

# Exploring the Pivotal Role of Next Generation X-rays in Bridging the Scale-Gaps in Next Generation Energy Materials under Extremes

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2014 NSLS/NSLS2/CFN User's Meeting Workshop

May 19, 2014



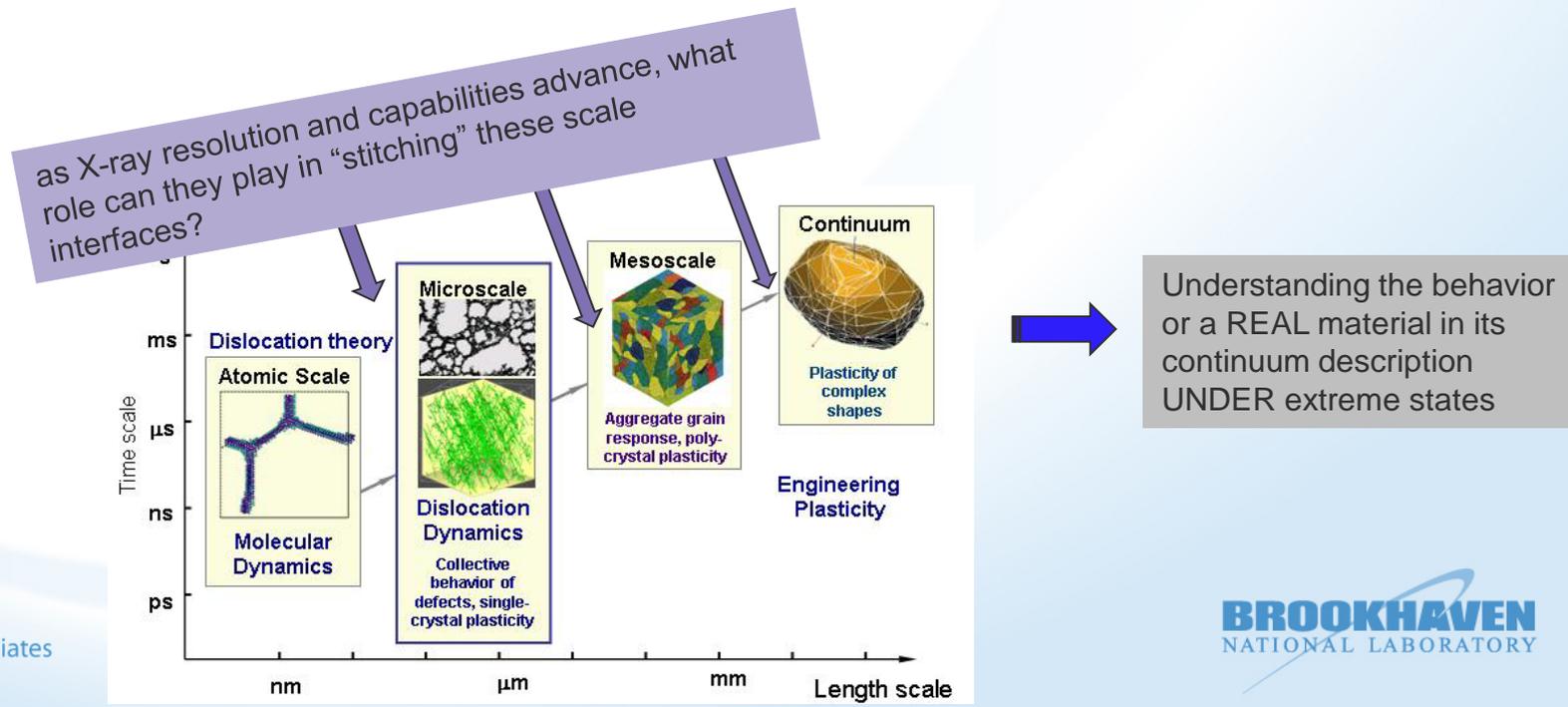
# WORKSHOP OBJECTIVE

Prompted by US DOE's interest in solving this "lingering" problem or challenge

Identification of synergies, interfaces and coupling between the x-ray field and

- a) the simulation world that spans the scales from atomistic to continuum
- &
- b) the science of materials under extremes

Aiming to identify the pivotal role and frontier science that X-ray techniques can play towards the scale-bridging challenges leading to a comprehensive understanding the behavior of next generation energy materials under extremes (nuclear, high pressure/temperature, etc.)



