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An Overview of Computational Materials Science & Engineering Department 1814

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NNSA National Nuclear Security Administration

Sandia National Laboratories

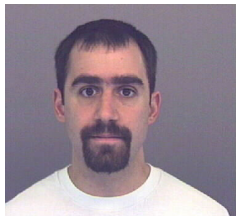
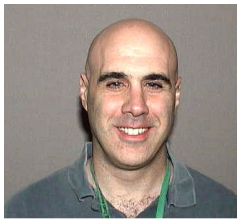
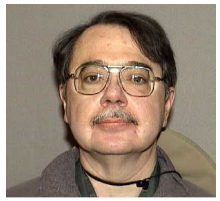
Department 1814 Computational Material Science & Engineering

Manager

Allen Roach

OAA

Cher Porter

	Atomistic	Grain Scale	Experiment
Hard Materials	 Stephen Foiles  Ed Webb	 Corbett Battaile  Liz Holm	 Luke Brewer  Tom Buchheit
Soft Materials	 Mike Chandross  Amalie Frischknecht  Frank van Swol	**Post Docs**  Joanne Budzien  Remi Dingreville  David Olmsted	

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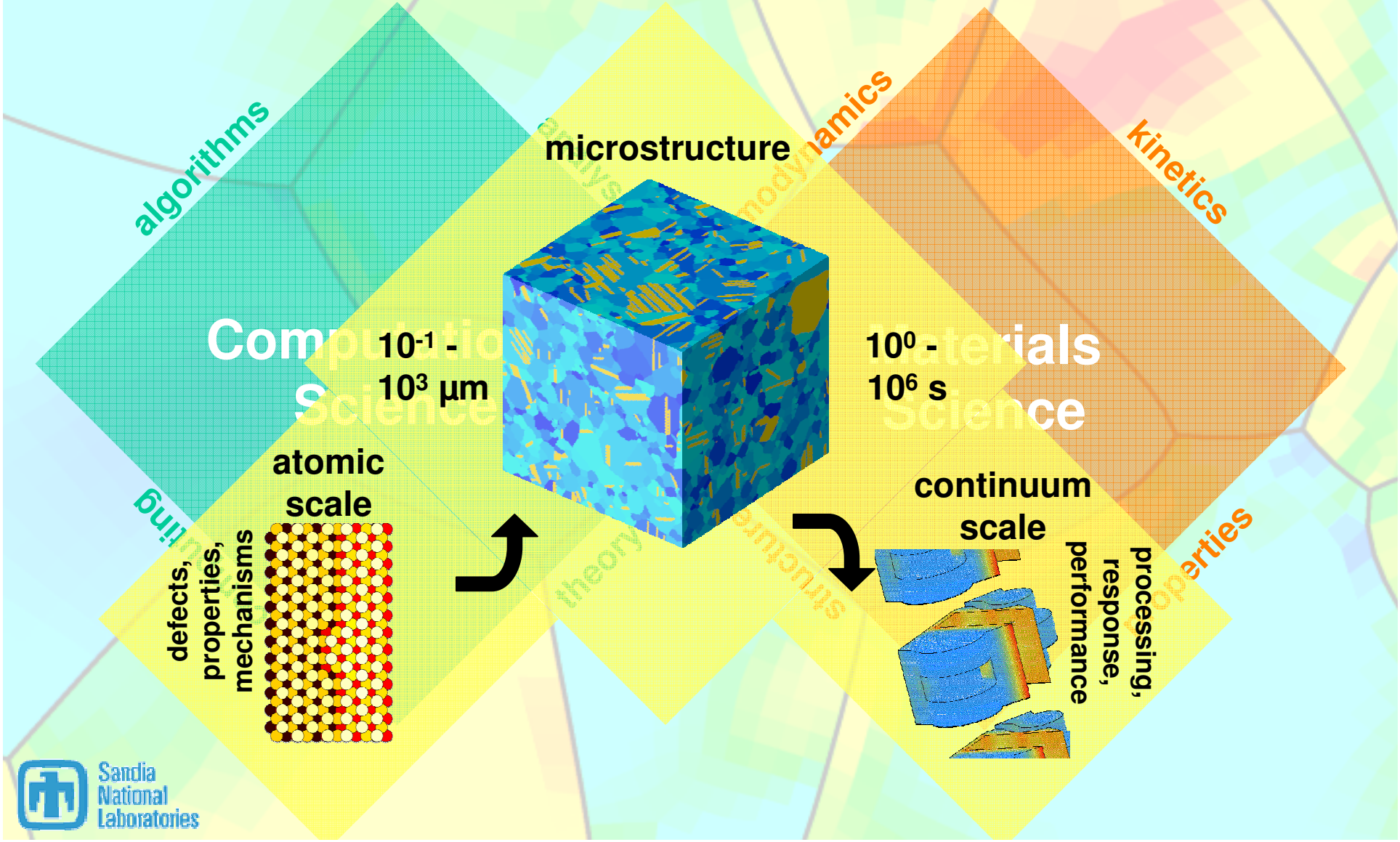
Computational Materials Science at the Mesoscale



