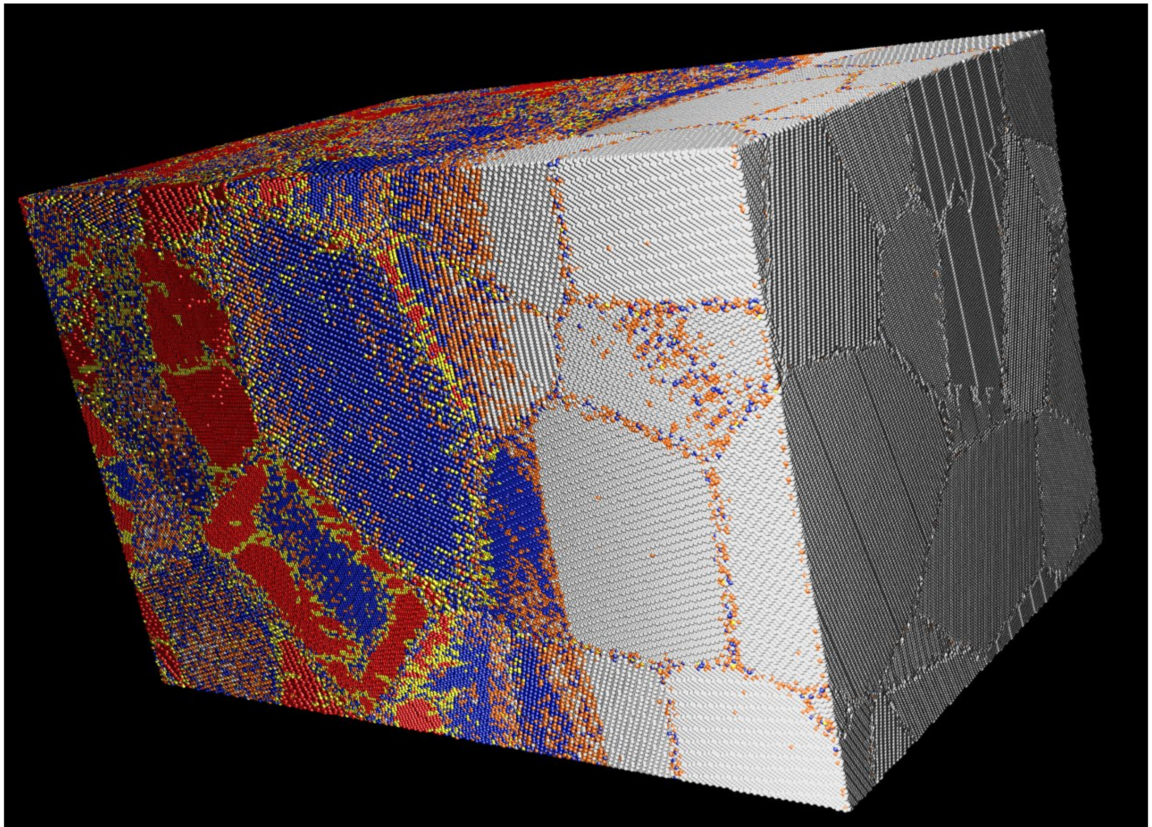
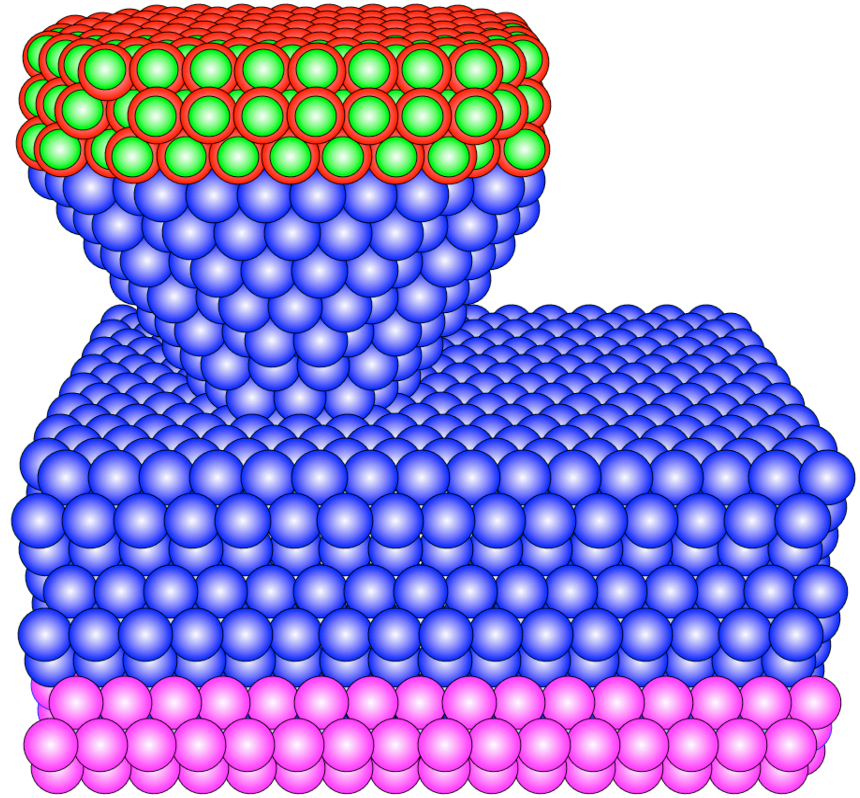


