MaRIE:

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

An Experimental Facility Concept Providing Transformational Materials Solutions for Today's and Tomorrow's National Security Needs

P/T Colloquium 6/3/09

Outline

- The Why/What/How of MaRIE
  - Mission Driver: observation → control
  - Vision for Success: micron frontier
  - Integrated Facility Definition: whole greater than sum of parts
- MaRIE FY09 Status & Plans
  - Opportunities for your engagement
- Prelude to a series of P/T Colloquiua

June 11: MPDH/Barnes

June 18:FFMF/Bourke

June 25: M4/McCleskey

July 9: TMC/Chadwick

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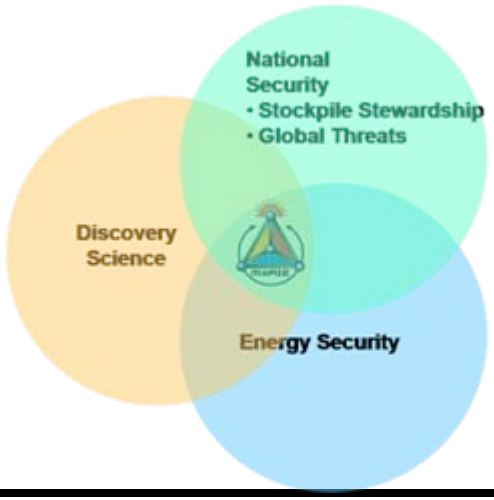
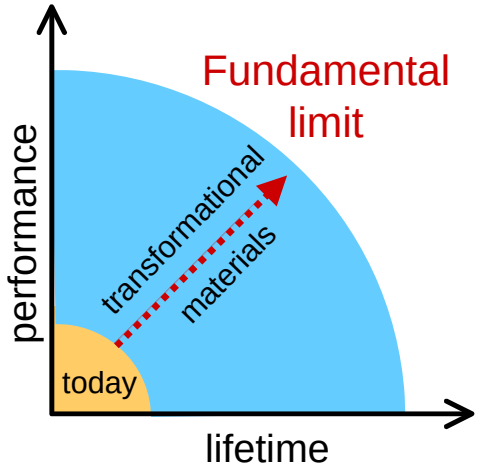
MaRIE: Materials R&D Capability for 21st Century National Security and Energy Security



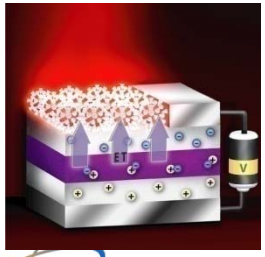
MaRIE addresses materials challenges across missions

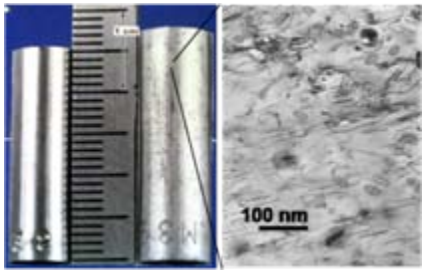
MaRIE enables the transition from "observation" to "control"



MaRIE will transform the science of microstructure, interfaces, and defects

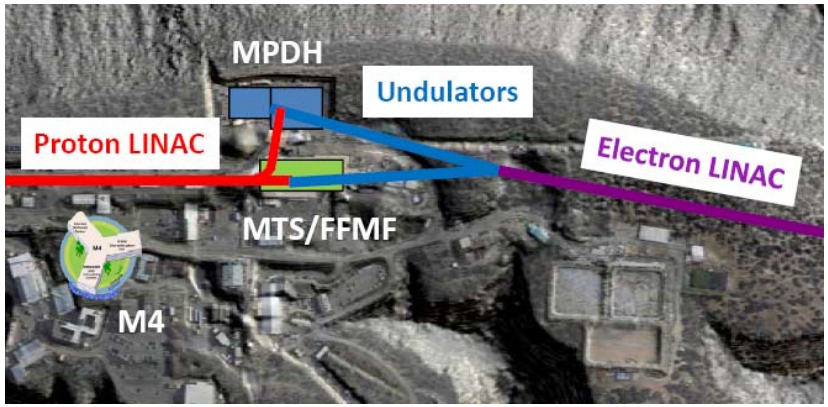
Next-generation solar cell architecture



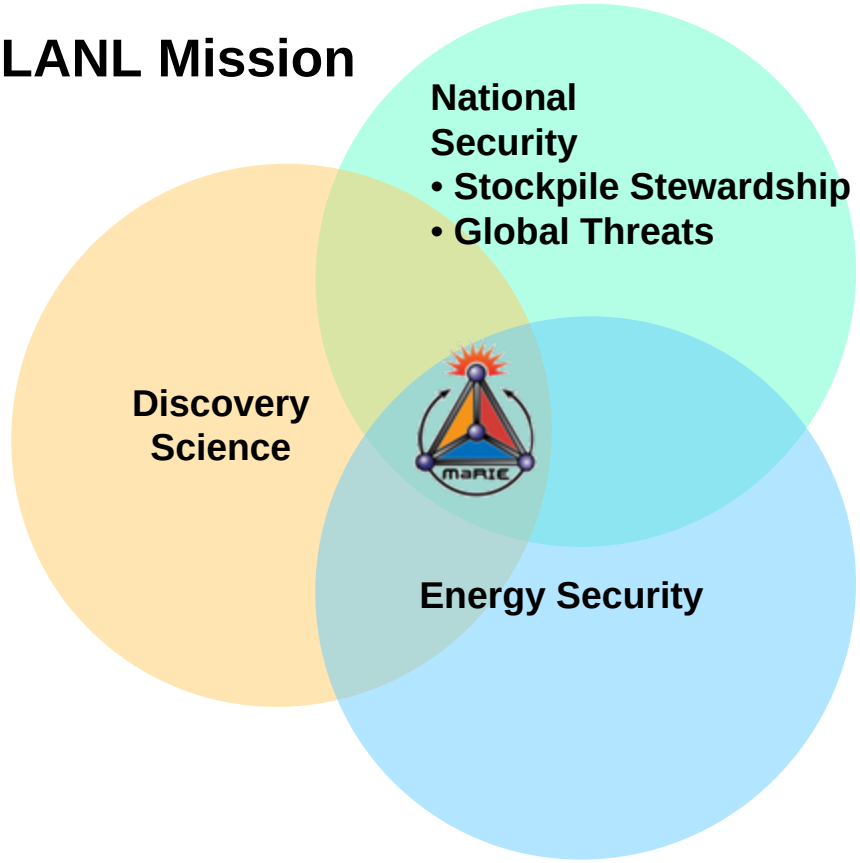


Radiation-induced swelling

MaRIE provides tools for transformational materials performance in extremes



MaRIE addresses decadal research frontiers and challenges of critical importance to Los Alamos' national security missions



National Grand Challenges

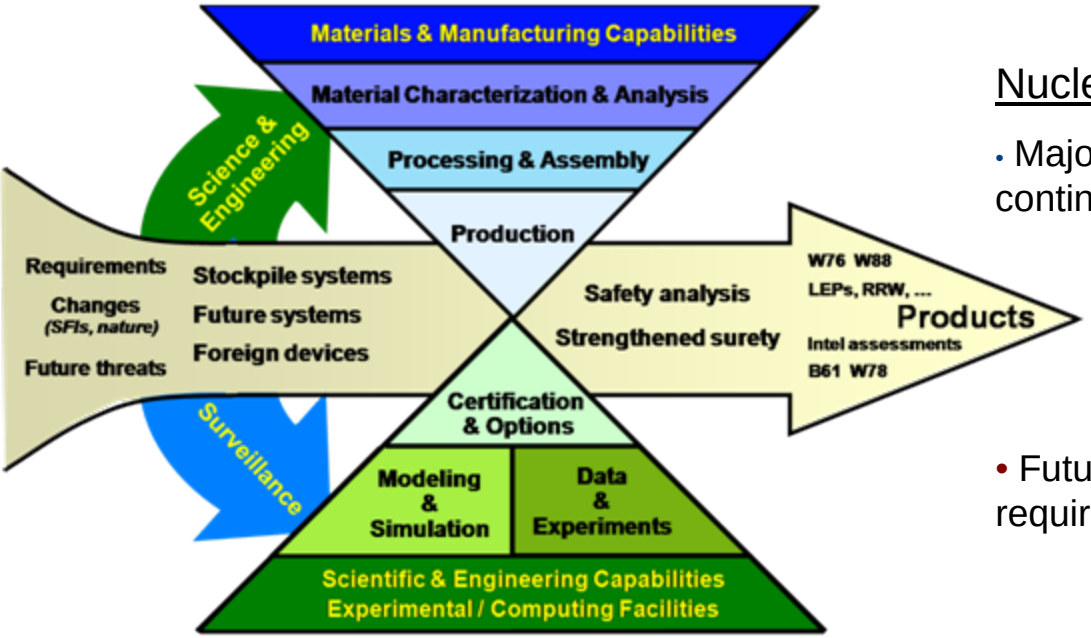
- **Transform the nuclear weapons enterprise: Define process-aware materials performance**
- **Close the 10 TW Gap between the energy we have and the energy we need: From fission & solar to fusion**

Materials Matter!
Material Requirements Central to National Grand Challenges

Materials Recognized as a Core LANL Capability

Enabling Materials-Centric National Security Science for the 21st Century

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



Dynamic processes dominate and are poorly understood today

Experimental capabilities to validate multi-scale models, especially on the meso-scale, are needed

Nuclear weapons program challenges

- Majority of stockpile issues have been and will likely continue to be materials based
  - Strength, damage: microstructure matters
  - Cast/wrought, weld, alternate material
- Future stockpile manufacturing and certification requires a "process aware" understanding of materials
  - Materials compatibility/substitution
  - 9 of top 11 NM RRW technical risks materials-related

MaRIE will be the first capability with unique co-located tools necessary to realize transformational advances in materials performance in extremes

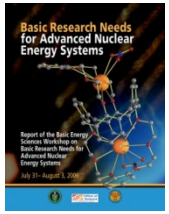
The transition from "observation & validation" to "prediction & control" is a central mission challenge AND the frontier of materials research

FESAC Priorities, Gaps and Opportunities for Magnetic Fusion Energy

- ***"…understand the materials and processes that can be used for replaceable components that can survive the enormous heat, plasma and neutron fluxes without degrading the performance of the plasma."***
- ***"… The potential for alternative irradiation facilities to reduce or possibly eliminate the need for the US to participate as a full partner in IFMIF needs to be assessed."***