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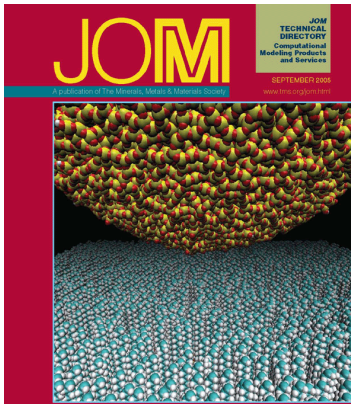
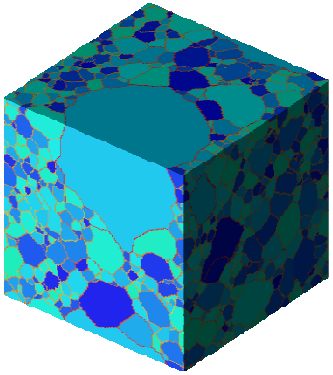
Modeling and Simulation through ASC is integral to our materials efforts

Integrate state-of-the-art modeling techniques, experimental validation, and high performance computing to:

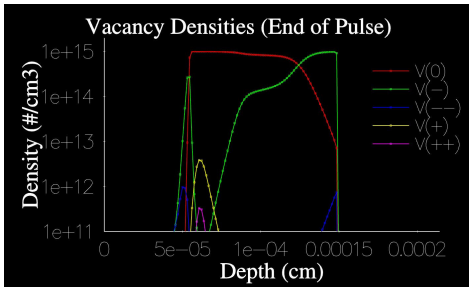
- **Elucidate mechanisms of materials behaviors**
- **Describe details in materials processing**
- **Predict material properties**
- **Design material substructure for desired performance**



Interface chemistry

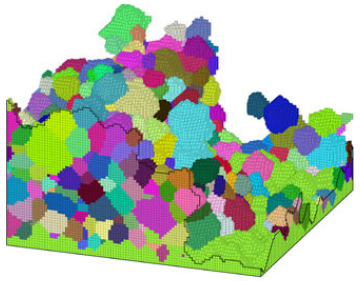


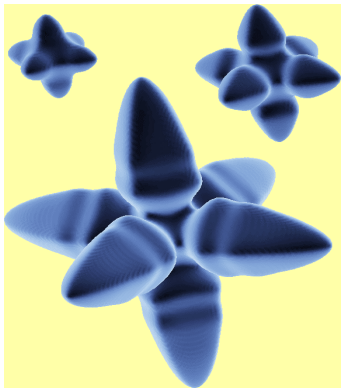
Recrystallization



Radiation Effects

Fracture

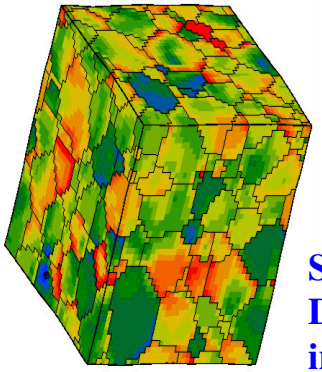




Dendrite formation in welds

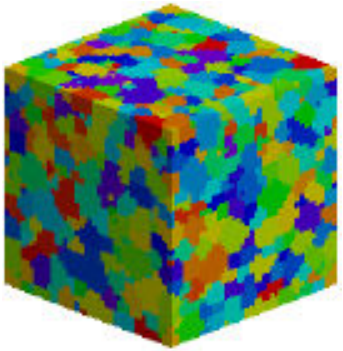
Add insight from validated materials models to higher level continuum models