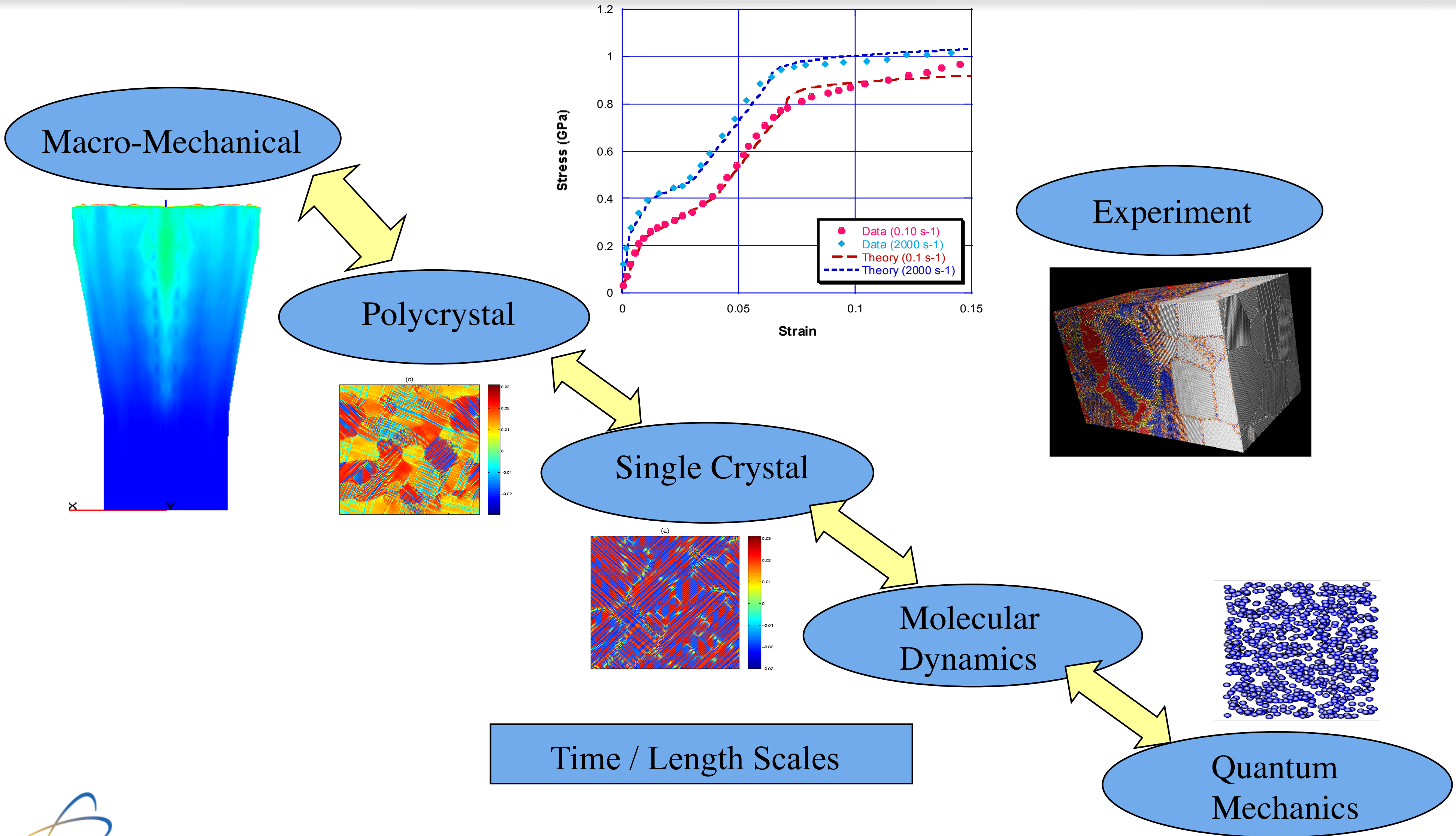
Materials Modeling at Los Alamos

Compiled by Joel D. Kress
Theoretical Division
June 15, 2017
LA-UR-17-24809

Abstract

This briefing describes some the materials theory, modeling and simulation capability at Los Alamos National Laboratory.

Multiscale materials modeling

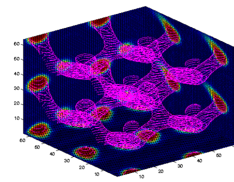


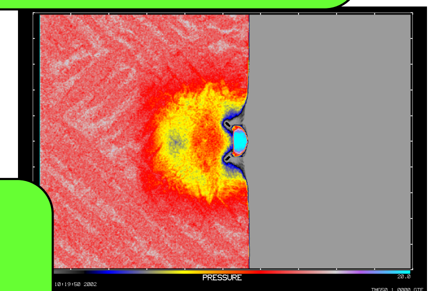
We are staffed to meet complex materials problems with interdisciplinary approaches: taking theory to models to numerical implementation to production codes

Multiscale modeling of polymers

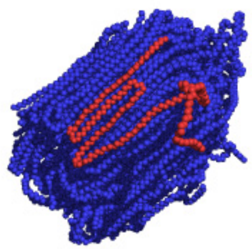
- Polymers present inherently multiscale modeling issues
  - Long relaxation times and physical / chemical aging
  - Entangled / frustrated systems
  - Complex phase diagrams for multiblock systems

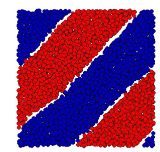
Continuum simulations



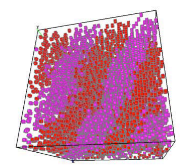


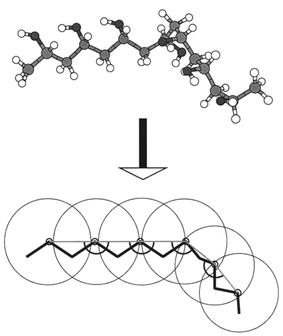
Mean-field computations

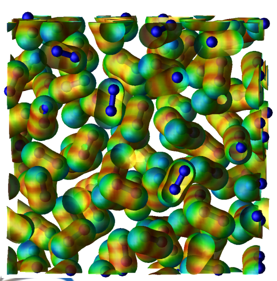




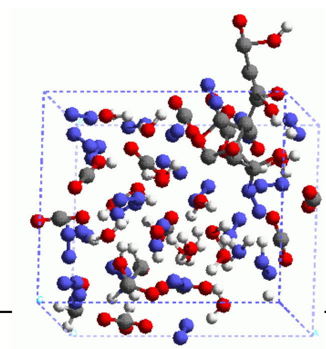
Coarse grained particle-based simulations