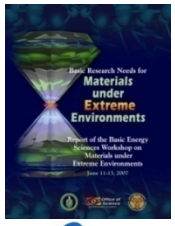
R&D Needs and Required Facilities for the Development of Fusion as an Energy Source

Report of the Fusion Facilities Review Panel
October 2008



Next-generation nuclear fission reactors require materials capable of withstanding higher temperatures and higher radiation flux in highly corrosive environments for long periods of time without failure

ANES Report http://www.sc.doe.gov/bes/reports/list.html



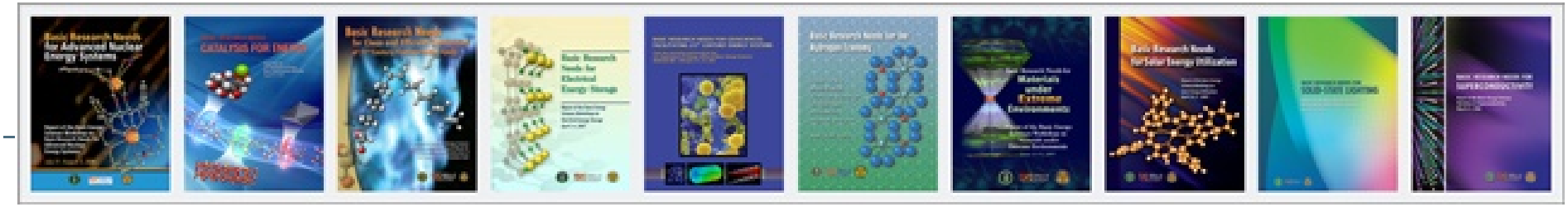
…(challenge is) to understand and control chemical and physical phenomena in multi-component systems from femto-seconds to millennia, at temperatures to 1000ºC, and for radiation doses to hundreds of displacements per atom.

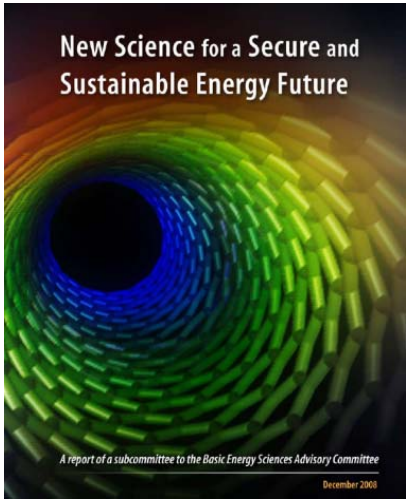
MUEE Report http://www.sc.doe.gov/bes/reports/list.html

MaRIE will address high priority materials challenges identified by fission and fusion energy communities

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

http://www.sc.doe.gov/bes/reports/list.html





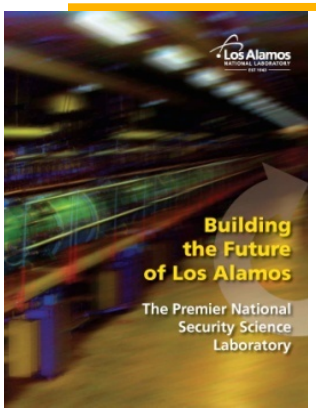
By engaging thousands of scientists around the world in a series of workshops, BES has defined 5 key grand challenges for materials research

- Control the quantum behavior of electrons in materials
- Synthesize, atom by atom, new forms of matter with tailored properties
- Control emergent properties that arise from the complex correlations of atomic and electronic constituents
- Synthesize man-made nanoscale objects with capabilities rivaling those of living things
- Control matter very far away from equilibrium

"The intersection of control science with high-functioning materials creates a tipping point for sustainable energy"

MaRIE provides to the user community the needed "beyond nano" tools for discovering and controlling complex materials

LANL's materials strategy defines focus areas for materials-centric national security science consistent with these national drivers

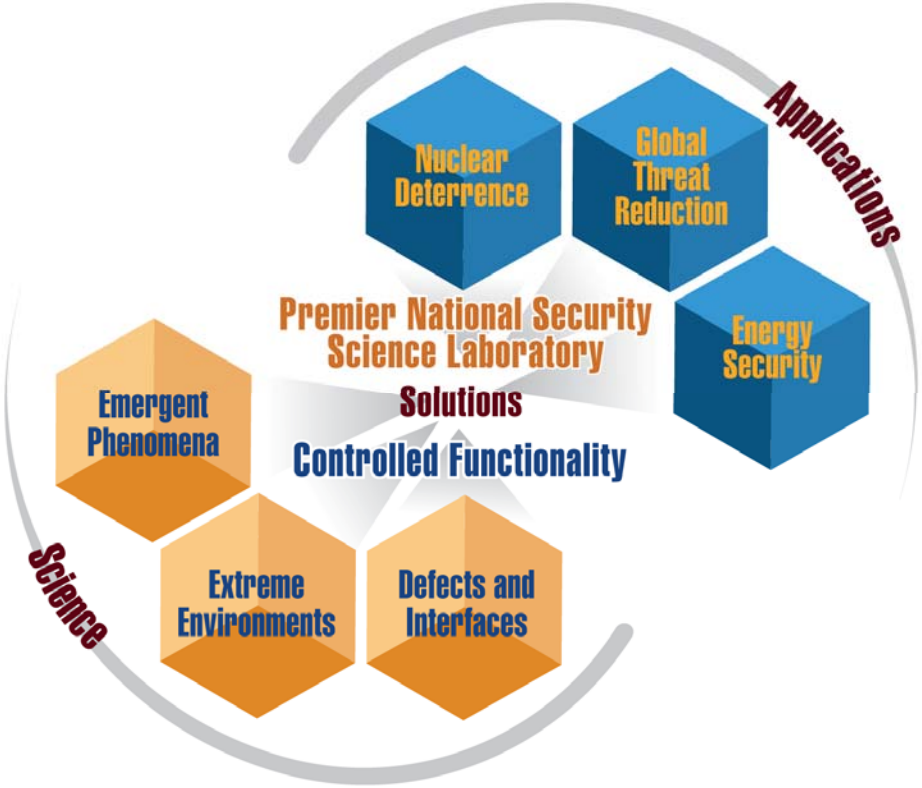


To achieve our vision of Los Alamos as the National Security Laboratory of choice, we have identified three strategic thrusts within "**Science that Matters**":

Information science and technology enabling predictive science,

Experimental science focused on materials for the future, and

Fundamental forensic science for nuclear, biological, and chemical threats.



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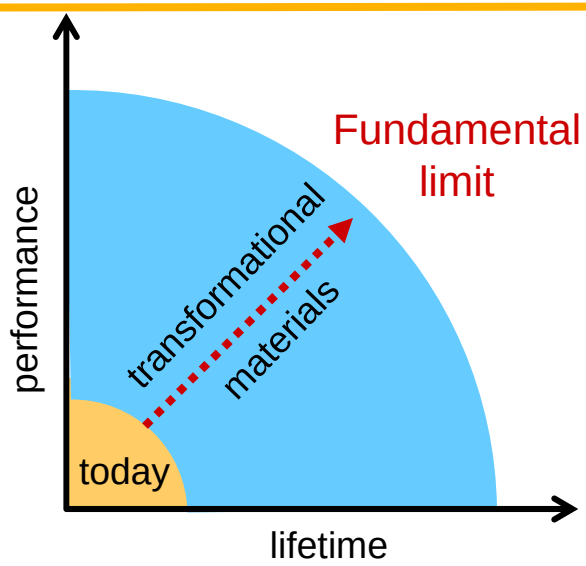
The transition from "observation & validation" to "prediction & control" is a central mission challenge AND the frontier of materials research

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

with an emphasis on Radiation-Matter Interactions
-Nuclear is special for LANL and for the world
-LANSCE is key to our uniqueness in materials-centric national security science

MaRIE will be the first capability with unique co-located tools necessary to realize transformational advances in materials performance in extremes

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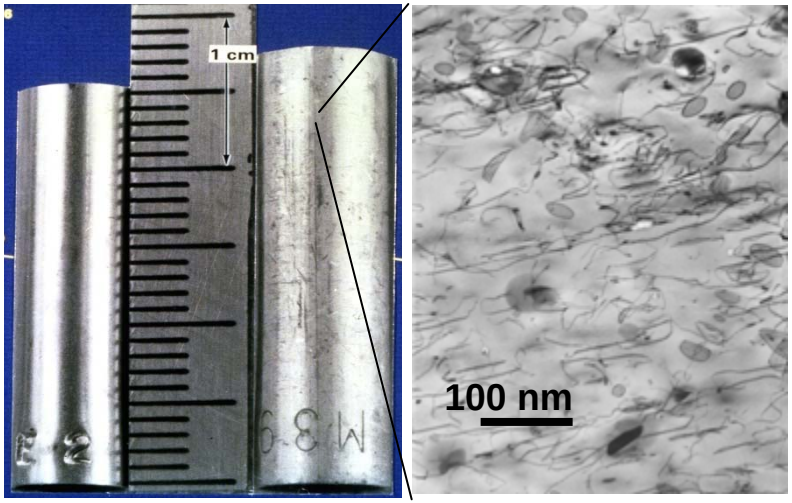
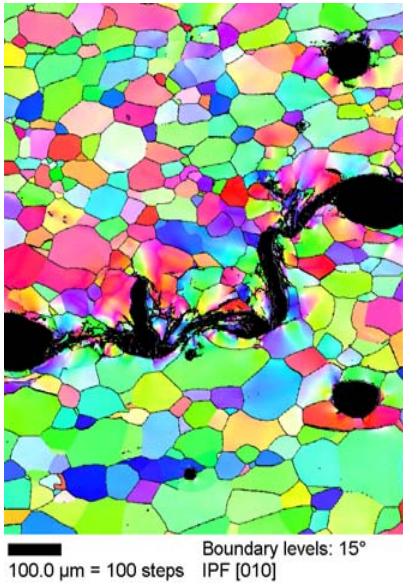
The “micron frontier:” Bridging the gap between atomic understanding and bulk performance

~ 1 μm is the domain of defect consequences and microstructure interactions that drive materials strength, damage evolution, etc.





