LA-UR-13-25735
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Title:	MaRIE 1.0 70th Anniversary talk
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Intended for:	70th Anniversary Talk, 2013-07-27 (Los Alamos, New Mexico, United States)
Issued:	2013-07-23

70 YEARS OF CREATING TOMORROW

Los Alamos NATIONAL LABORATORY

MaRIE 1.0

*Ma*tter *R*adiation *I*nteractions in *E*xtremes 1.0

Mary Hockaday

70th Anniversary
July 27, 2013

UNCLASSIFIED

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NNSA National Nuclear Security Administration

Los Alamos:
Where Great Mission and Science frontiers meet

Our strategy as a multi-program national security capability laboratory **is to develop and apply the best science, technology, and engineering solutions to the toughest national security missions:**

- Multidisciplinary science, technology, and engineering challenges
- Problems demanding unique experimental and computational facilities
- Highly complex security issues requiring fundamental breakthroughs

The signature facility MaRIE is part of our strategy to meet the future

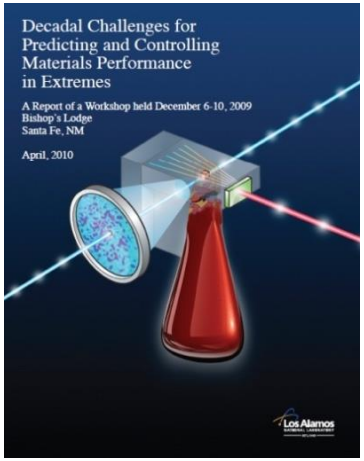
The confluence of unprecedented experimental capabilities and simulation advances are providing remarkable insights at length and time scales previously inaccessible

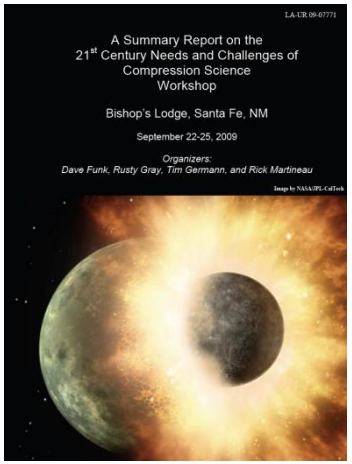
meso2012.com

science.energy.gov

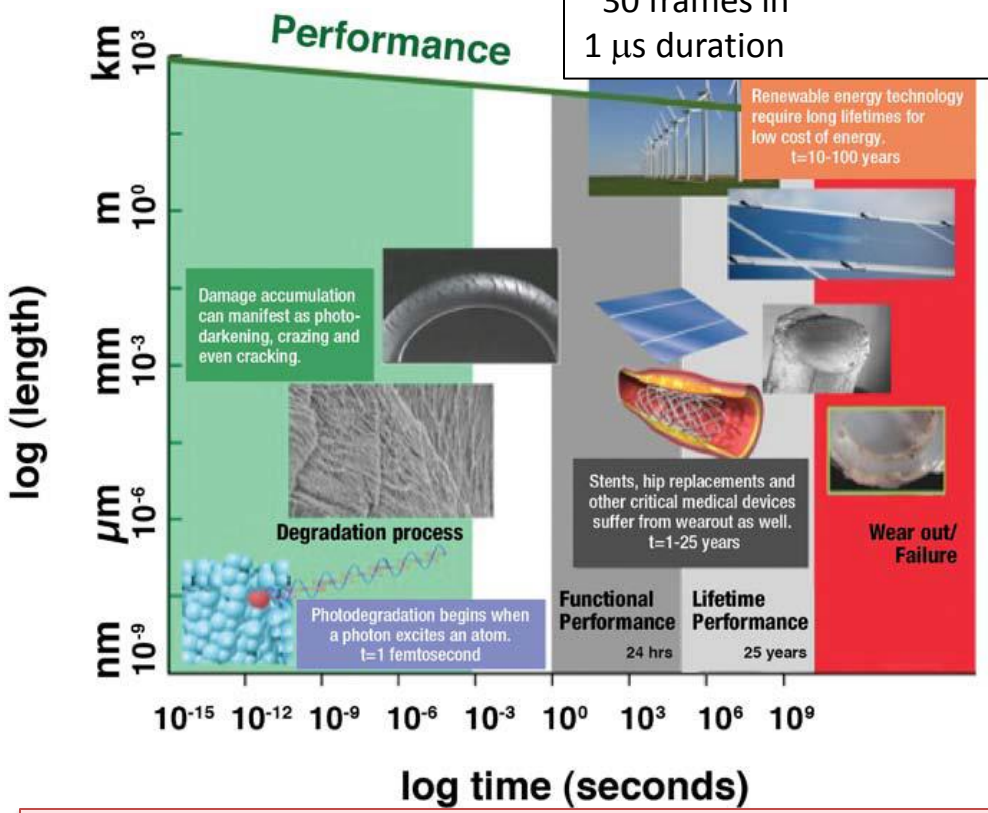
Materials Genome

Whitehouse.gov



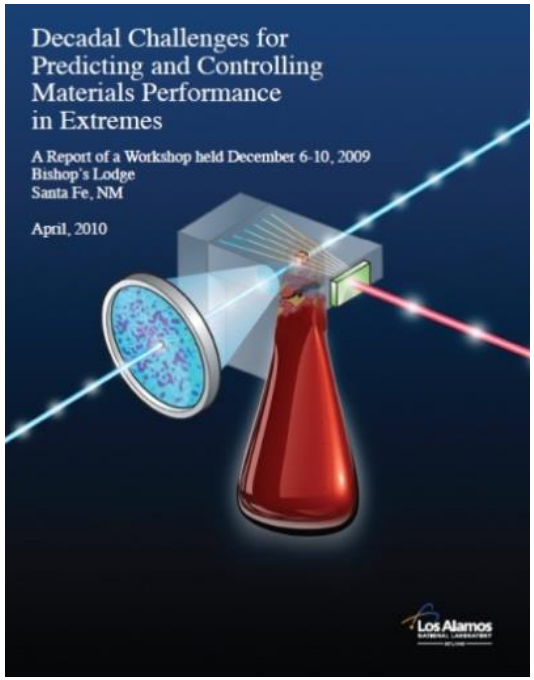


Sub-μm resolution
100's – 1000's μm samples
Sub-ns resolution,
~30 frames in
1 μs duration