## Gratitude

BNL Photon Sciences and CFN UEC

Stony Brook University

BSA

→ PS organization staff that took care of every detail and logistical challenge

## Logistics

Would like to have all the talks from the workshops to post on the NSLS website and link to the meeting summary which will be in the June issue of **e-News**. Please indicate/approve the use of your talk presented during the workshop (or if you can provide a useable copy of the talk)

Also, objective of the workshop organization is to generate a White Paper where everyone presenting is welcomed to be part of the process

Workshop may be considered as the next step to a previously organized workshop at BNL on materials under extremes

# Characterization of Advanced Materials under Extreme Environments for Next Generation Energy Systems

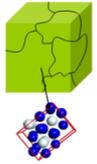
**Advanced Characterization of Materials Under Extreme Conditions Using Next Generation Probes**

**Ben Larson**  
Materials Science & Technology Division, ORNL

Workshop on  
Characterization of Advanced Materials Under Extreme Environments for Next Generation Energy Systems

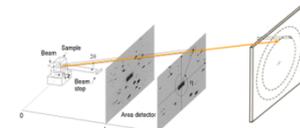
September 25-26, 2009  
Brookhaven National Laboratory

**3DXRD Vision**



- 3D characterization of individual grains within bulk polycrystals
  - Volume
  - Crystallographic orientation (intragranular ODF)
  - Grain boundary morphology (3D mapping)
  - Elastic strain tensor
  - Structural refinement
- Statistics over 100-1000 structural units
- In-situ annealing and deformation studies(4D)

**3DXRD set-up**



Detector I  
L = 5-10 mm  
Position and Orientation

Detector II  
L = 40 cm  
Orientation and Strain

Acq. time: 1-10 sec / 10-100 msec

Characterization of Advanced Materials under Extreme Environments for the Next Generation Energy Systems Workshop  
Brookhaven National Laboratory, Sept. 25-26, 2009

**Atomistic and Continuum Simulations of Phase Stability of Alloys - Advanced Models and Simulations of Nuclear Fuel Materials**

**Marius Stan**  
Computational Physics Group  
Los Alamos National Laboratory

Los Alamos UNCLASSIFIED NNSA

## Computational Approaches: Models and Simulations

James Glimm

Stony Brook University and Brookhaven National Laboratory

## Computational Modeling of Defects and Microstructure Dynamics in Materials under Irradiation

Anter EL-AZAB

Computational Science & Materials Science Programs  
Florida State University

Materials Under Extreme Conditions with Application to the Generation of Nuclear Power

National Spallation Light Source Workshop  
Characterization of Advanced Materials under Extreme Environments for Next Generation Energy Systems  
Brookhaven National Laboratory, September 25, 2009

**Fundamental Challenges in Multiscale Materials Modeling and Simulation**

**Sidsey Yip**  
Nuclear Science and Engineering and Materials Science and Engineering  
Massachusetts Institute of Technology

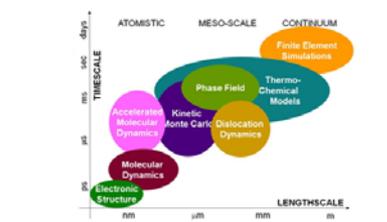
**A New First-Principles Computational Method for Disordered Materials**



**Wei Ku**  
CM-Theory, CMPMSD, Brookhaven National Lab  
Department of Physics, SUNY Stony Brook

**Tom Berlijn, Dmitri Volja**  
CM-Theory, CMPMSD, Brookhaven National Lab  
Department of Physics, SUNY Stony Brook

Multi-scale theoretical and computational methods<sup>1</sup>



Time Scale: 10<sup>-15</sup> s to 10<sup>10</sup> s  
Length Scale: 0.1 nm to 1000 nm

Methods: Acceleration Molecular Dynamics, Kinetic Monte Carlo, Dislocation Dynamics, Phase Field, Thermo-Chemical Models, Finite Element Simulations, Molecular Dynamics, Electronic Structure.

Los Alamos NNSA

<sup>1</sup>M. Stan, J. Nucl. Eng. Techn., 43 (2009) 38-52.  
<sup>2</sup>M. Stan, et al., J. Alloy Comp., 444-448 (2007) 415-423