Dynamic, stochastic processes in extreme environments dominate the phenomena that we do not understand

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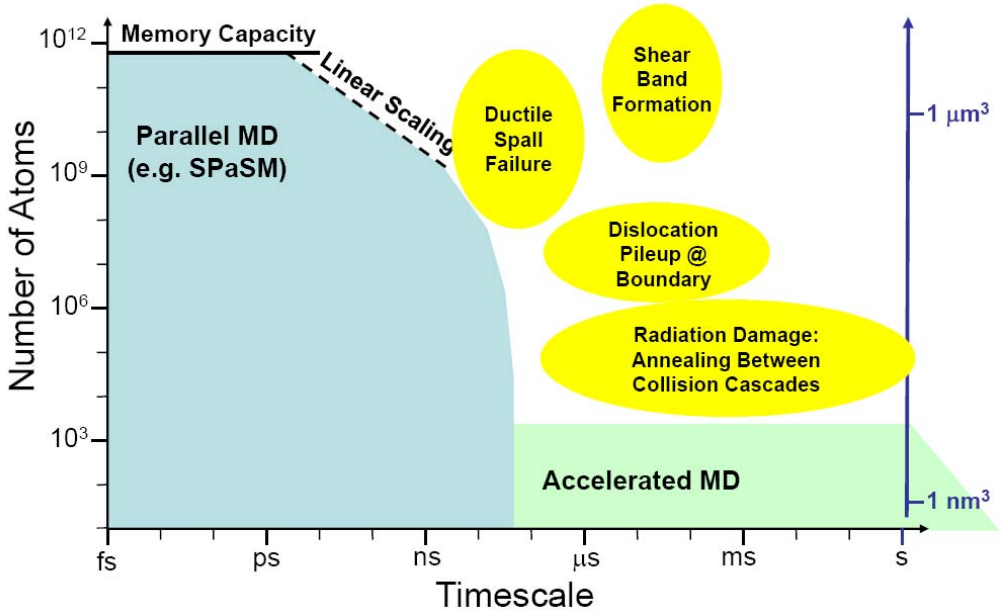
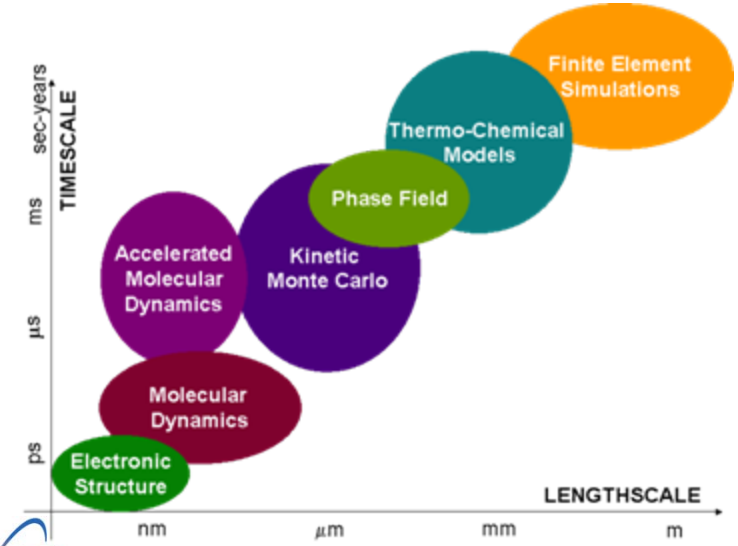
Experimental tools with unprecedented resolution are needed to validate and test the limits of modeling and simulation

One of the greatest challenges in multi-scale modeling is the physically-based treatment of defects and interfaces

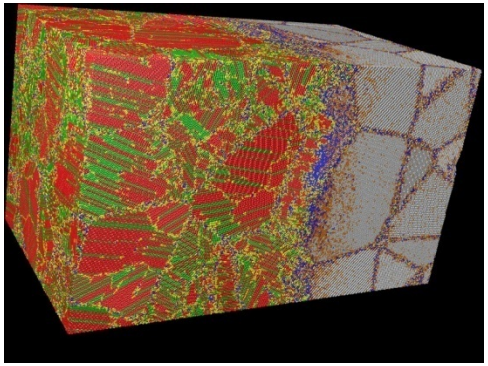




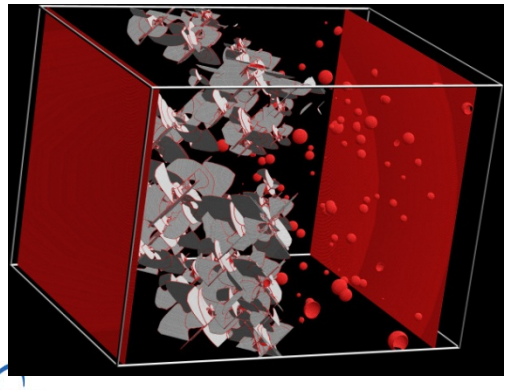
Anticipated advances in petaflop/s and exaflop/s computing – with advanced models - put us on the verge of accessing new phenomena on the micron scale

IS&T Methods Accelerate & Improve Model Development

SPaSM MD simulations of bcc -> hcp/fcc phase transitions, in polycrystal Fe



SPaSM MD simulations of dislocation loops nucleating from voids, in Cu



SPaSM provides modeling capability using trillions of atoms and billions of timesteps, but the quantity of data cannot be stored and analyzed intensively.

IS&T developments are needed to identify “significant” events in real time using advanced anomaly detection and classification algorithms, and develop analyses of the data during the calculation.

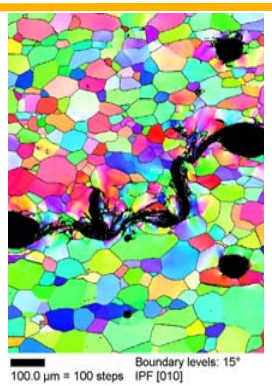
Models are sensitive to potential functions, defect concentrations, initial crystal arrangements and grain boundaries, but their roles have not been quantified

Model evaluation techniques are needed to assess sensitivity, quantify uncertainty, and facilitate development of realistic potential functions, defect distributions, grain orientations, and boundaries.

IS&T and UQ provide the framework to efficiently integrate information from experiment, theory,& simulation, & accelerate model development

MaRIE : What does success look like?

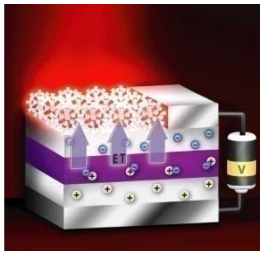
- **Predicting materials performance, including failure, in extremes of pressure and strain for multi-phase materials**



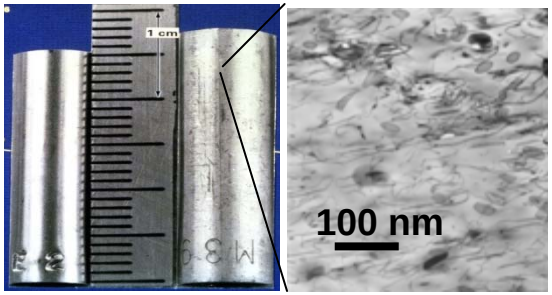
Materials failure under dynamic load

- **Developing radiation resistant structural materials and fuels by design**

- **Exploiting complex materials and architectures for next generation electronics**



Next-generation solar cell architecture



Radiation-induced swelling

Understanding and Controlling the Complexity of Real Materials

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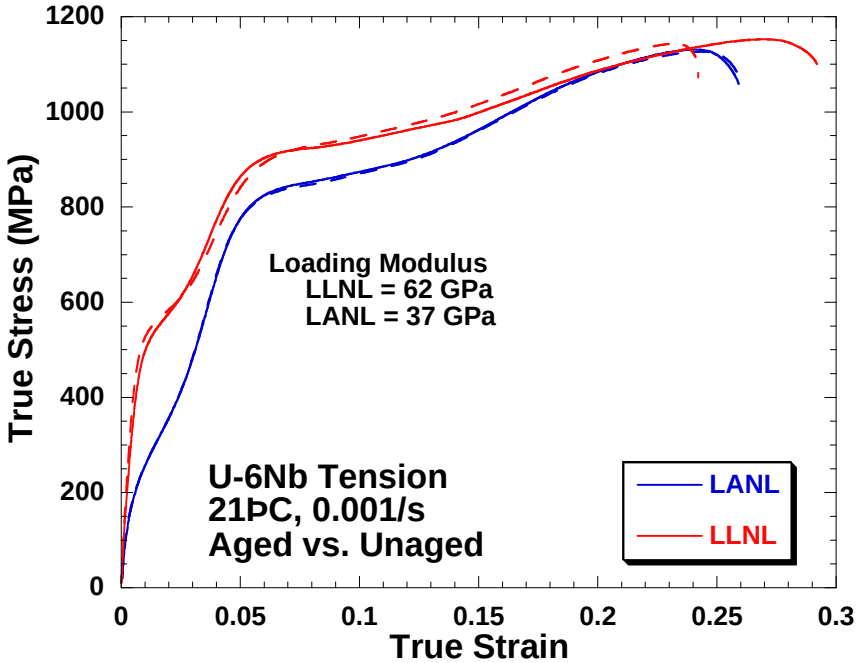
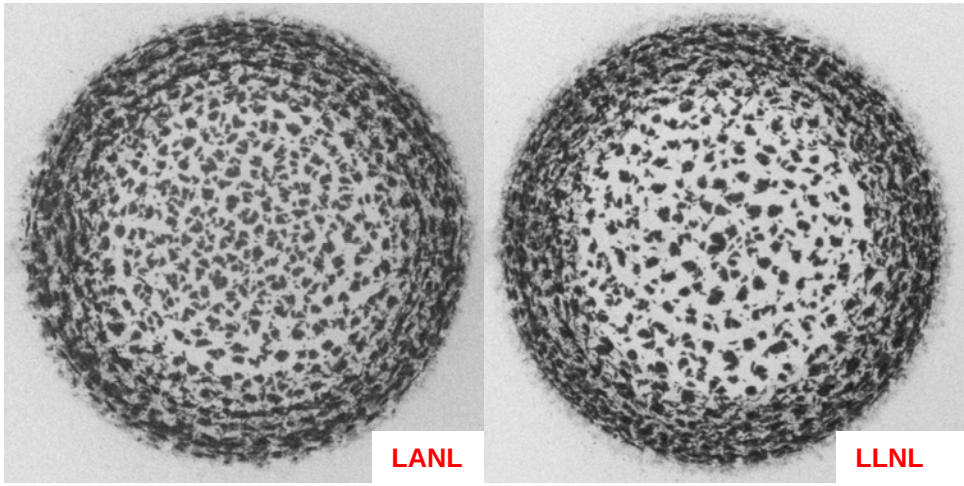
Mechanical behavior and HE-driven fragmentation of U-6Nb show strong influence of metallurgical state