The challenge is to observe the dynamic evolution of polycrystalline materials at the granular and sub-granular level

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



MaRIE brings together the new capabilities 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

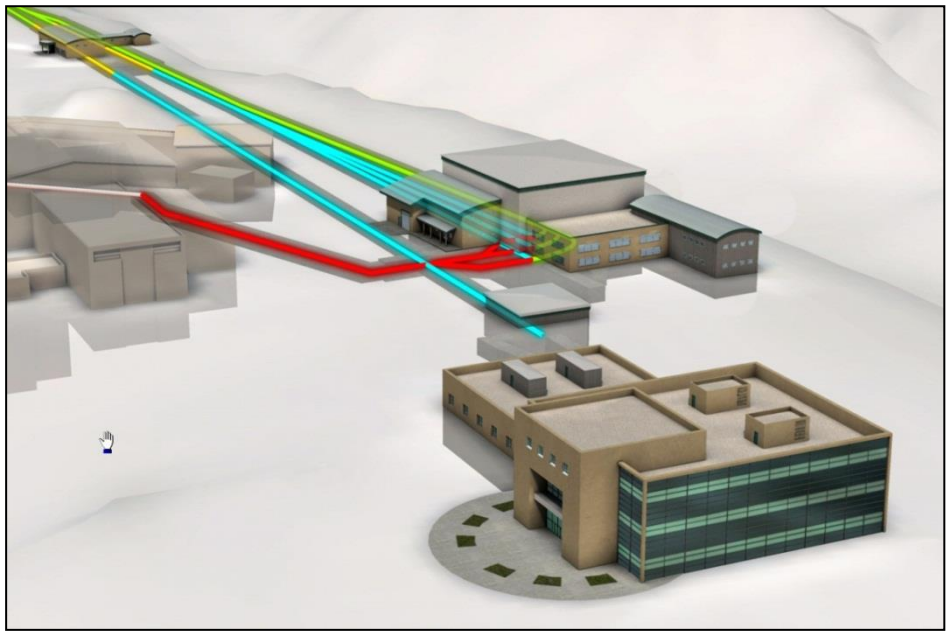
dynamic loading, irradiation

coupled with predictive modeling and simulation

materials design & discovery

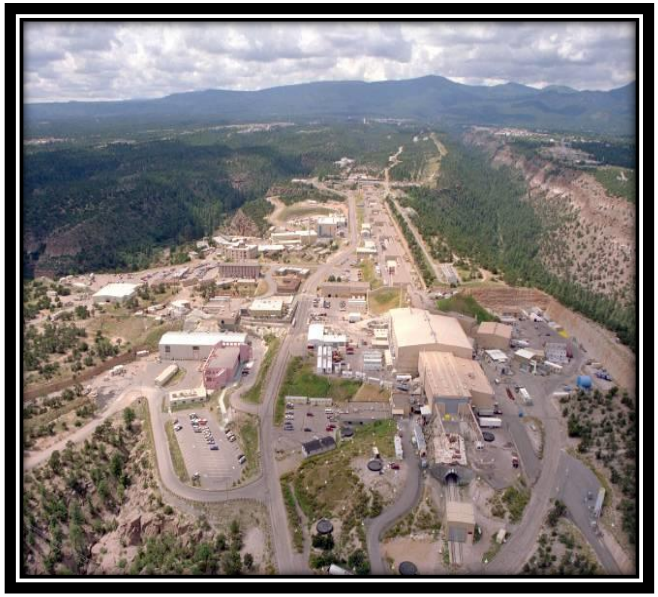
MaRIE 1.0 is the first phase of MaRIE focused on Stockpile Stewardship

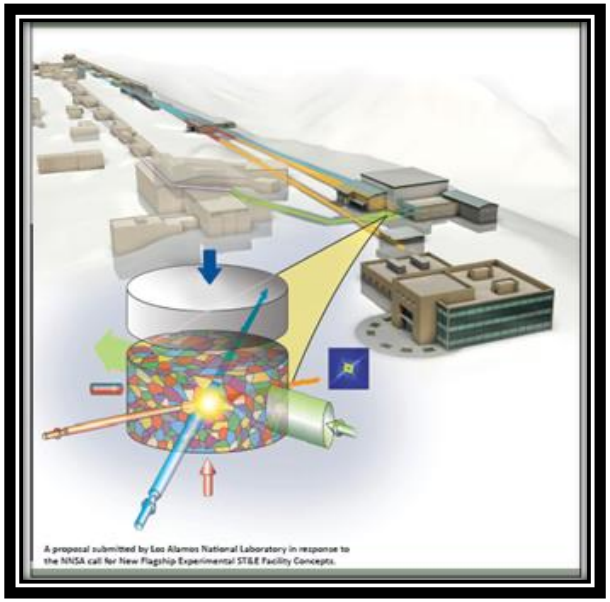
- **the world's first very hard (42-keV) XFEL**;
- **a new Multi-Probe Diagnostic Hall (MPDH)**, coupling hard, coherent, brilliant x-ray photons with 12-GeV electron and 0.8-GeV proton radiographic tools in dynamic extremes; and
- **a unique Making, Measuring, and Modeling Materials (M4) Facility** for materials synthesis and characterization with high-performance computational co-design focused on the mesoscale.



MaRIE 1.0 facility definition derives from "First Experiments" functional requirements and identified performance gaps