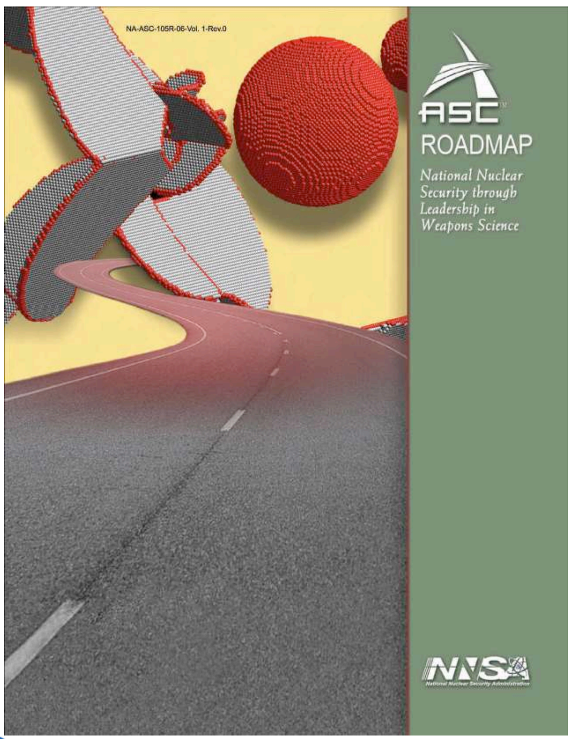
Quantum, MD & MC simulations



Large-scale molecular dynamics simulations

Fundamental probe of collective effects arising from large numbers of interacting particles or agents in a wide variety of systems

1) Plasticity and phase transitions in materials subjected to high strain-rate loading (e.g. shock)
2) Fluid instabilities (e.g. Rayleigh-Taylor, Richtmyer-Meshkov)
3) Agent-based modeling of disease spread, crowd dynamics, …

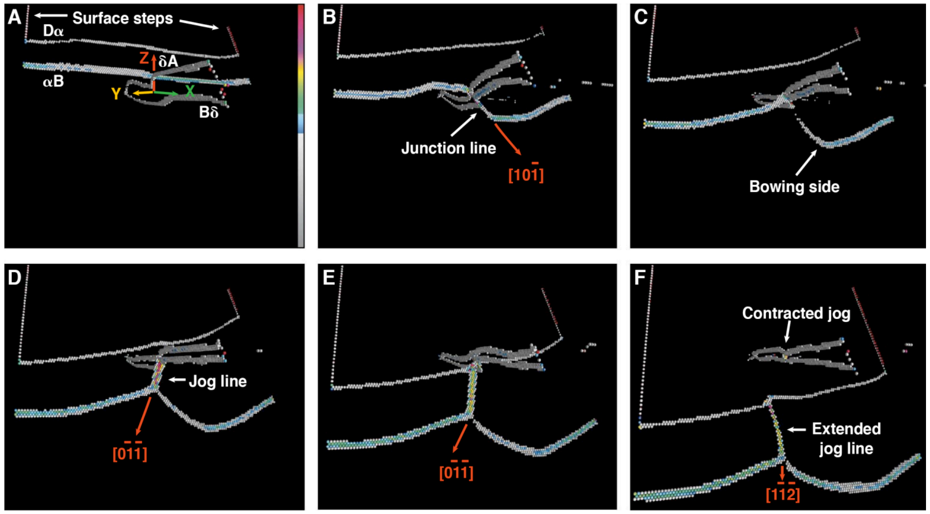


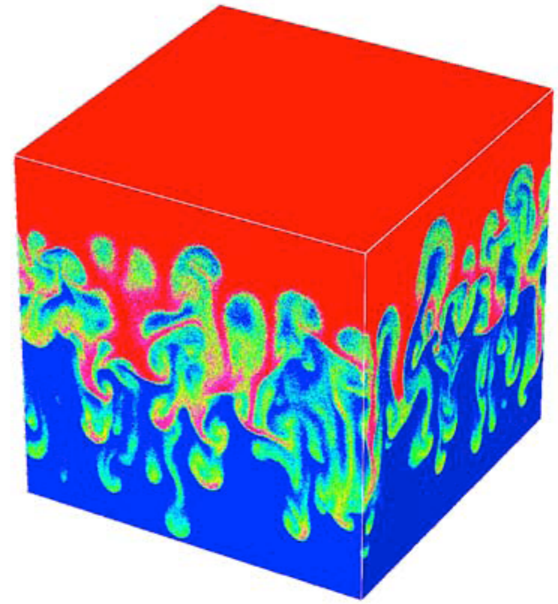
Large-scale molecular dynamics techniques for simulation of mesoscale systems using the high-performance SPaSM (Scalable Parallel Short-range Molecular dynamics) code.

SPaSM has exhibited linear scaling and high performance (4-time finalist, 2-time winner of the IEEE/ACM Gordon Bell Prize) up to 10^{12} atoms on platforms including BlueGene/L and Roadrunner.

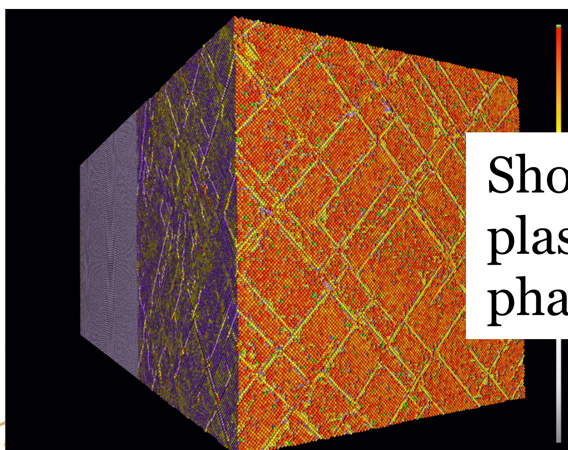
Large-scale molecular dynamics simulations