LANL = Solution treated / Quenched

LLNL = Solution treated / Quenched + Aged





Quantitative analysis reveals 6σ difference in open area between images

Process-aware understanding of materials performance is lacking

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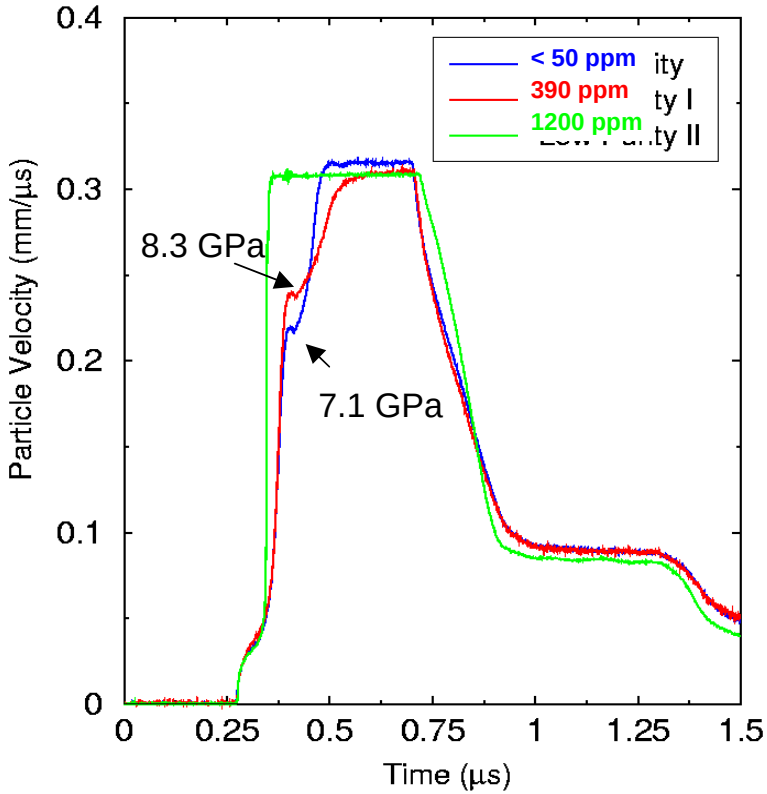
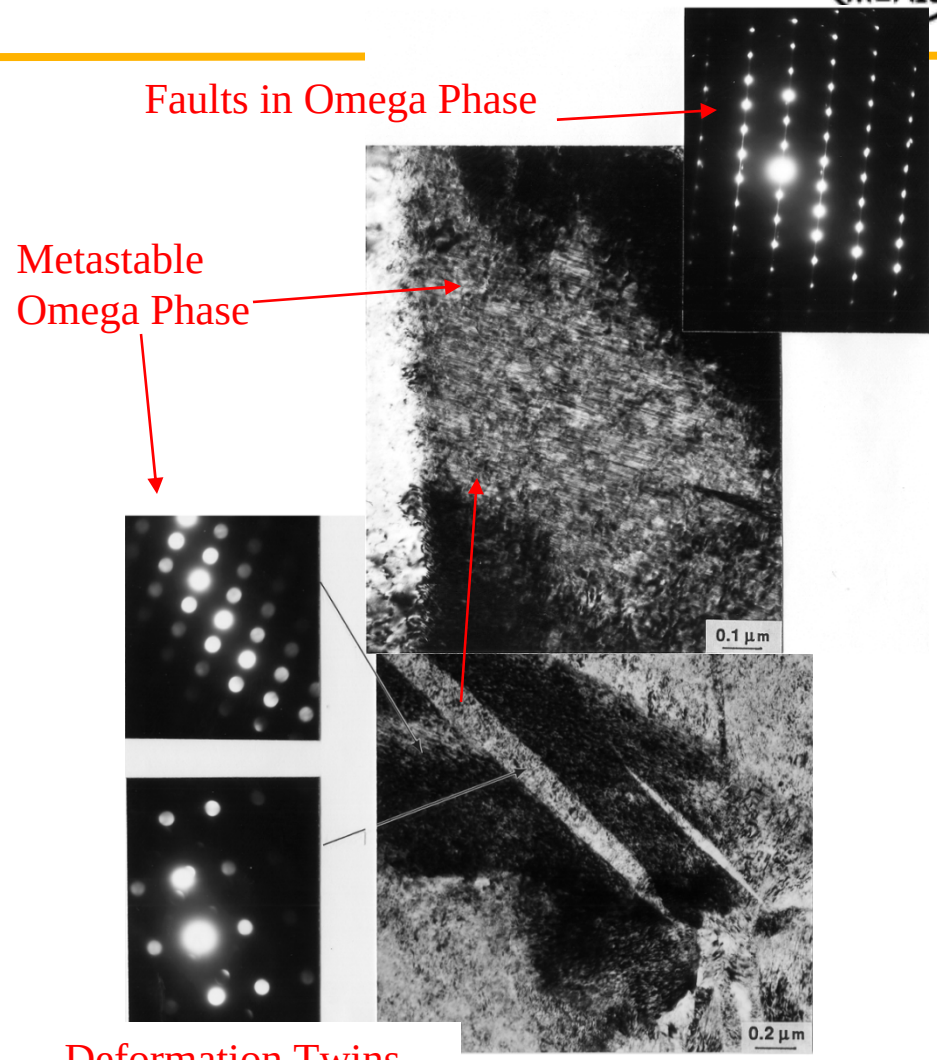
Shock-induced phase transitions - spatially complex processes with strong materials sensitivities

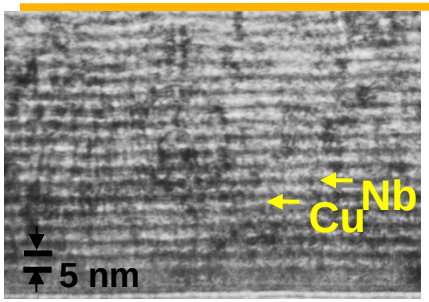
Oxygen content suppresses the α–ω phase transition in Zr





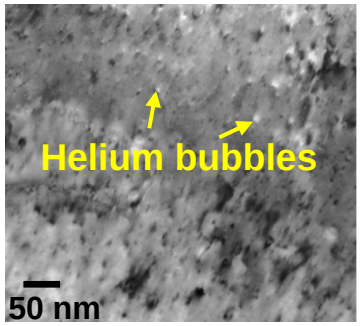
Predictive models must acknowledge that solids are an assembly of crystals that deform according to their local state of stress

Frontiers of materials discovery: Interface/structure manipulation produces enhanced strength and radiation resistance

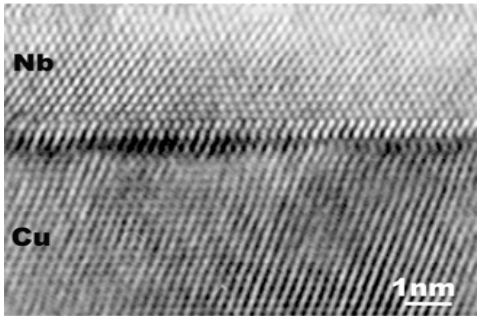


Nanolayer architectures produce materials strength that exceeds theoretical “limits”

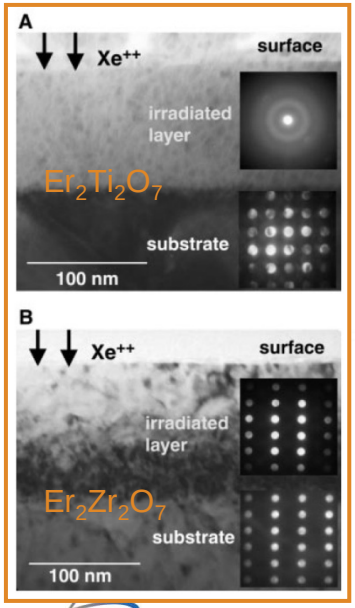
Same structures produce extreme radiation resistance by actively eliminating point defects

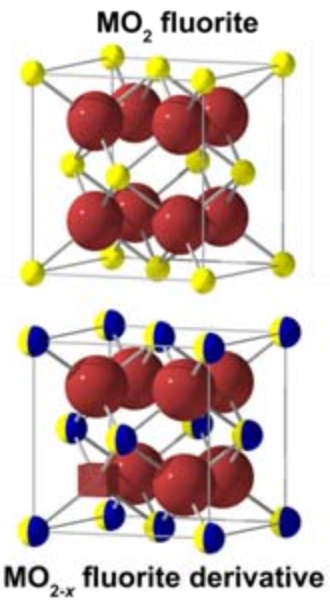


Pure Cu



5 nm layer thickness Cu-Nb multilayer



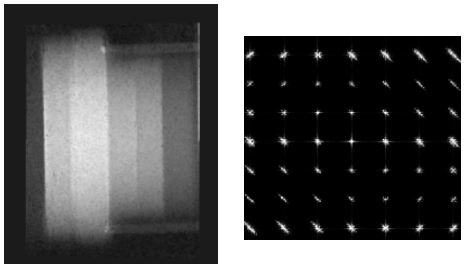


← Challenge is to translate these insights to bulk systems

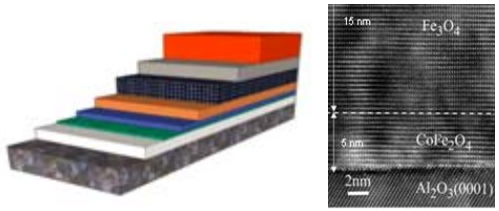
How do we discover ‘by design’ bulk materials that embody these principles and observe and manipulate their defect structures in ‘real’ deformation and irradiation extremes?

MaRIE : What does success look like?