MaRIE builds on LANSCE's success

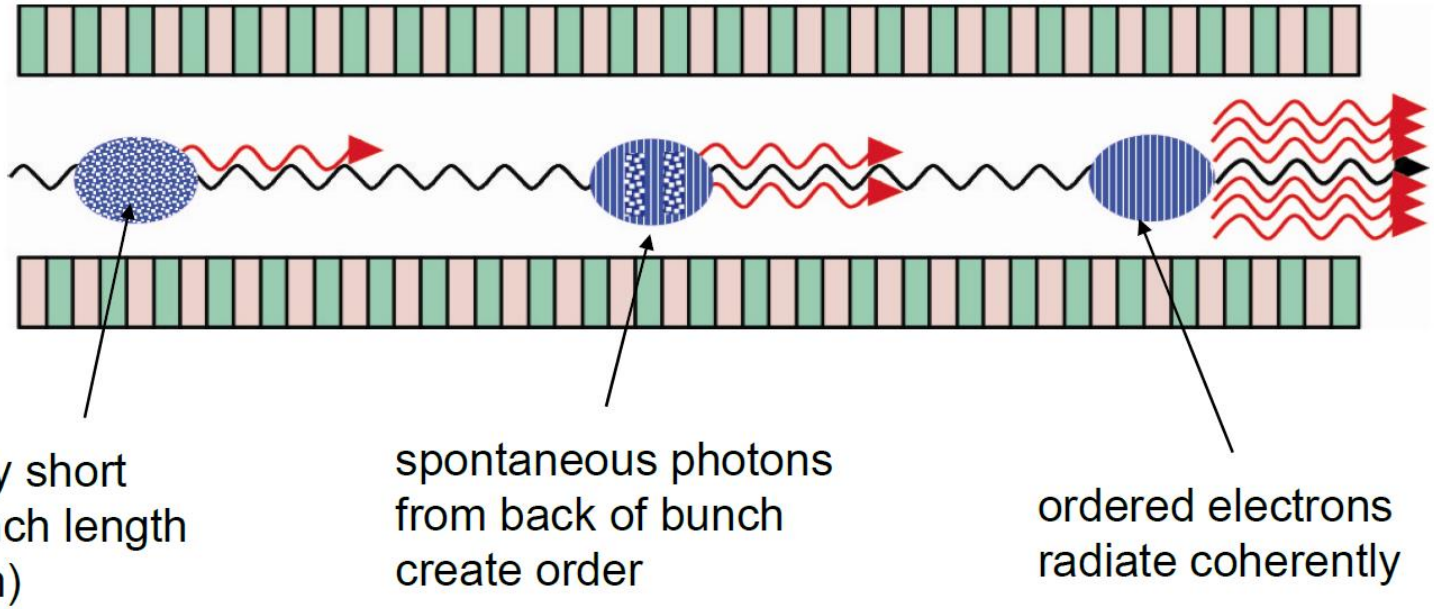




- Provides ~$1B infrastructure site credit towards MaRIE
- Expertise in mission materials (Pu, HE,…) in a classified environment
- Experience optimizing the co-existence of basic and classified research
- Proven track record in running large accelerator based facilities

A Free Electron Laser (FEL) is NOT Your Ordinary LASER

- Intense, coherent radiation output definitely LASER* like
  - Complete tunability because electrons are free from atoms
- Send electron bunch produced by a linear accelerator through a very long undulator



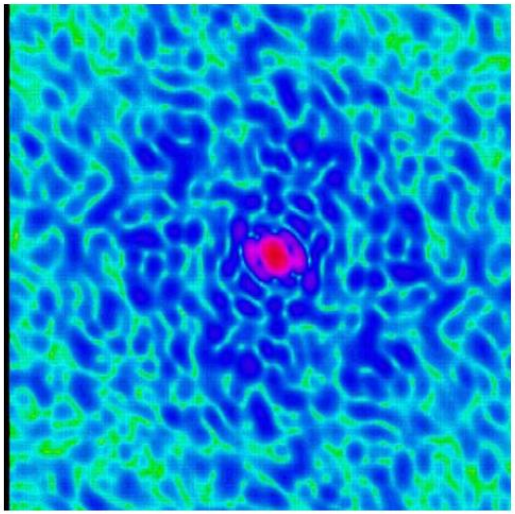
* Light amplification by stimulated emission of radiation

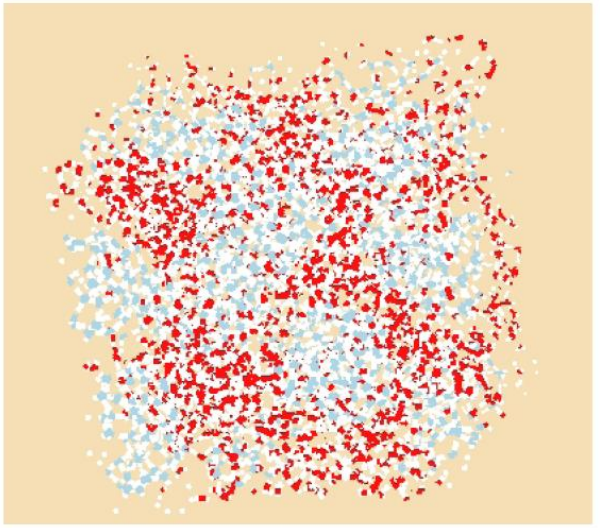
The MaRIE 1.0 XFEL is a unique source of very hard, coherent, brilliant photons

Current preconceptual reference design leverages SLAC expertise in XFEL design, construction

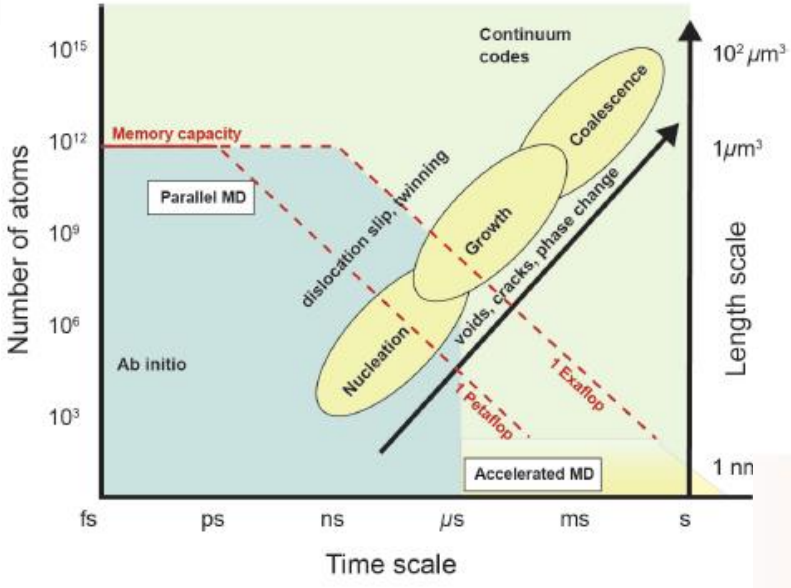
What We Can Do With an 'Ultra-Fast, Ultra-Bright' X-ray Source

- Make movies of the chemistry in action during material synthesis
- Study the structure and time-resolved function of single molecules
- Do 3D imaging and dynamical studies of materials
- Characterize the transient states of matter created by radiation, pressure, fields, etc.