Strength of metals

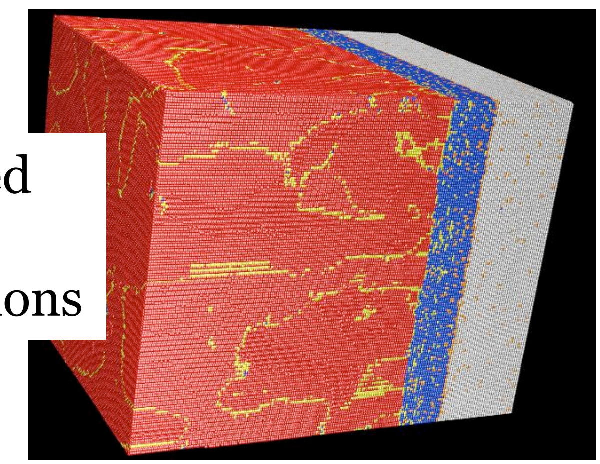




Fluid instability and the onset of turbulence



Shock-induced plasticity and phase transitions

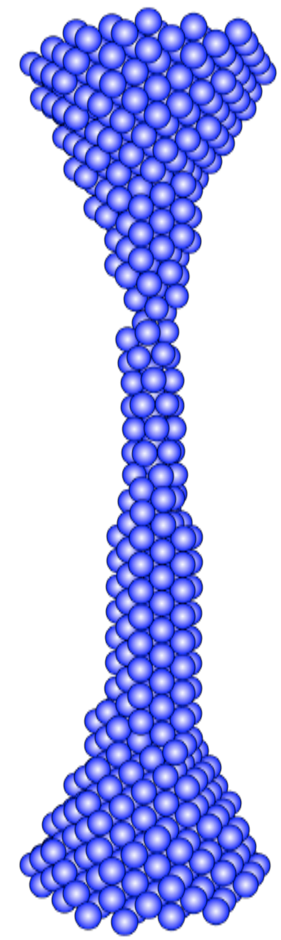


Accelerated molecular dynamics

1) Conventional molecular dynamics simulations
2) Rate theory calculations (barriers, prefactors, rates)
3) Self-Learning Hyperdynamics
4) Parallel-Replica Dynamics for static and driven systems
5) Integration with Ab initio codes like VASP and CP2K
5) Integration with the Roadrunner hybrid architecture

For small systems (~1000 atoms) Parallel Replica Dynamics routinely reaches microseconds of simulation time on small commodity clusters and was shown to reach milliseconds on petascale supercomputers like Roadrunner (when using empirical potentials).

On workstations, hyperdynamics was shown to provide speedups between tens and millions over conventional molecular dynamics.



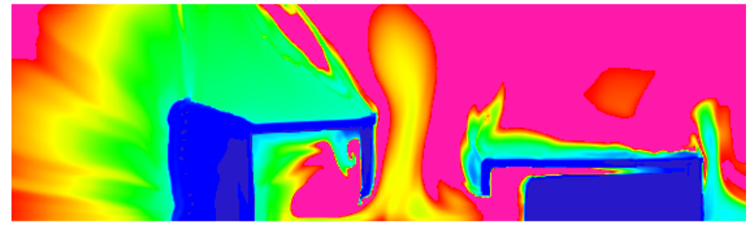
Roadrunner simulation of nanowire stretching

Multiphysics modeling

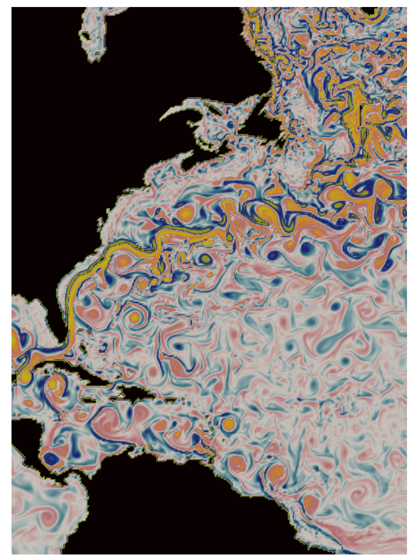
Methods Development
- Multi-physics & multi-scale methods development
- Multi-phase & multi-material dynamics modeling
- Chemically reacting flow modeling

Climate Modeling and Simulation
- Ocean and ice system dynamics
- High-resolution global and regional climate modeling
- Abrupt climate change science
- Biogeochemistry

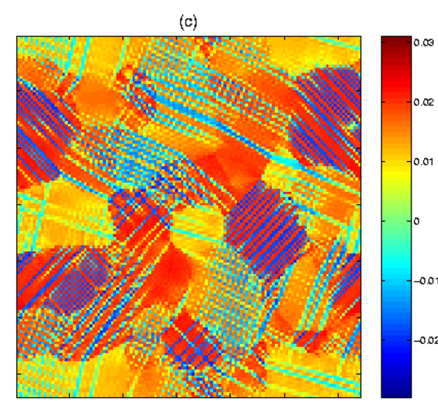
Materials Model Development
- Materials modeling and continuum mechanics
- Crystal plasticity and damage modeling
- Dislocation, defect, and interface dynamics
- Methods development for multi-scale modeling