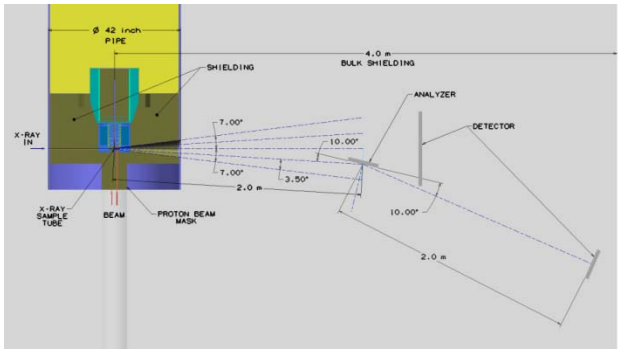
- **Predicting materials performance, including failure, in extremes of pressure and strain for multi-phase materials**
- **Developing radiation resistant structural materials and fuels by design**
- **Exploiting complex materials and architectures for next generation electronics**



Simultaneous diffraction
& dynamic density imaging



Defect manipulation in multiphase materials



In situ characterization
in extreme environments

MaRIE provides the first comprehensive set of co-located tools to realize transformational advances in materials performance in extremes

First x-ray scattering capability at high energy and high repetition frequency with simultaneous charged particle dynamic imaging

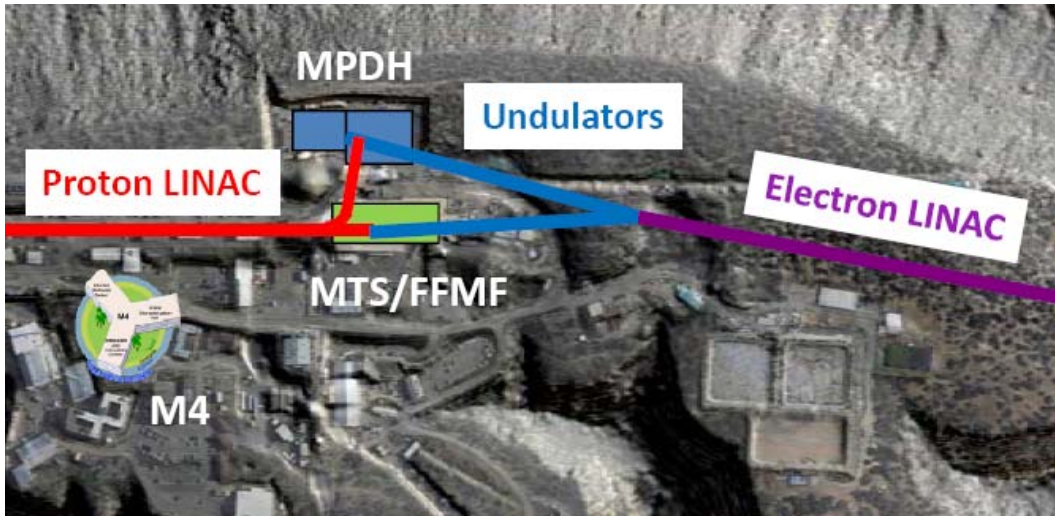
(Multi-Probe Diagnostic Hall)

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

(Fission and Fusion Materials Facility)

Comprehensive, integrated resource for materials synthesis and control, with national security infrastructure

(M4 Facility)



MaRIE will provide unprecedented international user resources

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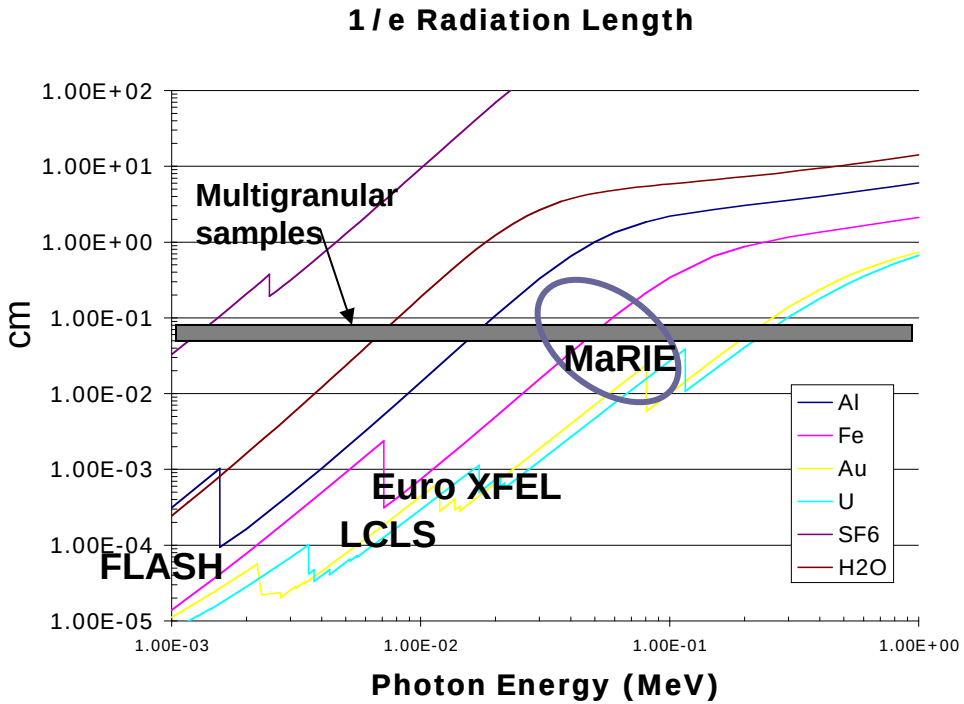
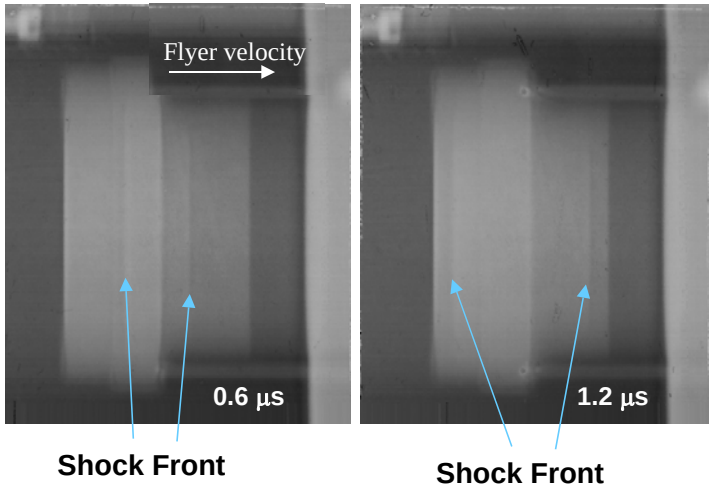
Through Multi-Probe Diagnostic Hall, MaRIE provides unique scattering and imaging capabilities to bridge the micron gap in extreme environments

A high-energy-photon (50-115 keV) XFEL allows multigranular sample penetration and multipulse dynamics without significant sample perturbation



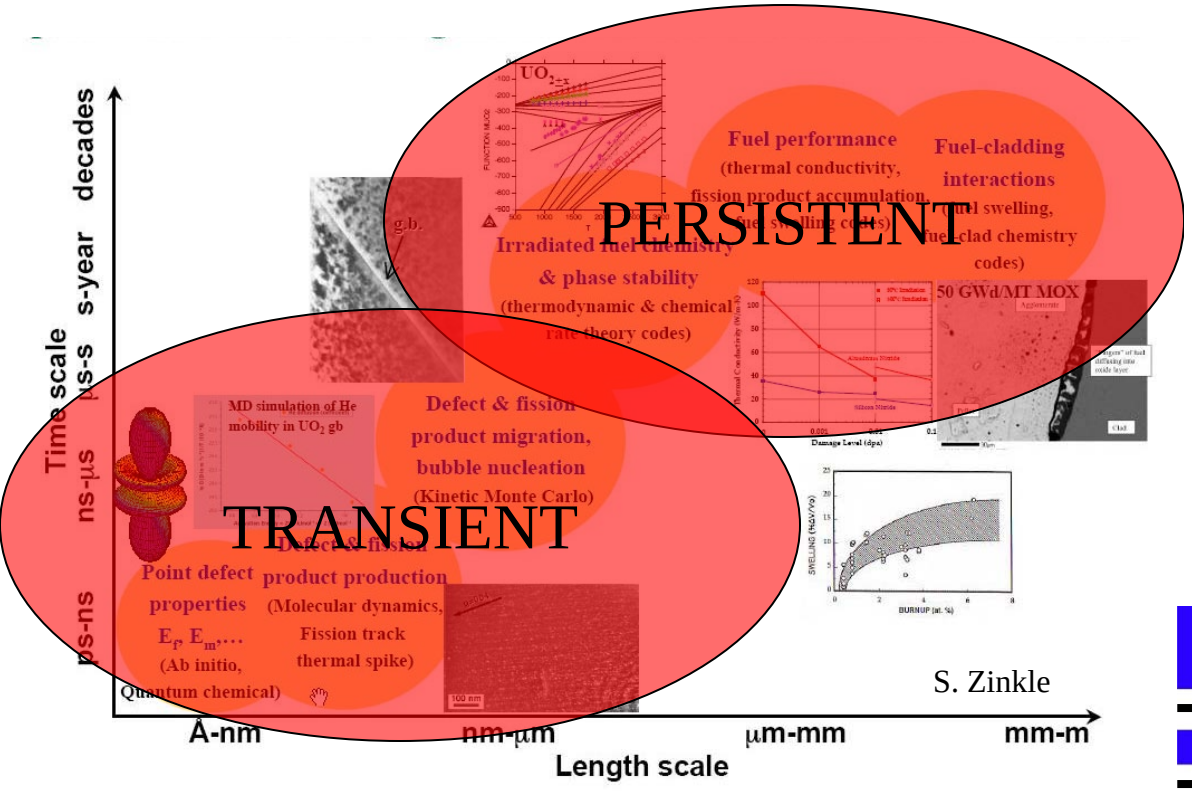


pRad absolute Density:
$\rho = 3.07 \pm 0.03$ g/cm^3 (1.1%)

Meanwhile, charged particle radiography can provide absolute density and velocities through the sample volume

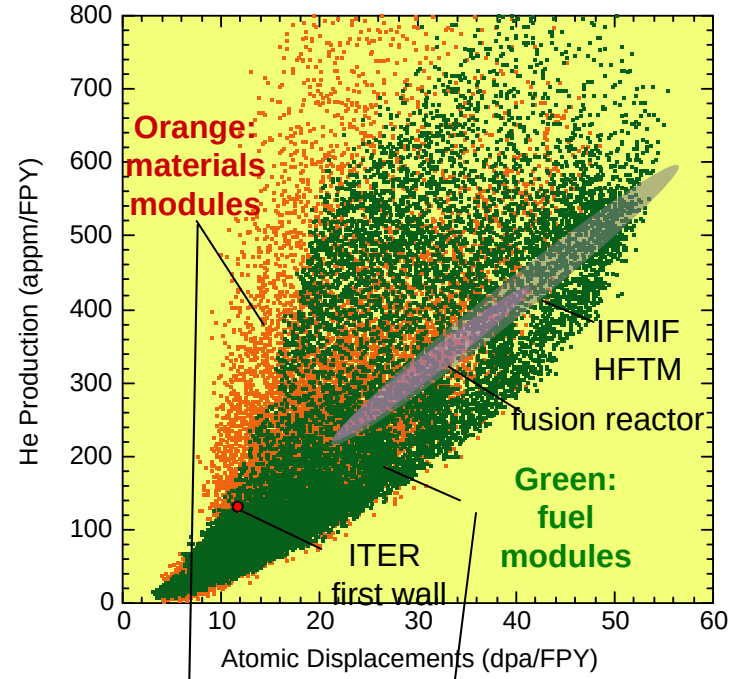
Through Fission Fusion Materials Facility, MaRIE creates extreme radiation fluxes and advances the frontiers of radiation damage science through in situ measurements