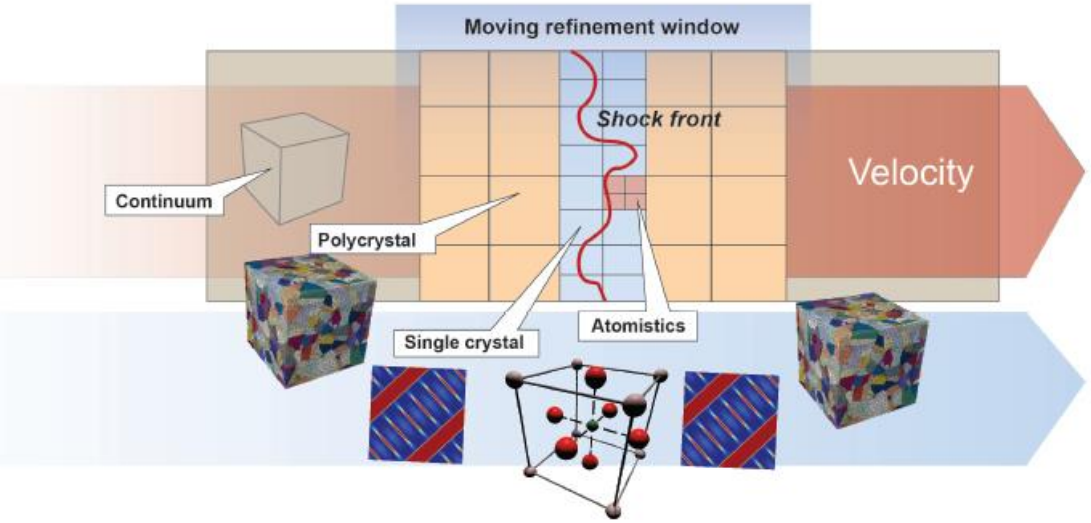


There is a symbiotic relationship between MaRIE and advanced computational power to achieve self consistent modeling of newly manufactured materials & components



Mesoscale materials phenomena need extreme-scale computing

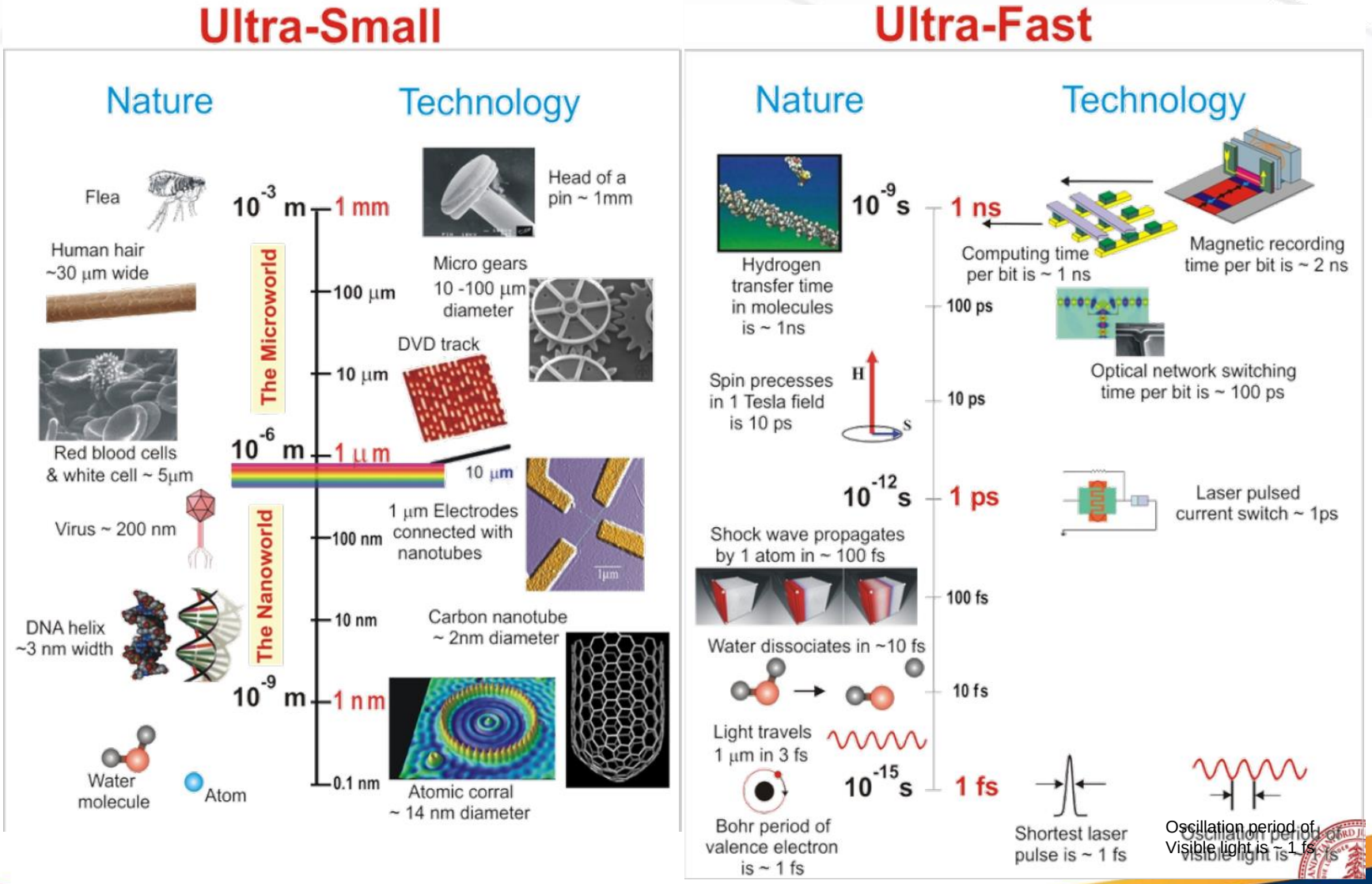
Variable-resolution models are synergistic with multi-probe, in-situ, transient measurements



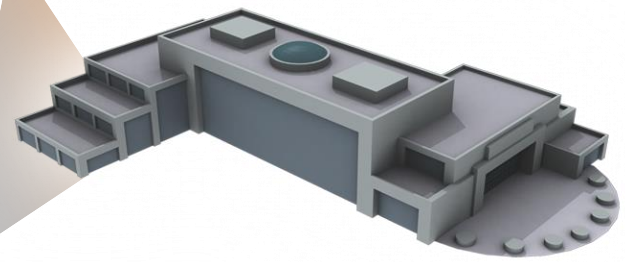
"First Experiments" define mission-driven functional requirements and reveal facility performance gaps