Microstructure-Based Materials Modeling
Mesoscopic Approach



Crystal Plasticity

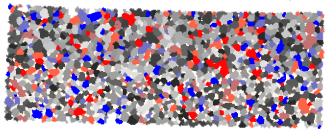
Stress Distribution in Grains

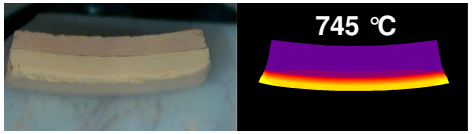


Microstructure

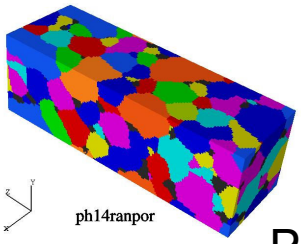
Ceramic Sintering

Bi-layer Microstructure

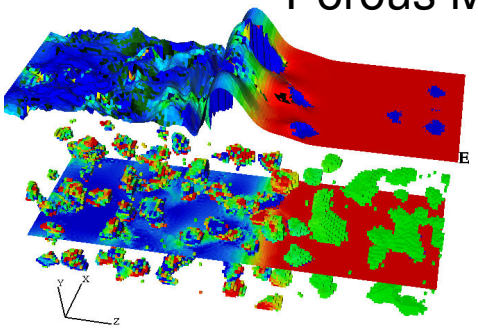




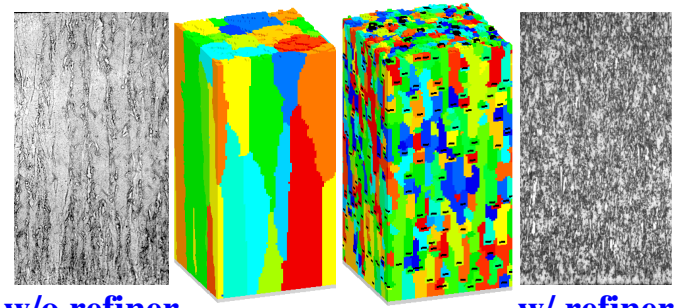
Experiment FEA



Shock Response in Porous Material



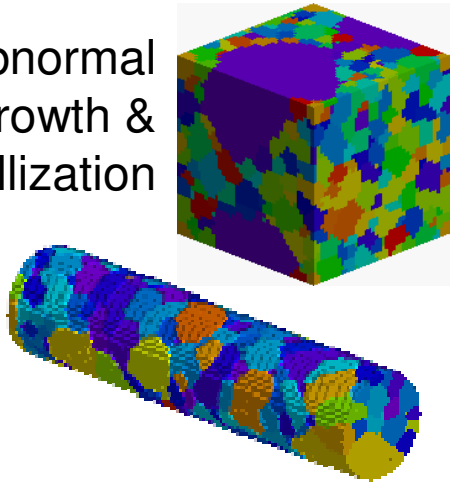
Electrodeposition



w/o refiner (Sulfamate)

w/ refiner (Watts)

Abnormal Grain Growth & Recrystallization



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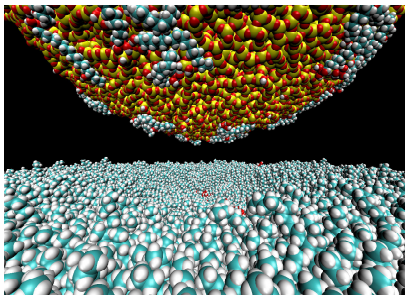
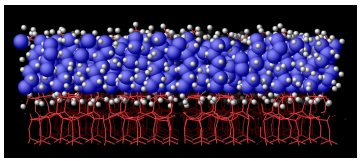
Microstructure-Based Materials Modeling
Atomistic Approach