Fluid-solid interaction

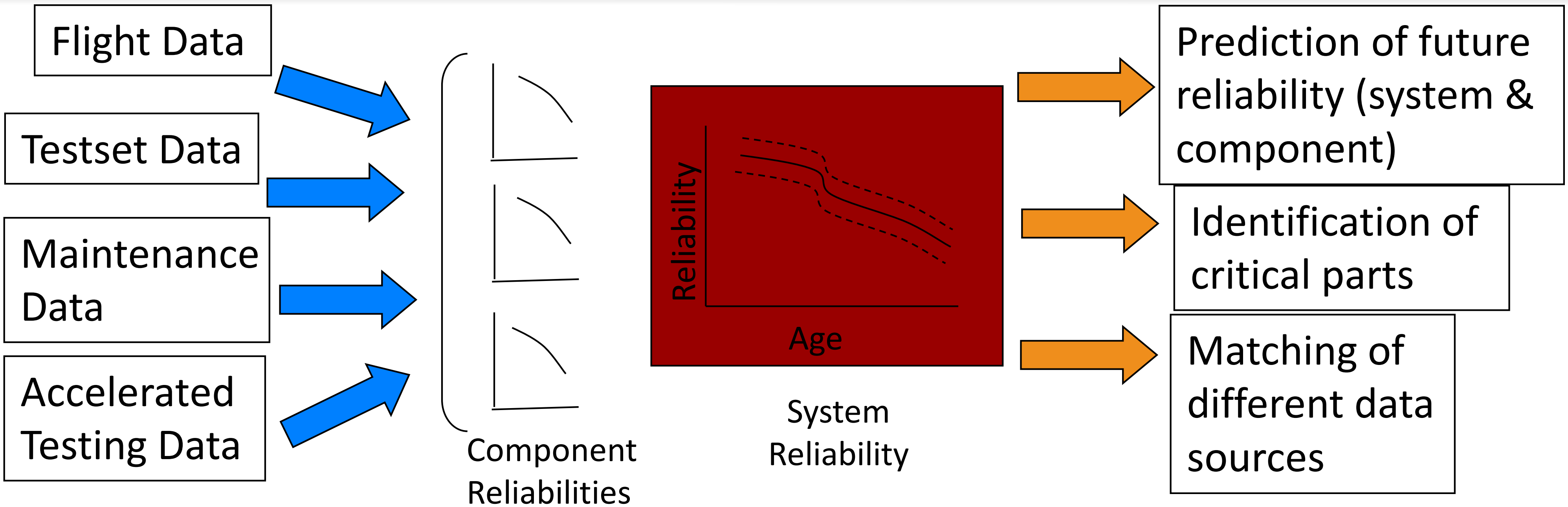


Evolving surface vorticity in a global ocean simulation (western North Atlantic shown)

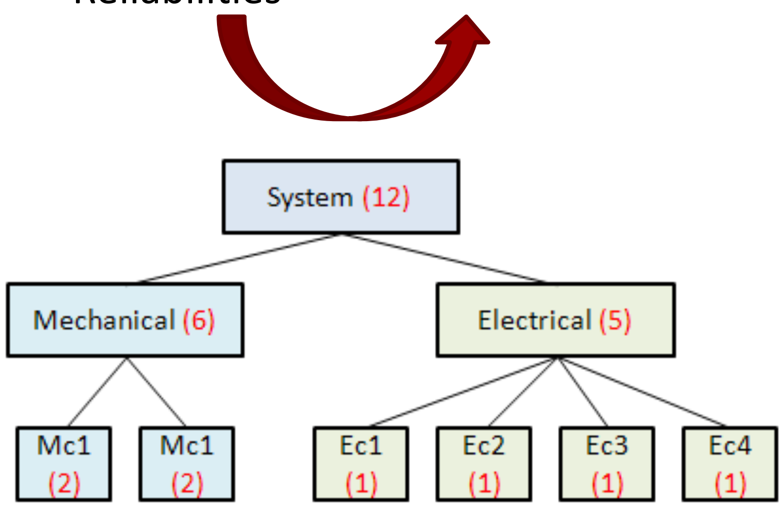


Twinning in a polycrystalline metal

Reliability (Change with Age) Using Multiple Data Sources



Key elements:
- Analysis combines subject matter expertise with statistical methods
- Careful assessment of model assumptions and comparison to reality
- Leveraging data from multiple sources



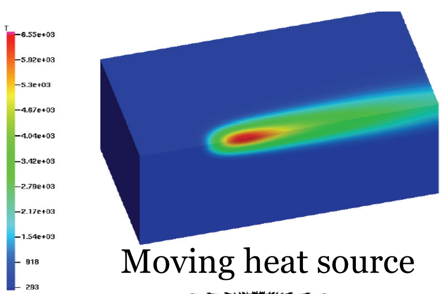
Benefits of Bayesian approach:
- Uses data already available and thought to be relevant
- Check on consistency of information from different sources
- Allows inclusion of external information
- Appropriately propagates uncertainty at all levels

Long-term vision: process aware Additive Manufacturing modeling and simulations

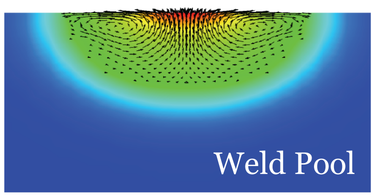
Process Modeling ⟷ **Microstructure Modeling** ⟷ **Properties Modeling** ⟷ **Performance Modeling**

Process Modeling

TRUCHAS code
3D multi-physics microstructure-aware solidification capability



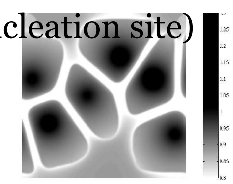
Moving heat source



Microstructure Modeling

Direct numerical simulation of grain growth

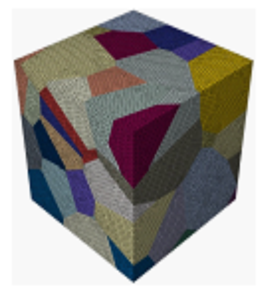
Initial grain distribution (Nucleation site)



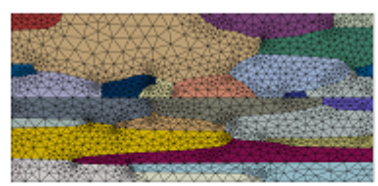
Final grain shape and composition

Properties Modeling

Polycrystal models to determine elastic/plastic/damage properties



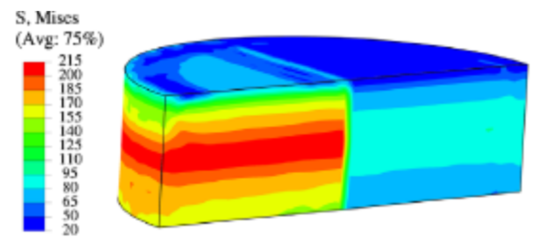
Polycrystal and grain boundary properties



AM specific interface properties

Performance Modeling

Thermal - mechanical models to predict elastic/plastic/damage and failure processes