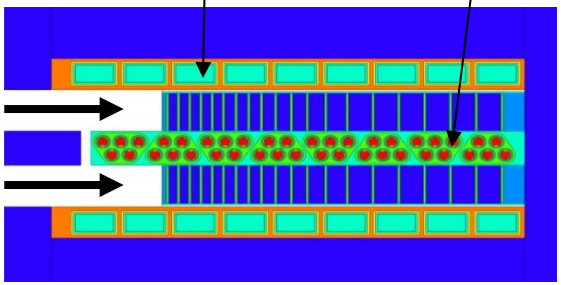
The same x-rays (protons) enable in-situ (near in-situ) measurements…



S. Zinkle

…in relevant environments





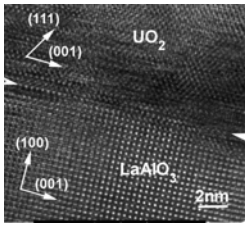
MTS target assembly

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

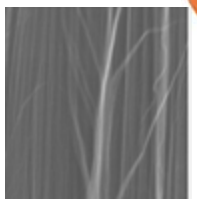
- Integrated synthesis, fabrication, and processing capabilities from molecules to nanoparticles to thin films to bulk crystals and architectures

- Rapid, flexible capability for new materials *designed from theory*
- *In situ* characterization during synthesis
- Robust structural and functional characterization capabilities

Thin film deposition
(PLD, PAD, IBAD, CVD, MBE, ALD)



FAB- 2-D lithography, FIB etching
Interface to circuits and patterning of surfaces



80 μm nanotube forest

Nano-architectures
Porous structures, nanoparticle synthesis, carbon nanotubes.

Single crystal growth
Casting

Tomorrow's multi-layered, 3-D structured devices

Molecular chemistry
polymer processing, soft materials, molecular receptors, catalysts.

Control

Integrated Synthesis Capability

Current MaRIE definition is pre-conceptual: Facility definition must be driven by community-identified performance gaps and functional requirements

- **Photons**
  - -with enough energy to penetrate micron frontier
  - -with enough brilliance & coherence to yield high quality data in an in situ snapshot
  - -with enough predictable pulses for a series of stroboscopic image

(20 GeV XFEL w/ 2 undulators → 50-100 keV photons)

  - -which also yields electrons for radiography

- **Protons & Spallation-derived Neutrons**
  - -with enough intensity to produce sufficient damage
  - -with enough energy for dynamic density imaging at the micron frontier

(800 MeV, 1 MW protons (post-MTS) → 800 MeV, 1.8 MW with MaRIE)

  - -and for broader purposes

- New Measurement Hall – MPDH (including dynamic drivers)
- Enhanced MTS → FFMF (in-situ/near in-situ/PIE measurement capability)
- M4 Facility: Materials synthesis & processing/crystal growth flagship; Gateway to MaRIE

Potential evolutions from current preferred alternative

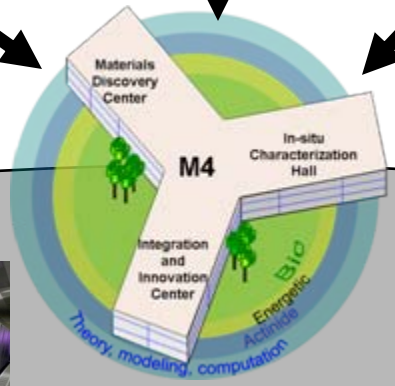
- Alternate scenarios for proton accelerator (higher energy, high-power superconducting linac)
- Alternate electron accelerator approaches (flat-beam transform, emittance exchange, pre-bunching)
- More undulators (directly to M4, and to enhance user capacity)

MaRIE: Integration is key – integrated facility capabilities and gateway to broader LANL

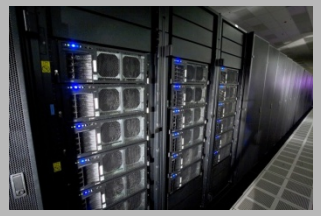
Portal to the External User Community

FFMF
- Pre and post irradiation characterization
- Radiation hard materials
- Materials synthesis in a radiation environment

MPDH
- Samples with controlled microstructure
- Complimentary ultrafast characterization
- In-situ characterization during synthesis