Mission Need	First Experiments	Functional Requirements	Performance Gaps
	Dynamic Materials Performance • Multiphase High Explosive Evolution • Dynamic Performance of Plutonium and Surrogate Metals and Alloys • Turbulent Material Mixing in Variable Density Flows **Process Aware Manufacturing** • Controlled Solidification and Phase Transformations • Predicting Interfacial Microstructure and Strain Evolution • High Explosive Functionality by Design	**Environments** • Dynamic pressure: 4–200 GPa • Strain rate: 10^{-3}–10^{7} s^{-1} • Stress loading > 200 ns • HE < 500g (< 30g with SNM) • Temperature rate 10^{5} °C/sec **Transient Multi-frame Measurements** **Imaging** • 0.1–1 µm, < 0.3 ns res over 0.1–1 mm • 0.1–1 nm, < 1 µs res over 10 µm • 1% density accuracy **Diffraction** • Defects: 1 nm res over 10 µm • Phase: 1–2 µm res over 100 µm • Lattice Strain: 10^{-5}–10^{-3} over 10's of µm **Thermo-Physical** • Temperature: 10 µm and 10–100 ns res • Chemistry 1 µm; < 100 fs **Synthesis with *in situ* Characterization** • Single crystals and 2D interfaces • Tailored microstructures with control of grain size, phase, and composition • HE and actinides, metal alloys • Real-time feedback during processing	**Integrated Driver Suite** **Repetitive 42-keV coherent x-ray source with 10^{10} photons in < 1ps focused to 1–100 mm** **Dynamic charged particle imaging with 12-GeV electrons and 0.8-GeV protons** **Synthesis, characterization, and processing with control of impurities and defects** **Integrated co-design and data visualization**

Static "Structure" Combined with Dynamic "Function"

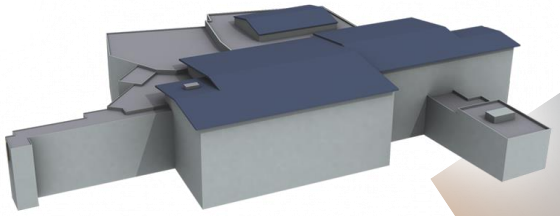


MaRIE's product and performance process for advanced materials



Multi-Probe Diagnostic Hall (MPDH)

- Performance
- Testing



Making, Measuring, and Modeling Materials Facility (M4)

- Fabrication
- Characterization

MPDH M4

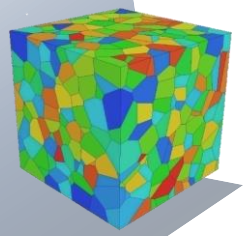
Materials Discovery and Fabrication

Process Theory

$$\text{where } K = \frac{\theta_c^2 p^2 \beta^2 X_0}{(14.1\,\text{MeV})^2}$$

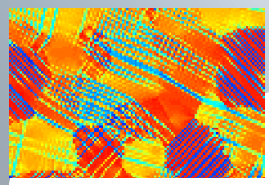
Theoretical Physics
Applied Mathematics
Plasma Physics
Solid Mechanics

Simulation



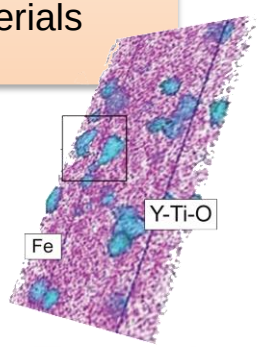
Computational Physics
Software Engineering
Systems Integration

In situ Characterization



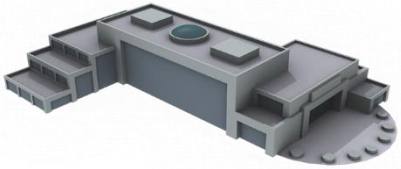
Materials Physics
Nuclear Science
Proton Radiography

Data Results



Process Data
Practical Applications
Nuclear Materials

Making, Measuring, and Modeling Materials Facility (M4)



MPDH M4

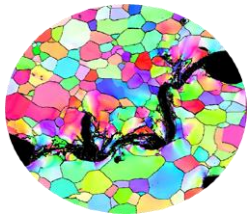
Performance and Testing

where $K = \frac{\theta_c^2 p^2 \beta^2 X_0}{(14.1\,MeV)^2}$

Performance Theory

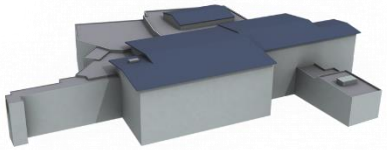
Theoretical Physics
Applied Mathematics
Plasma Physics
Solid Mechanics

Performance Data
Practical Applications
Nuclear Materials

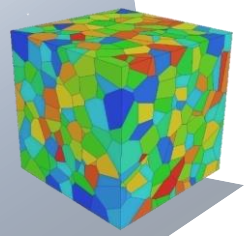


Results Data

Multi-Probe Diagnostic Hall (MPDH)