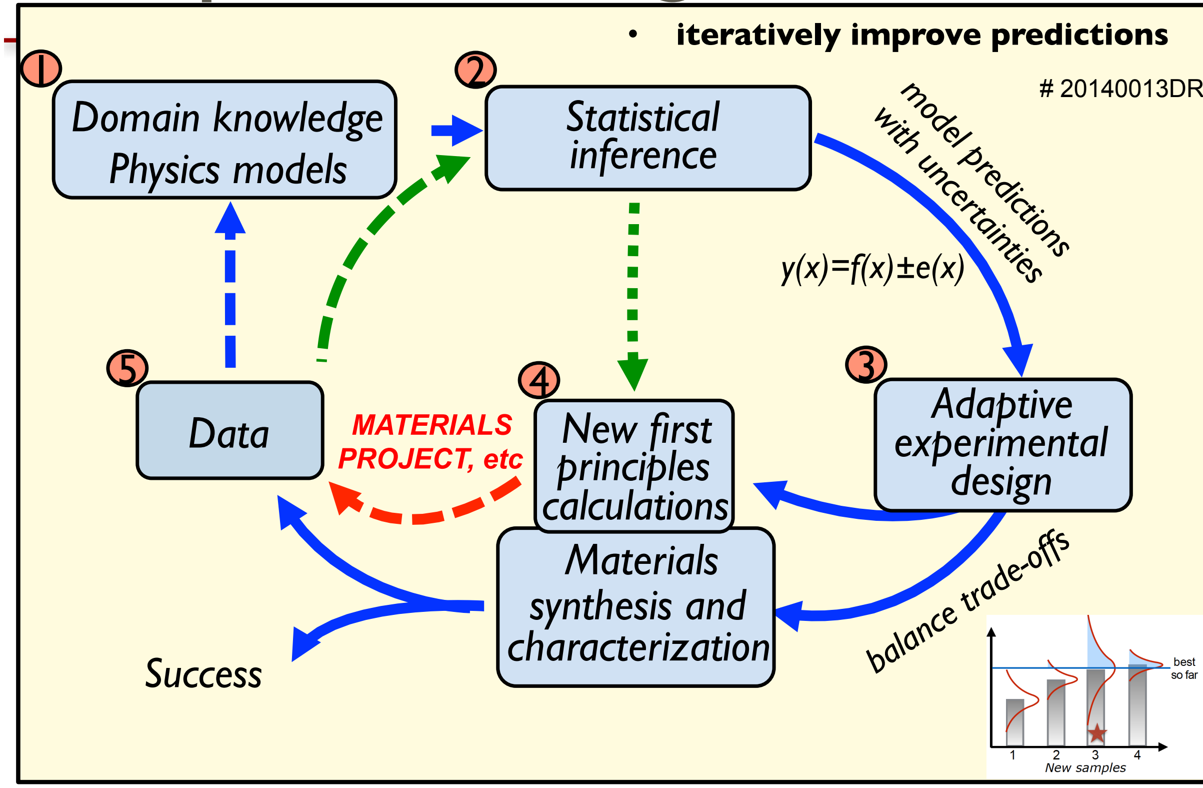


Mesoscale to macroscale prediction of performance

Liquid/solid phase change

Solid/solid phase transformation

Accelerated Materials Discovery via Adaptive Design

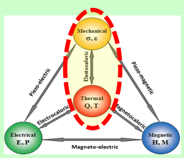


Goal:

Optimal learning of materials with targeted properties by guided experiments and calculations

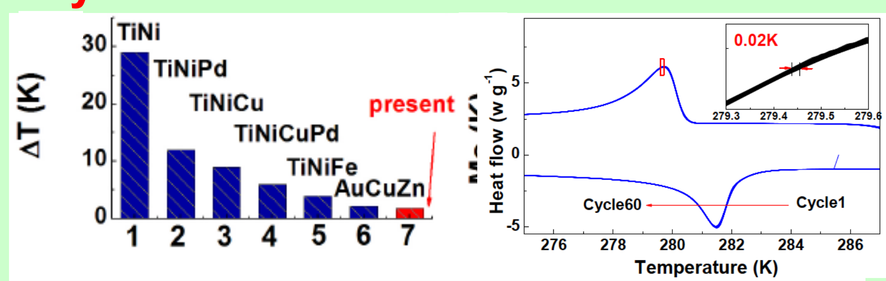
Approach:

- **'Exploit vs Explore' high dimensional search space of possible candidates via global optimization**