NHMFL

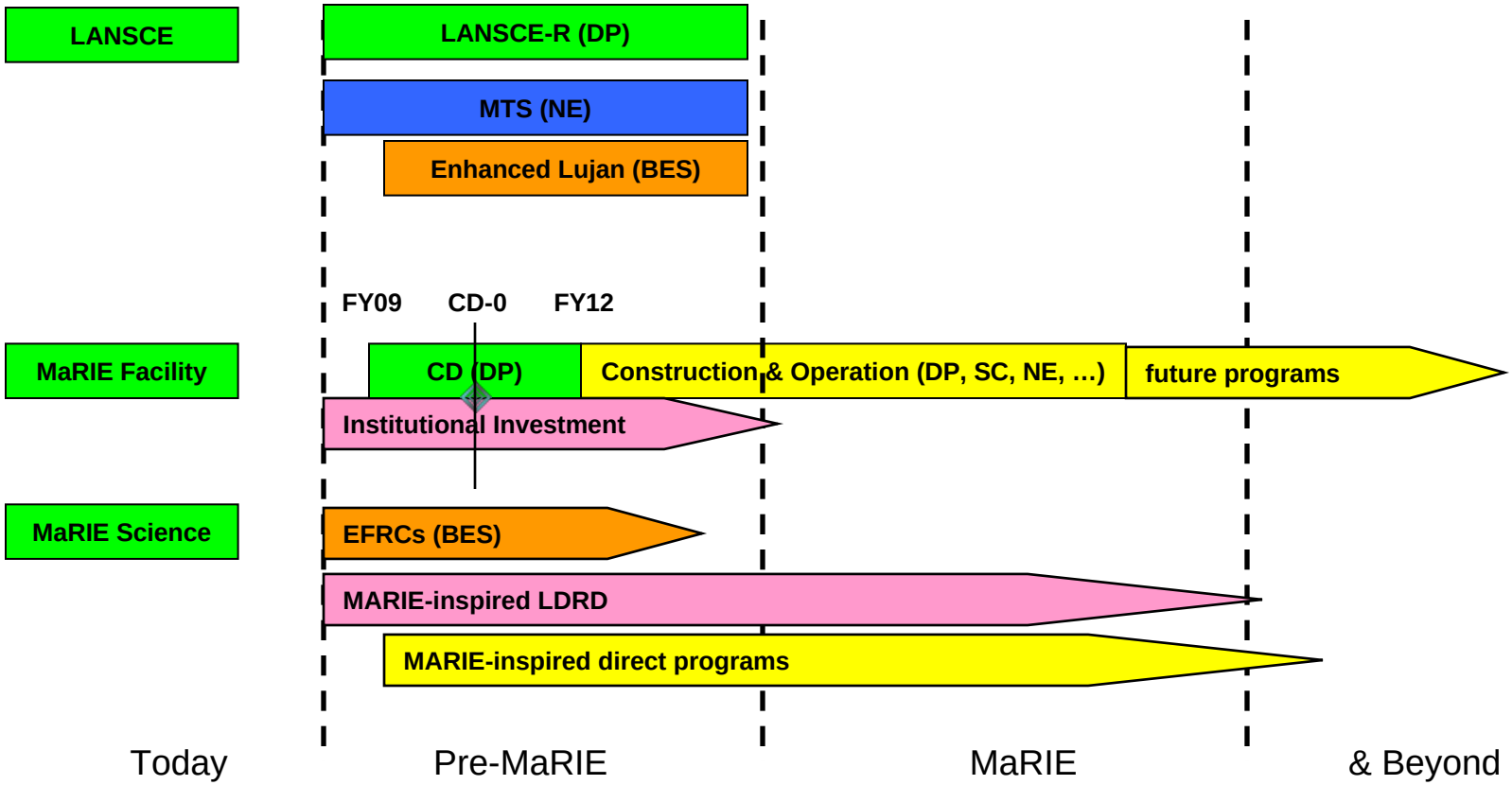

Roadrunner

Enhanced Lujan

CINT

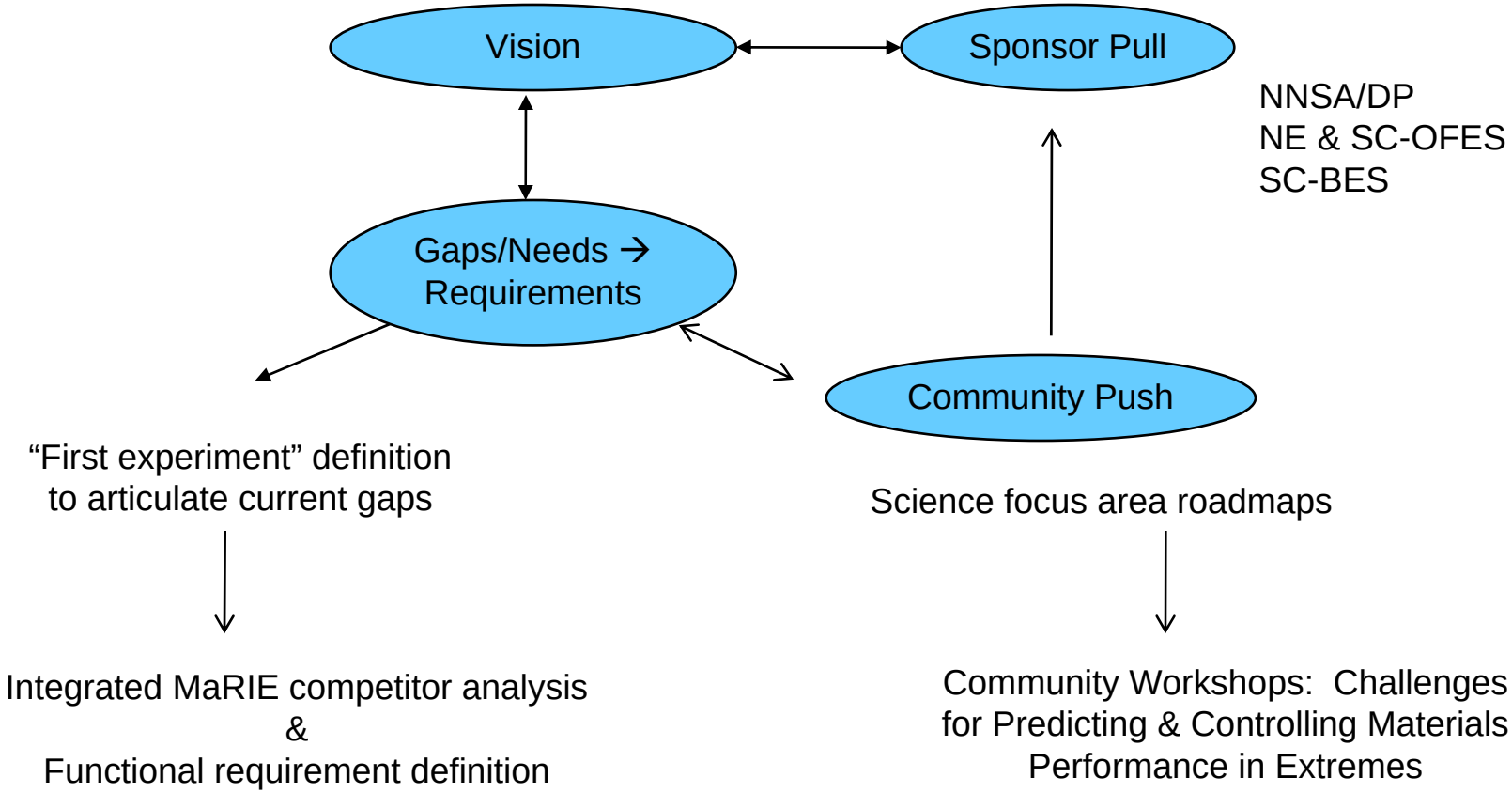
Integrated Solid State Solutions
- Materials with process aware controlled microstructure
- New radiation hard materials (self healing materials)
- Next generation photovoltaics/Advanced radiation detectors

MaRIE Acquisition Strategy Primary Planning Scenario: DP leadership is key



1) *Execute LANSCE-R + MTS + Enhanced Lujan Projects*
2) *Define Facility*
3) *Deliver MaRIE Science*

Current Facility Definition focus: On the road to CD-0



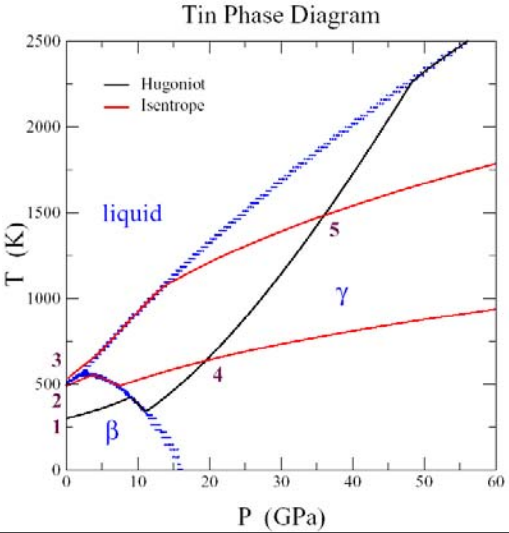
Success is seamless integration between/among these elements
The gold standard for Office of Science is NSLS-II

Gaps/Needs → Requirements

Frontier experiments identify performance gaps that form the basis of MaRIE's functional reqts

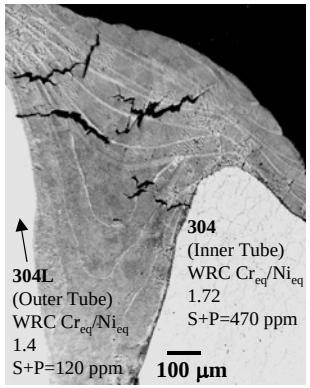
User Driven Science → Materiel Needs → **Functional Requirements** → Alternatives Analyses → **Performance Gaps** → Preferred Alternative & Roadmap → **Facility Concept**

Path dependence of strength



- 1 => 4, Shock loading (**high** strain rate & **solid-solid** phase transition)
- 2 => 4, Isentropic loading (**low**, variable strain rate & **solid-solid** transition)

Persistent observation of solidification/crystallization processes



Weld micrograph

Frontier Experiments define Functional Requirement Clusters

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*	*Ultrafast pump-probe; swept spectroscopy; nano-imaging*	*Multiple measurements over longer times*	*Intense ion beams*

Which Lead to Technical Alternatives

High-energy coherent x-ray imaging; dynamic electron microscopy; variable strain-rate drive; multiple surface diagnostics	Proton radiography; high-energy transient x-ray diffraction	Next generation temporal control for x-rays; optical ultra-fast lasers	Limits on duty cycle; phase contrast imaging	High-intensity ultra-fast laser system

C) Functional requirements - Frontier Experiments

To enable frontier experiments in …

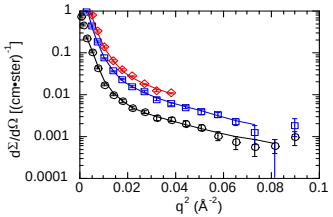
Corrosion	Swelling	Structural integrity	Phase Stability	Thermal Transport

Requires *in-situ* measurement of e.g. …

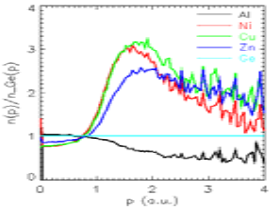
Corrosion *Growth rate* *Oxidation rate*	Void / Bubble *Total volume* *Nucleation* *Growth rate & size* *Spatial distribution*	Mech. properties *Creep strength* *Tensile strength* *Residual stress*	Phase *Composition* *Microstructure* Grain *Growth rate & size*	Thermo. properties *Heat capacity* *Conductivity* *Diffusivity*
layer *Thickness* *Composition*Fuel cladding *Interaction thickness*	Defects *Number* *Type* *Volume*	Cracks *Size* *Volume* *Shape*	Fission Product *Distribution* *Segregation* *Accumulation*	Temperature *Distributions*

In the laboratory environment ….

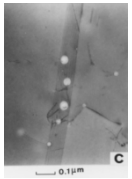
SANS / ASAXS



PAS



TEM



…. etc

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Frontier Experiments Define Functional Requirement Clusters

Frontier Challenges

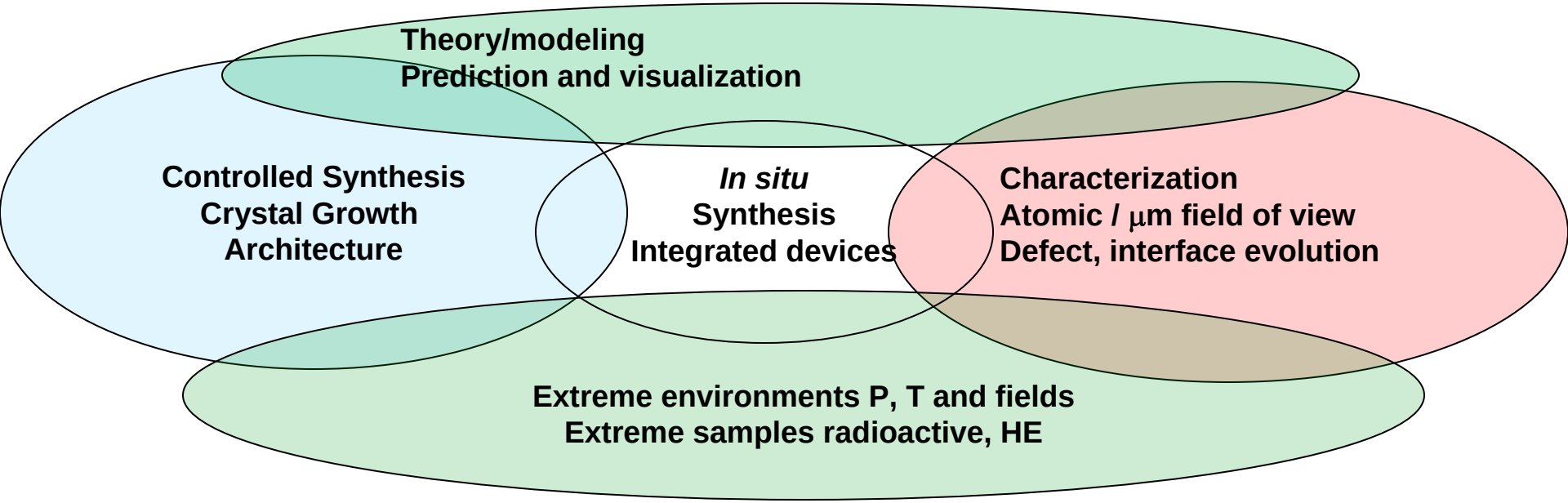
Energy Conversion and Storage

Radiation Extremes

Dynamic Extremes

Control of Complex Materials and Chemical Processes

Drive Functional Requirement Clusters



Define M4

Bulk single crystal growth

Flexible fabrication

High quality metastable materials

Nucleation and growth characterization

Multi-scale characterization of devices

Evolution of structure under irradiation

Dynamic structure-property relation

3.0 Building the Science Case

Deliverables for each:

- **Problem Statement**
- **Theory, Modeling, & Simulation Requirements Statement**
- **Solution Impact Statement**
- **Identify User Community**
- **Outreach**
- **Inreach**
- **Scientific Functional Requirements**
- **User Team Creation**
- **First Experiments Document**

Facility definition is being driven by community demand through validated performance gaps and functional requirements