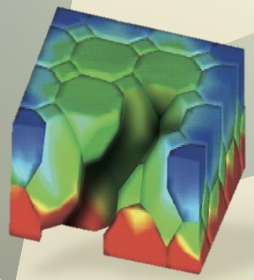


Simulation



Computational Physics
Software Engineering
Systems Integration

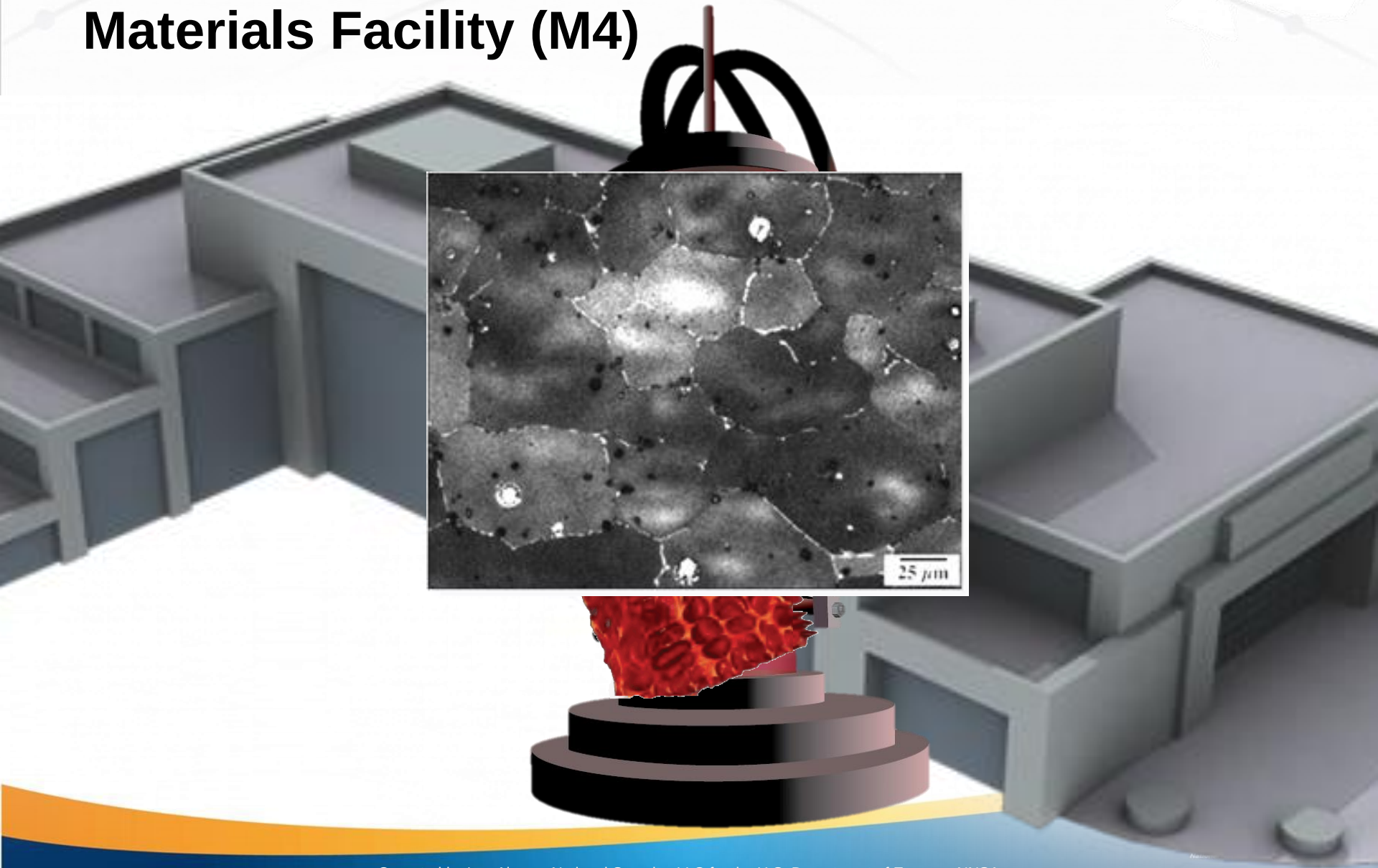
Experiment



Materials Performance
Materials Physics
Dynamic Phenomena

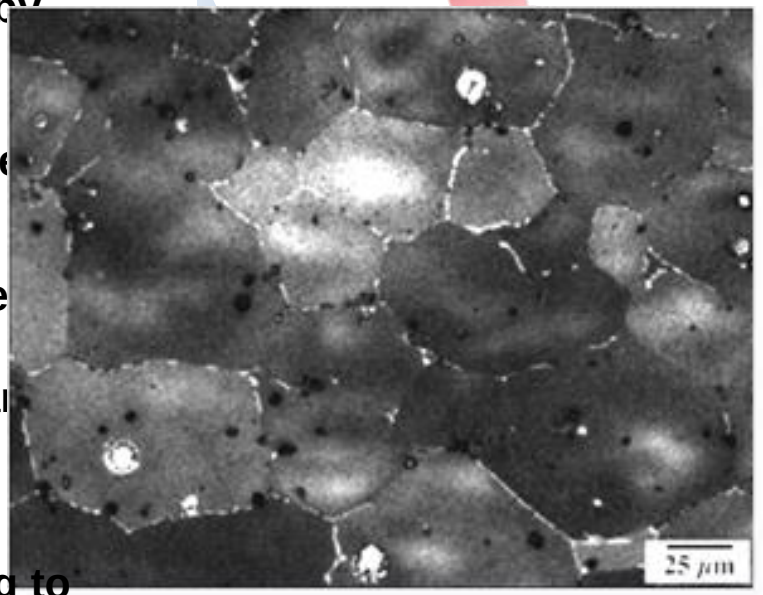
MPDH M4

Making, Measuring, and Modeling Materials Facility (M4)



Making, Measuring, and Modeling Materials Facility (M4)

- Enables discovery-by design of materials that have more durability in extreme environments
- Provides solid-state solutions for renewable energy a radiation detection
- Translates atomic-scale understanding to device performance



