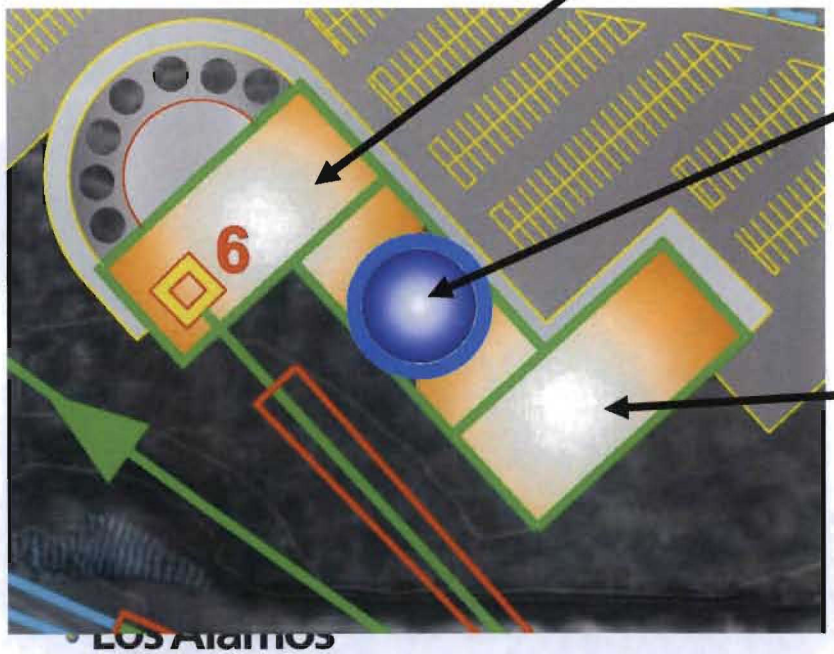




MTS target assembly

Through M4 Facility, MaRIE provides the directed synthesis of materials essential for defect/interface control and materials discovery





M4 XFEL end station
- Other Extremes (E,H, pH)
- In situ synthesis probes

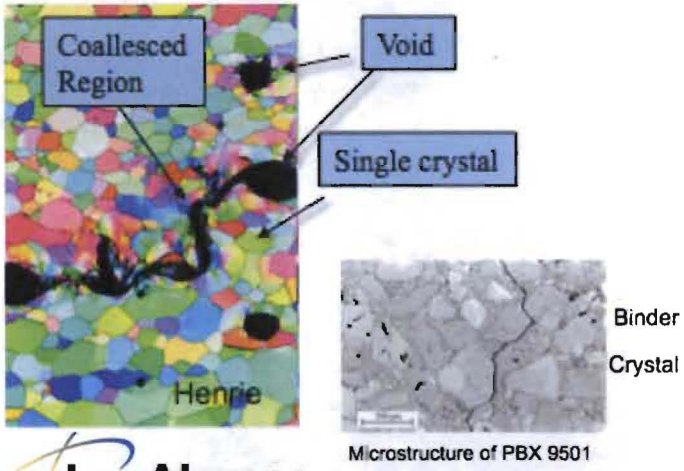
User Gateway
- Co-design Center
- Visualization Capability

Multi-scale Synthesis & Crystal Growth
- Characterization
- National Security Infrastructure

Measuring
Modeling
Making

Understanding materials in extreme environments is key to weapons program success in the future

MATERIALS MATTER



Microstructure of PBX 9501

Current Stockpile

- Prediction of materials lifetime & failure

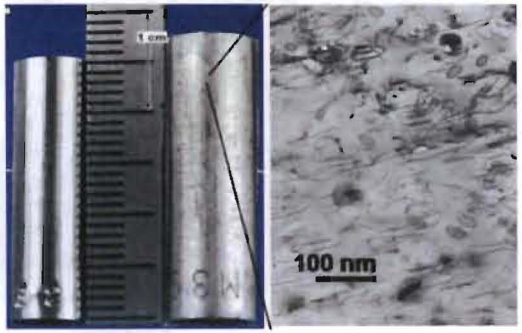
Rebuild & Lifetime Extension

- Materials 'by design' rather than re-learning old processes

Weapon performance

- Effects of microscale materials properties on dynamic performance for key physics