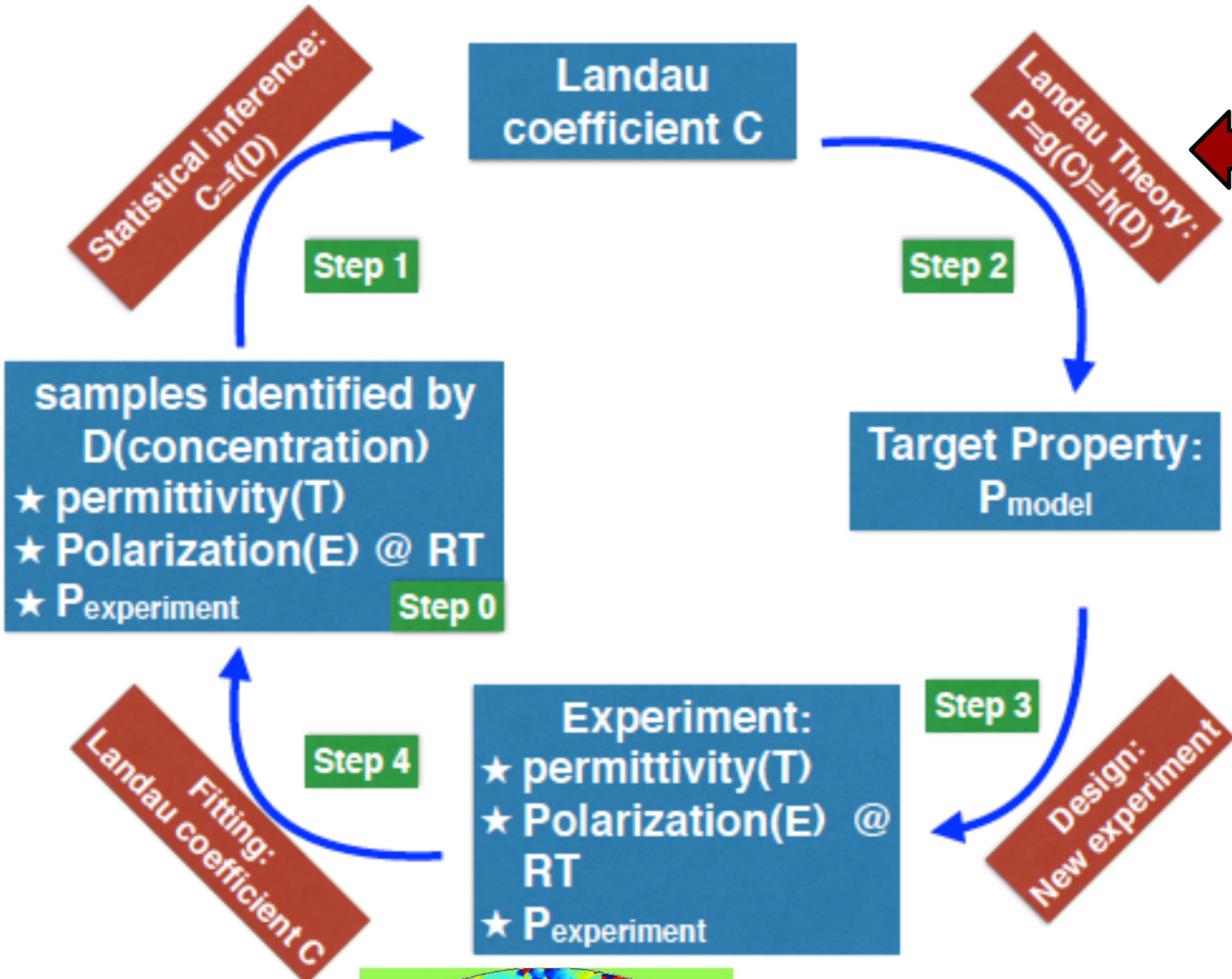


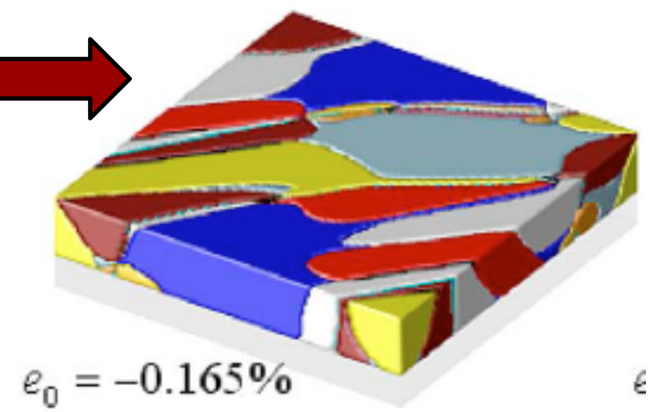
Findings: New ultra low dissipation smart alloys

9 prediction/synthesis/characterization iterations
(batch mode: 4 predictions/experiments at a time)
14 alloys better than the best in training data
(p value<.001)

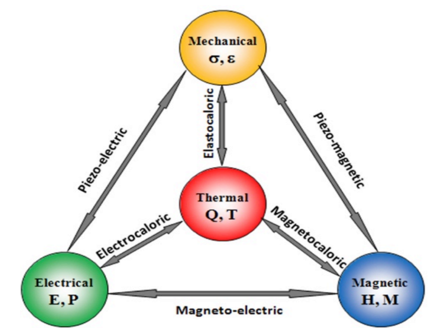


via Informatics, Synthesis and *in situ* Characterization



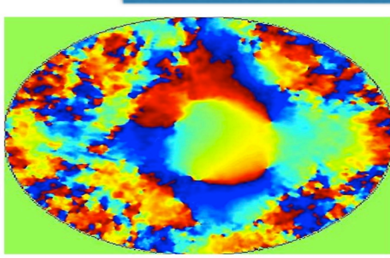


Phase field simulation



Applications to energy harvesting materials

- **ferroelectrics**
- **electrocalorics**
- **magnetocalorics**



In situ @ LCLS

Image maps

Polarization

Distortion

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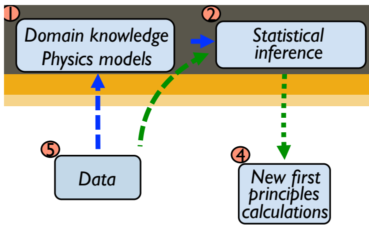
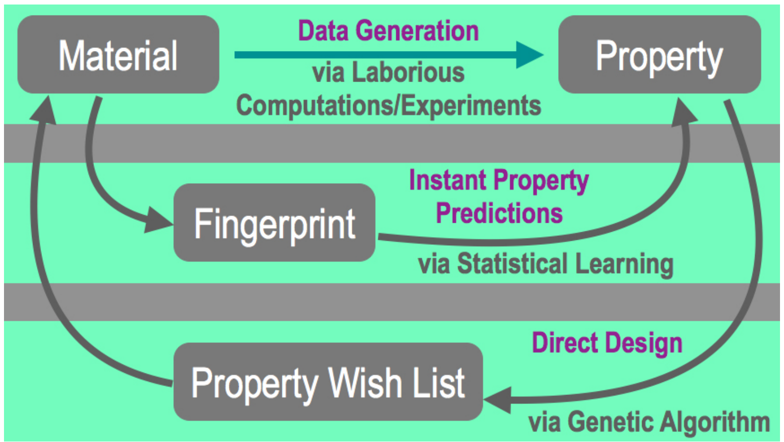
NNSA