1Å - Electronic Structure

lecular Dynamics

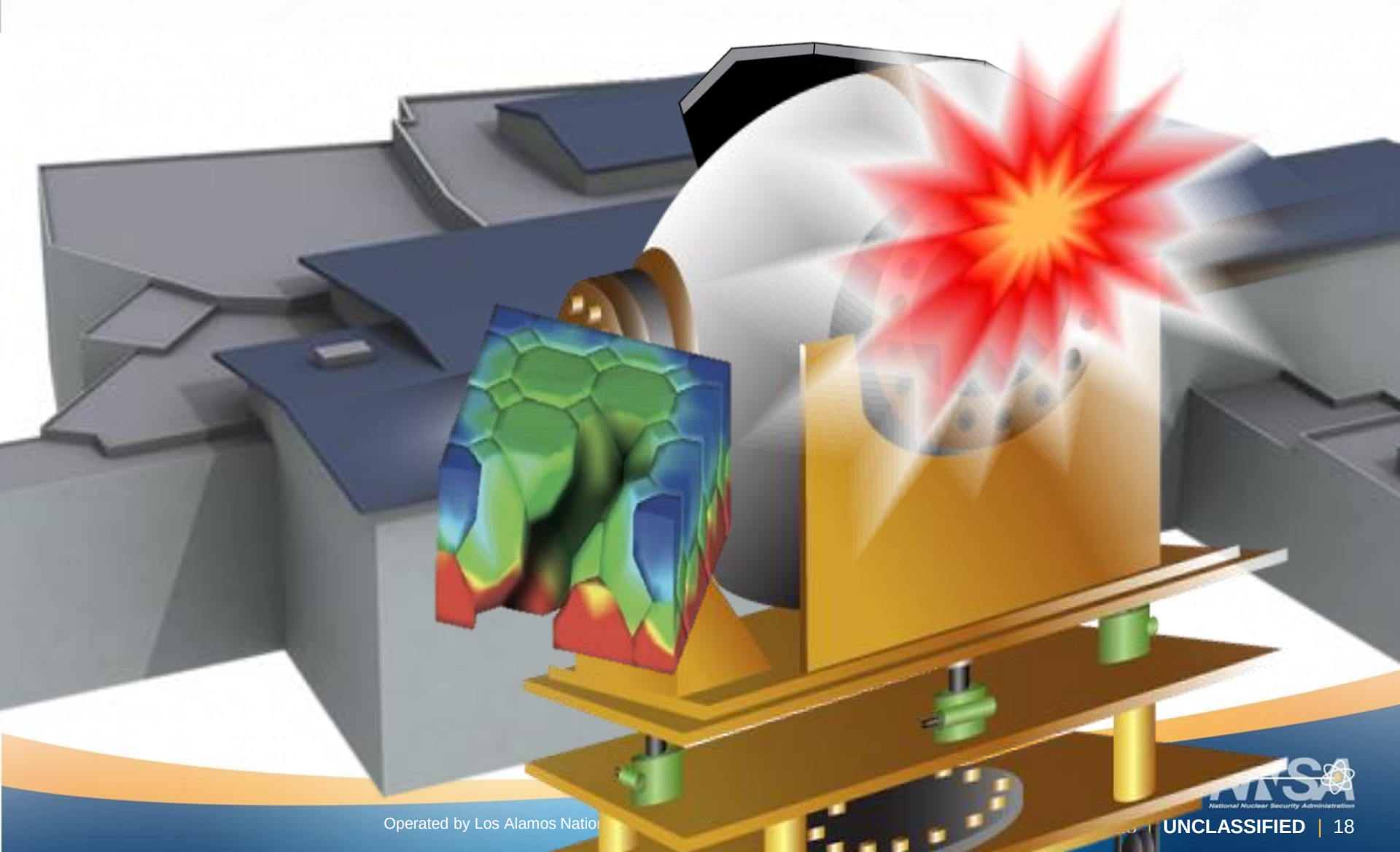
- Dislocation Dynamics

100μm - Single Crystal

1mm - Polycrysta

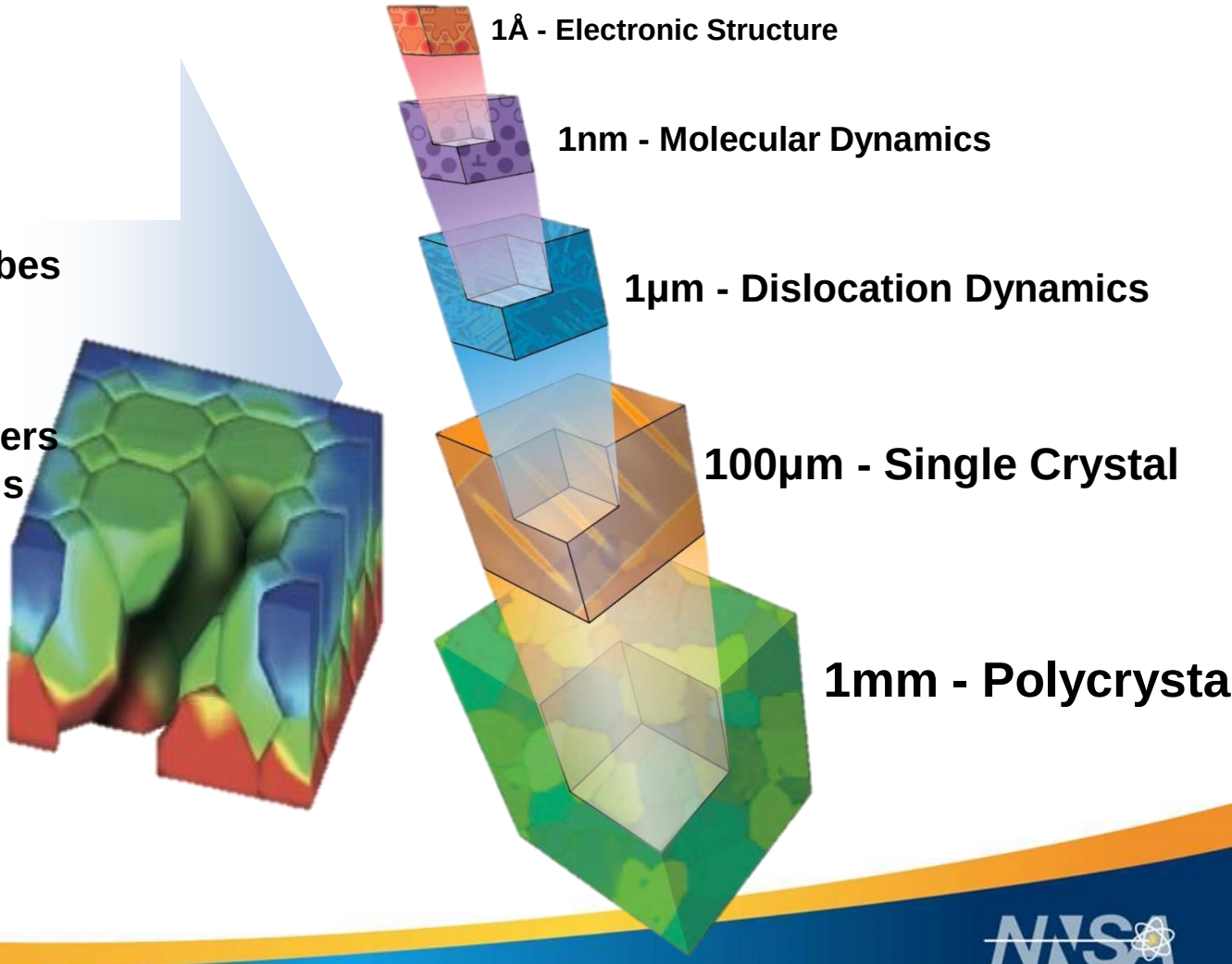
Multi-Probe Diagnostic Hall (MPDH)

MPDH M4



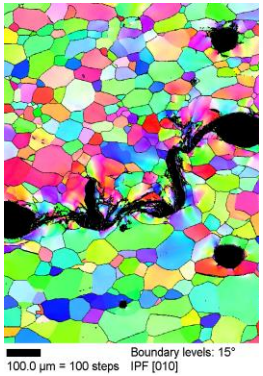
Multi-Probe Diagnostic Hall (MPDH)

- Unprecedented probes of matter under dynamic extremes
- Advances the frontiers of dynamic materials

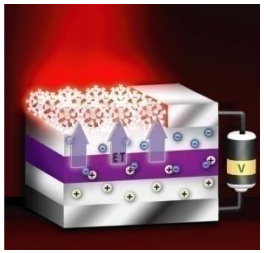


MaRIE : What does success look like?