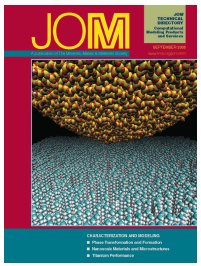
AFM Tip

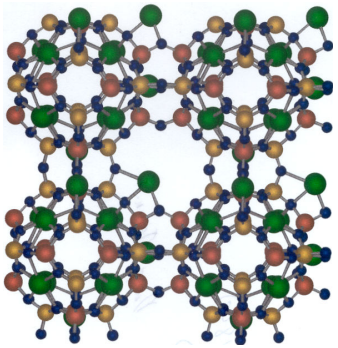


Polymer Coating



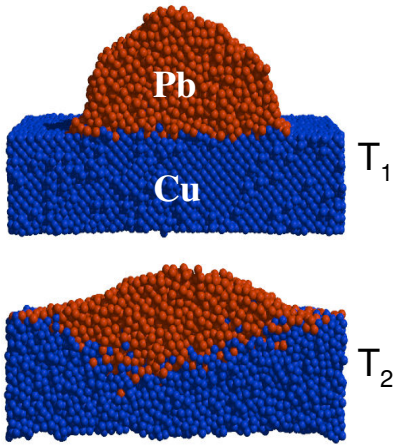
AFM Test on MEMS Coating

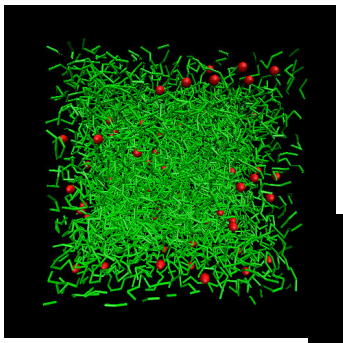




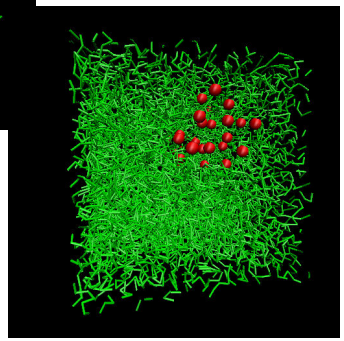
Quantum & Atomistic

Reactive Wetting

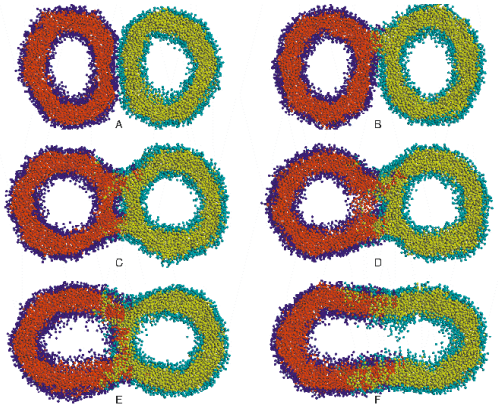




Nanoparticles in Polymer Thin Film

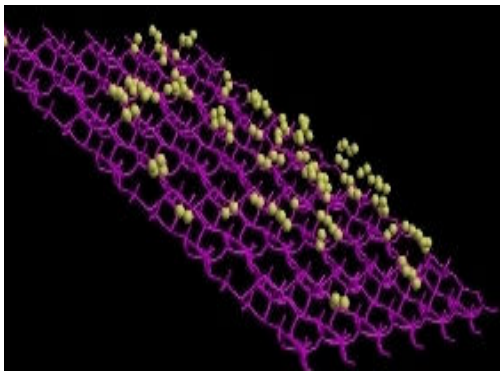


Molecular Biophysics



Fusing liposomes

Competitive Adsorption in Desiccant



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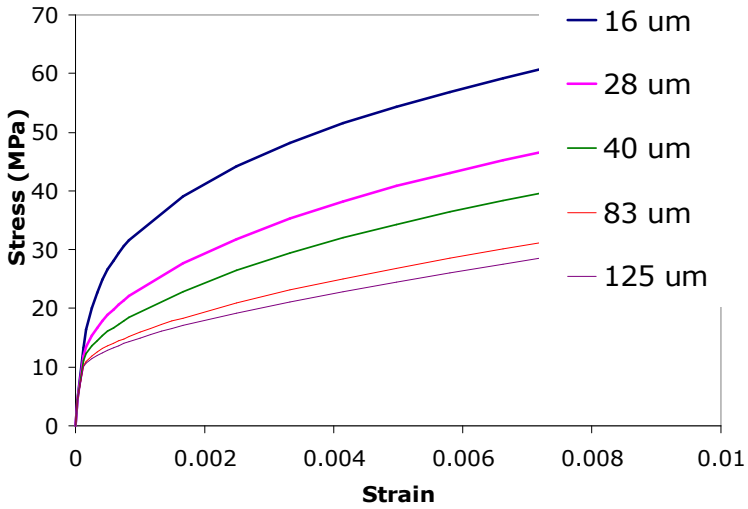
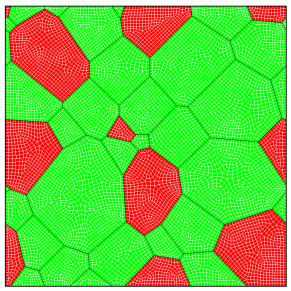