Materials behavior limits the performance of advanced energy systems needed for energy independence

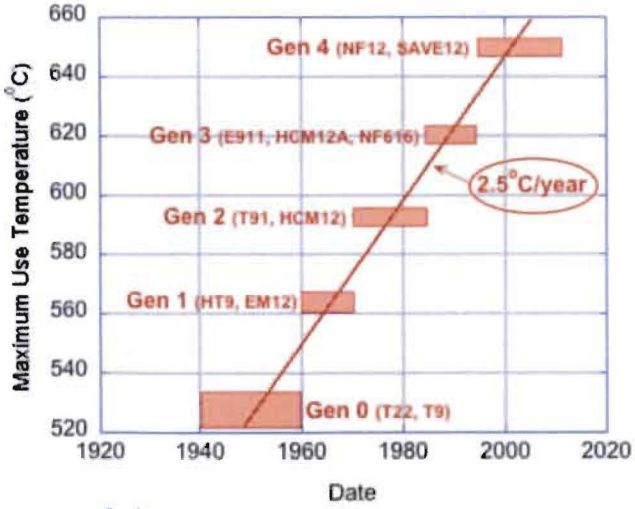


Life extension, safety of existing reactor fleet

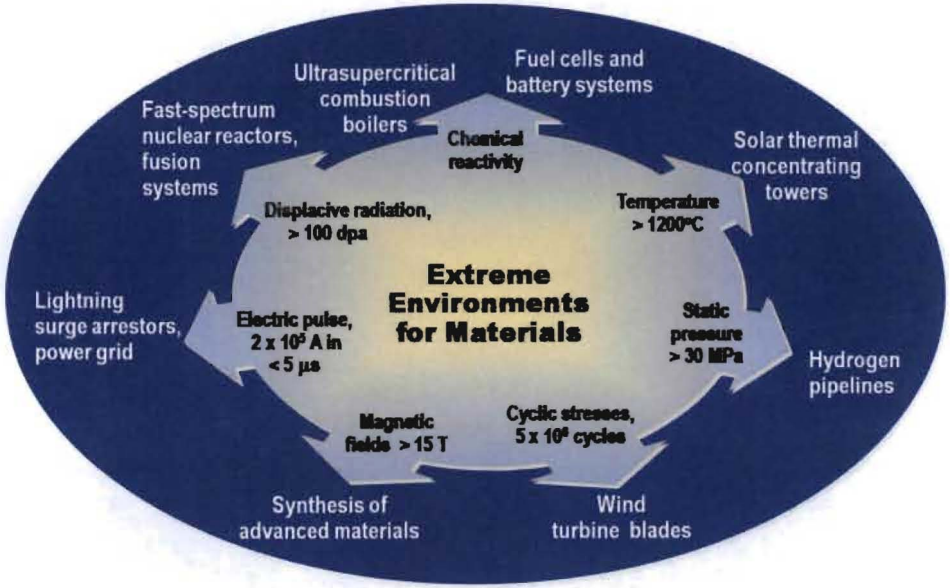
Improved affordability for new reactors

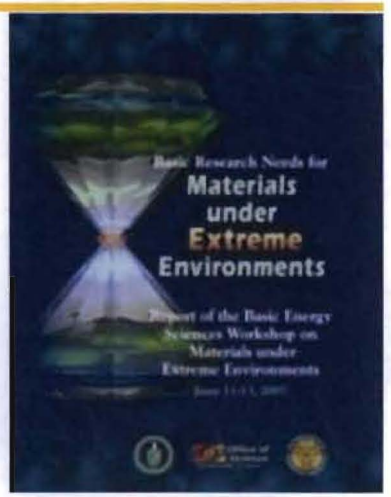
Sustainable fuel cycles

Fusion Reactor first wall materials



The needs for materials in extremes are many; the challenge is common: revolutionary advances in controlled functionality





We need to enable a transition:

from observation and validation

to prediction and control