- Predicting materials performance, including failure, in extremes of pressure and strain for multi-phase materials
- Exploiting complex materials and architectures for next generation electronics

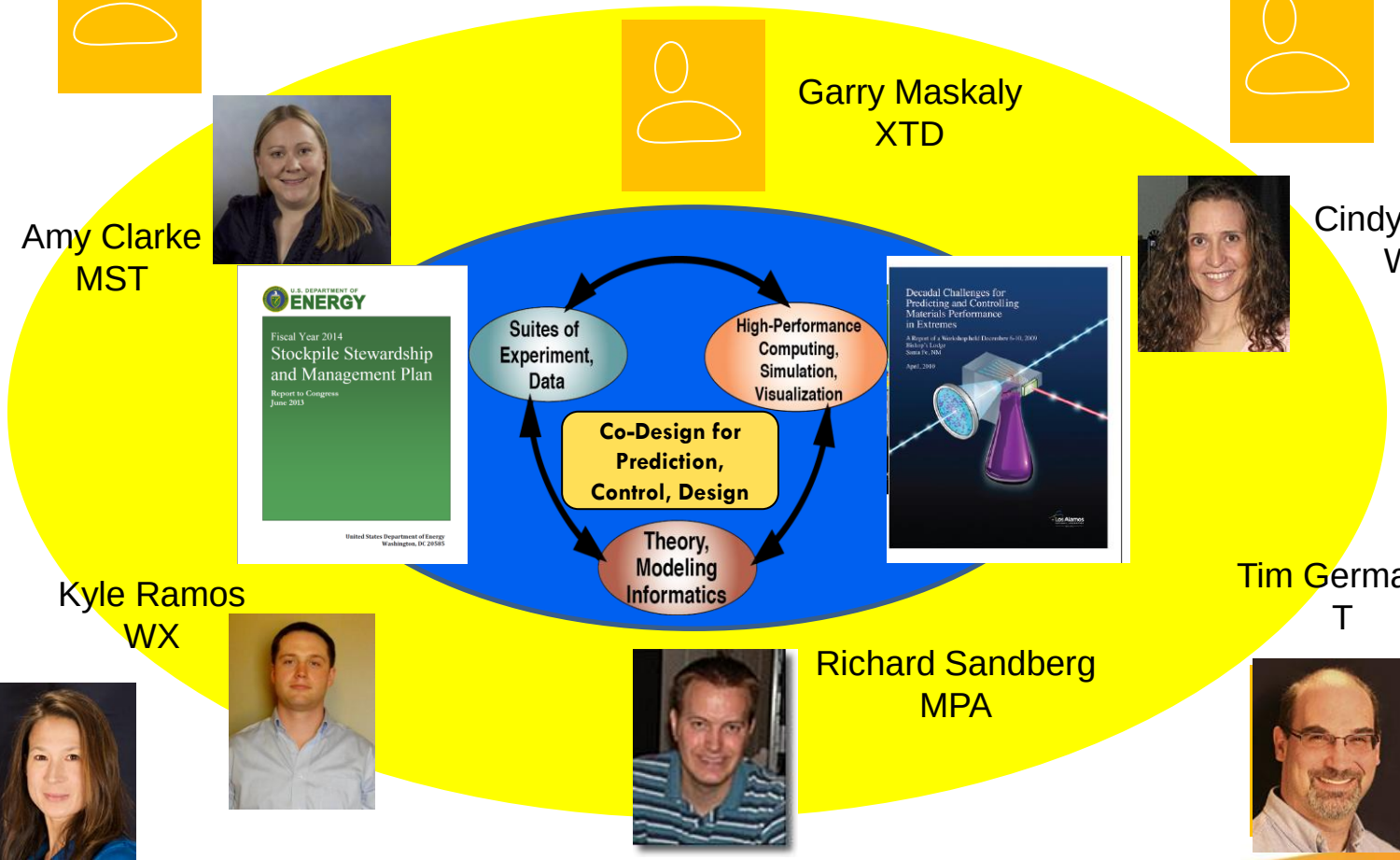


Materials failure under dynamic load


Next-generation solar cell architecture

Understanding and Controlling the Complexity of Real Materials

MaRIE 1.0 science and mission is already attracting the best and the brightest across broad disciplines



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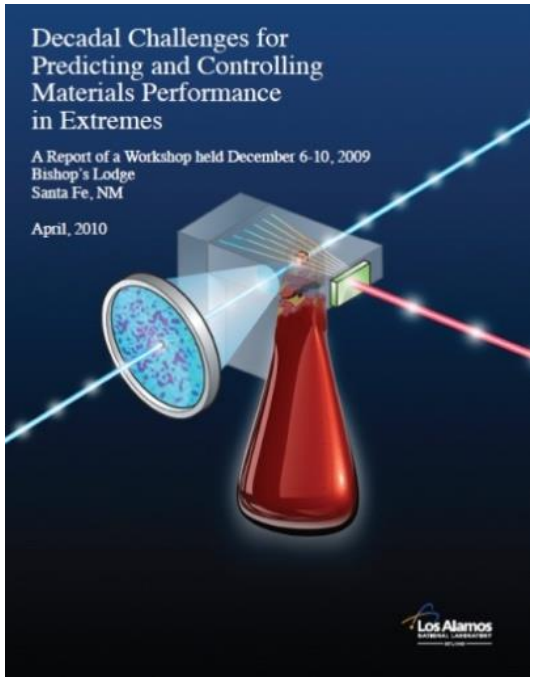

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