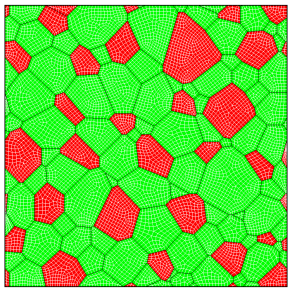
Example - Combining Microstructural Simulation with Experiment: Informing and Validating Model Development





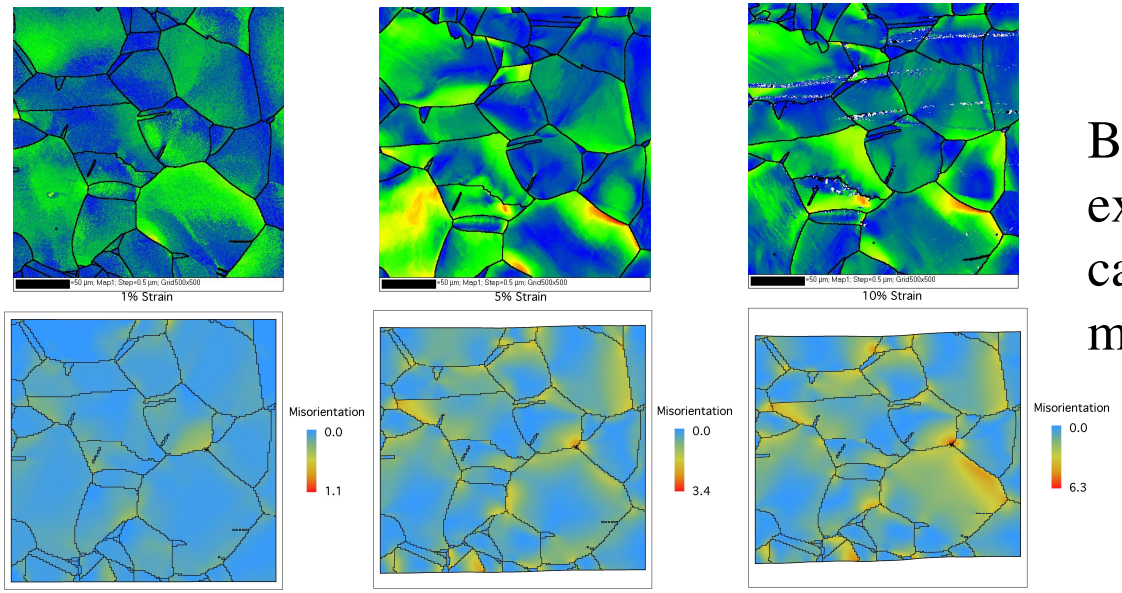
150 um



3.4 um

We can develop materials models that reproduce the expected behavior at the macro-scale?

But do they produce the correct result at the microstructural scale?



By combining microstructural experiments with simulations, we can quantitatively evaluate new models.

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Questions?

- Several Depts
- Many Material Codes

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