Capabilities on the road to MaRIE

Controlled Functionality; Process-Aware Certification; Transformational Performance

and BEYOND

DECADE

MPDH *FFMF* *M4*

pRad @ GSI
LCLS-MEC
DC-CAT
MTS
HFIR, ATR
JANNuS
NSRCs

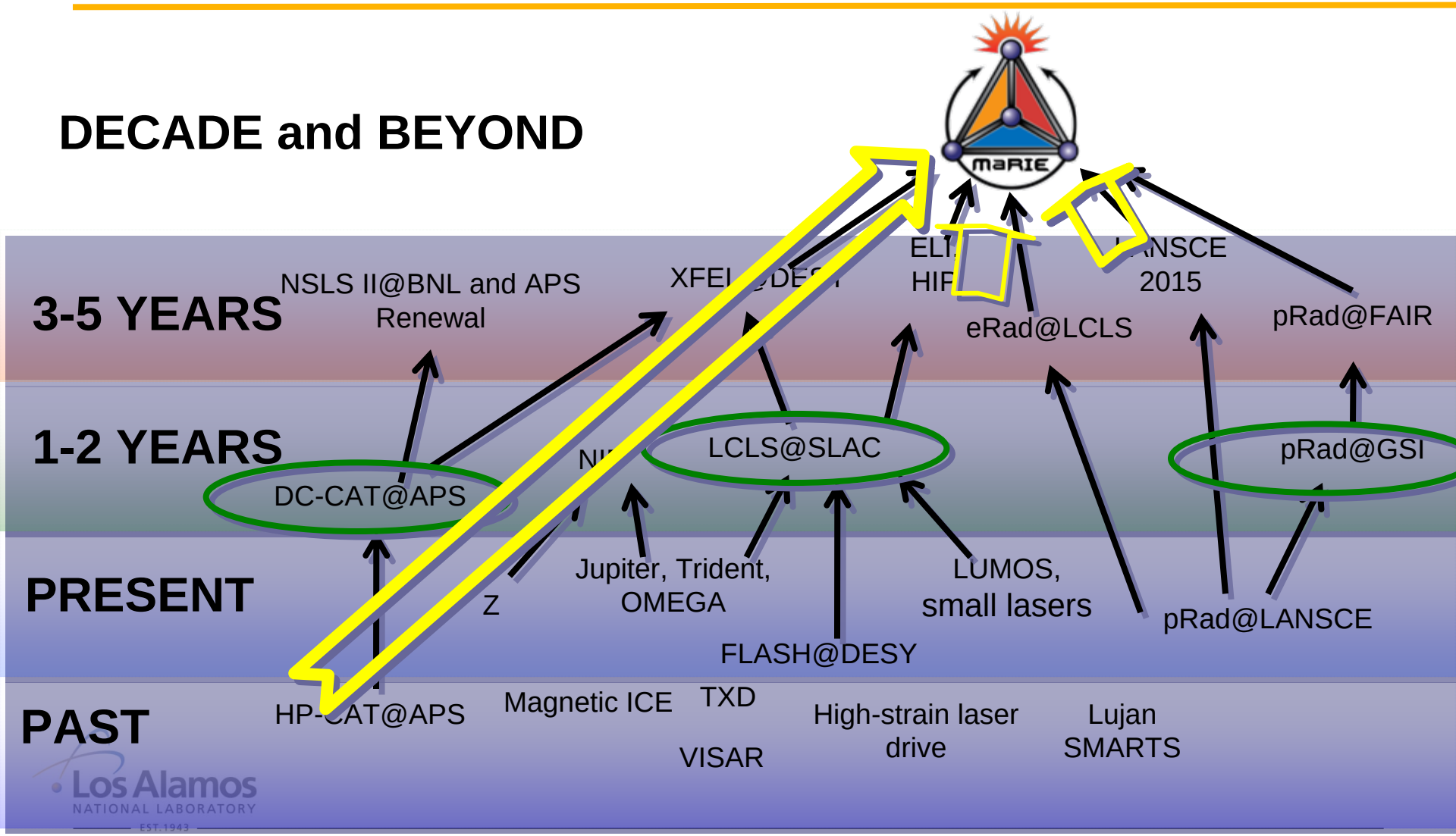
p, e- imaging	X-ray Sources	Lasers, Drivers	In-Situ Measurements	Relevant Doses	Lab-Scale Extremes	In-Situ Char.	Synthesis Capability

PRESENT

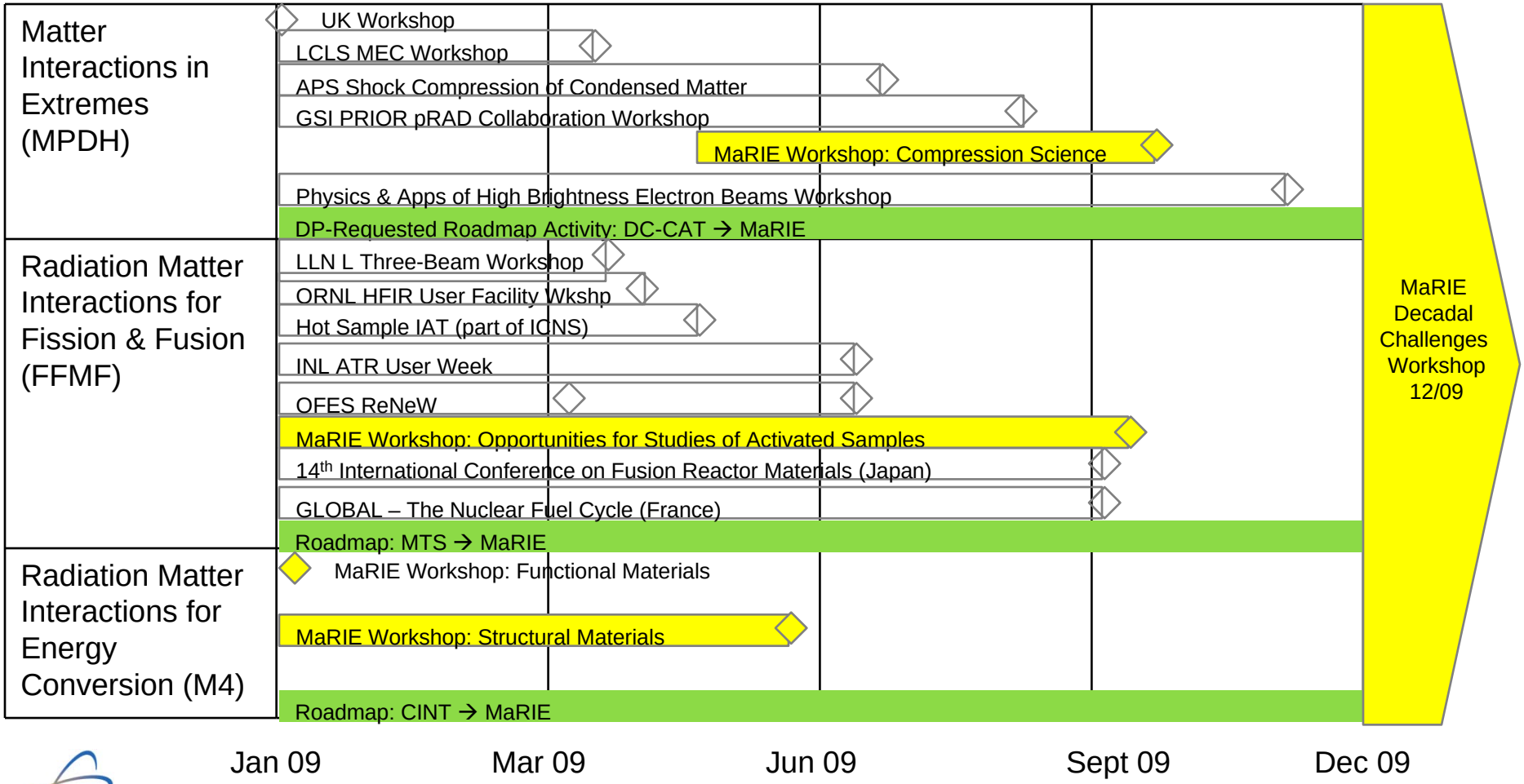
Multi-Probe Measurements **Extreme Environments** **Directed Synthesis** **Integration (esp. theory)**

Observation → Control

The Roadmap from DC-CAT to MaRIE



Community Engagement: Road to 12/09 Workshop



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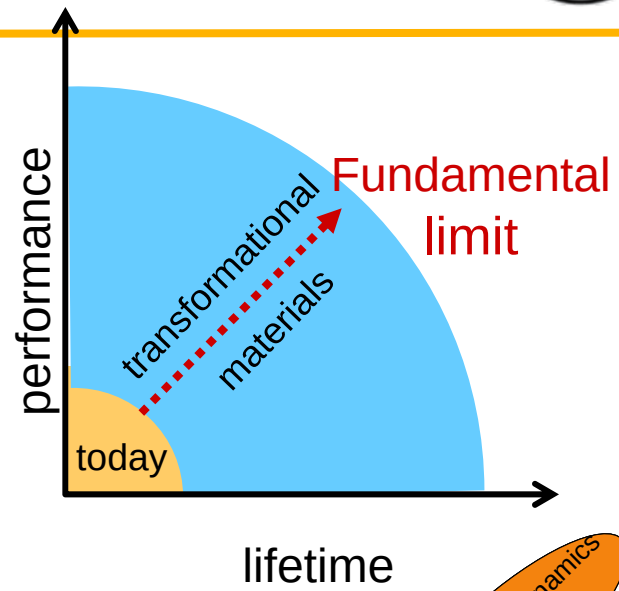
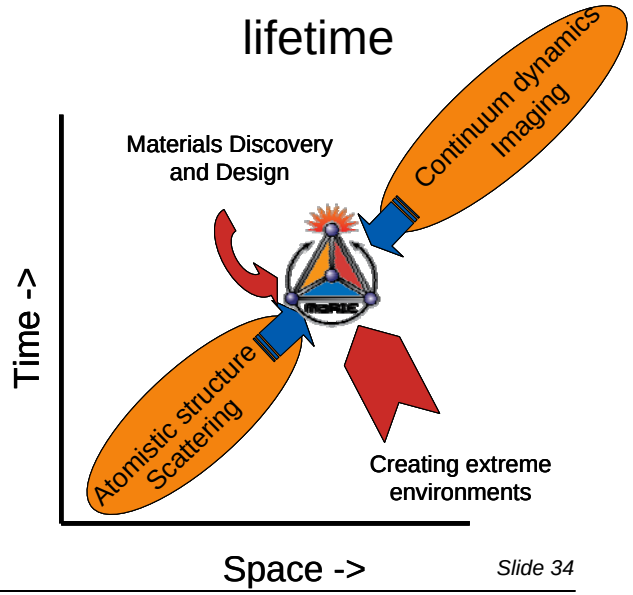
The transition from "observation & validation" to "prediction & control" is a central mission challenge AND the frontier of materials research

- **Conquering "the micron frontier" is essential for solving transformational materials grand challenges**
- **MaRIE will provide unique capabilities**
  - Simultaneous *in situ* imaging and scattering measurements
  - Accessing materials irradiation/damage extremes
  - Incubating materials discovery and solutions through control of defects and interfaces
- **LANSCE is essential for MaRIE's success**
- **Facility definition is being driven by community demand through validated performance gaps and functional requirements**





MaRIE will be the first capability with unique co-located tools necessary to realize transformational advances in materials performance in extremes