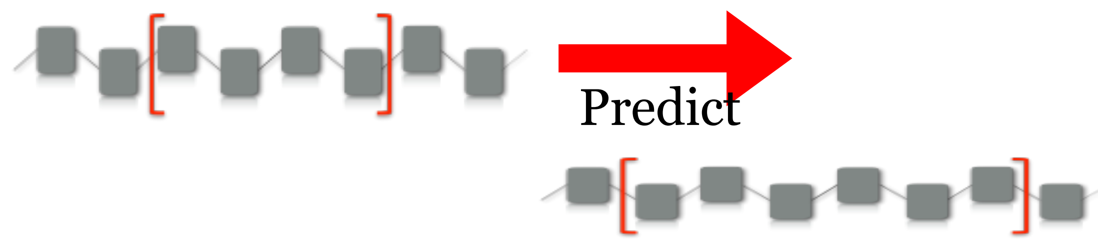


learning

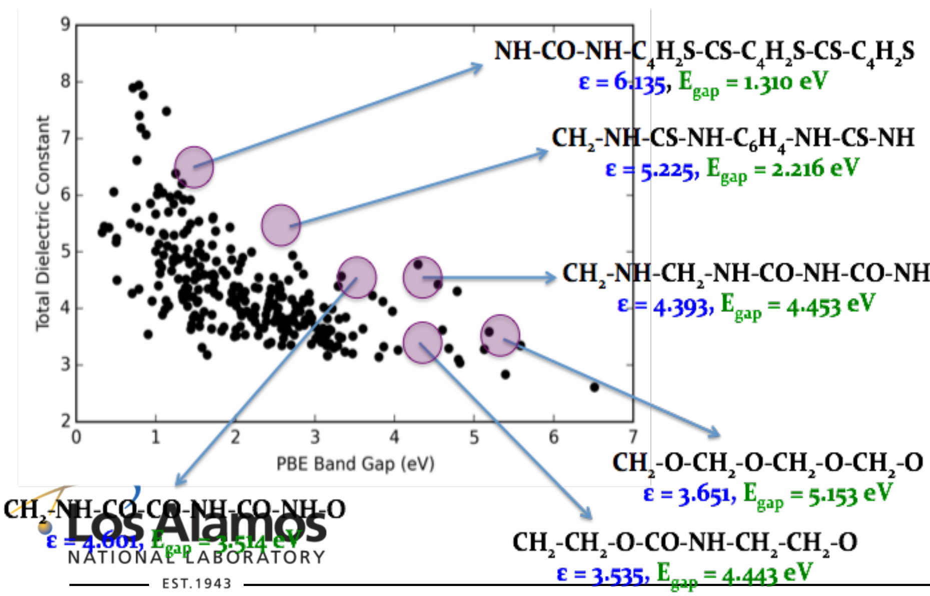
Goal: Polymers for high energy density capacitors and release: large wide band gap & dielectric constant

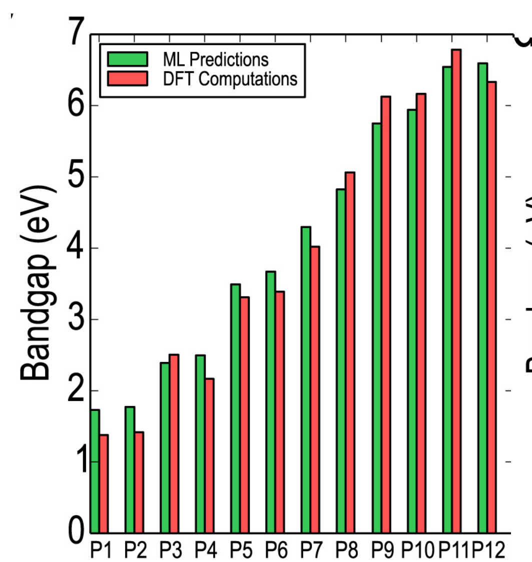
Maximum Energy Density $\alpha\ \varepsilon E_{bd}^2$

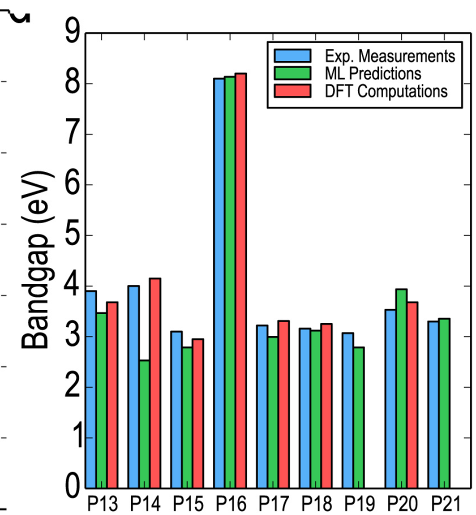




- **Learn from polymers with small repeat units to predict response for large repeat unit polymers**







Computational (Macro/Meso) Mechanics of Materials Performance

Curt A. Bronkhorst
Theoretical Division
Fluid Dynamics & Solid Mechanics

LA-UR-14-28159

8 October, 2014

Topical Overview

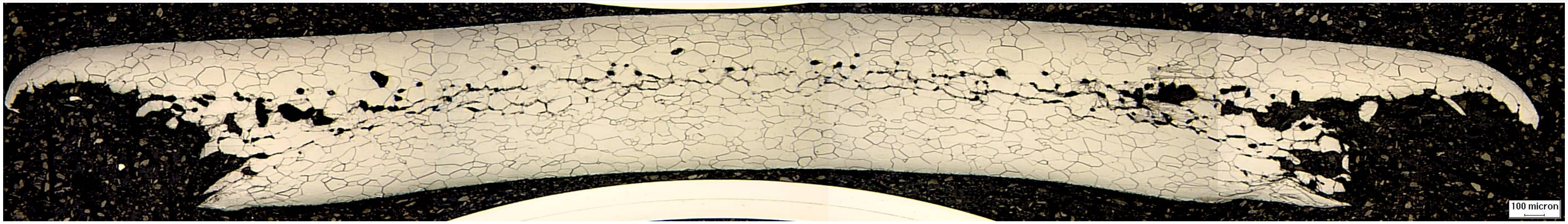
- Dynamic Damage and Failure of Metallic Materials
  - Porosity Based
  - Localization Based
- History Effects of Coupled Structural Transformation and Plasticity
- Manufacture and Modeling of Metallic Nano-Layered Composites
- Additive Manufacturing – metals modeling component (new)

Computational Interrogation of Dynamic Pore Nucleation in Polycrystalline Metallic Materials

C. A. Bronkhorst, D. J. Luscher, F. L. Addessio, E. Lieberman,
M. W. Schraad, E. K. Cerreta, V. Livescu, G. T. Gray III

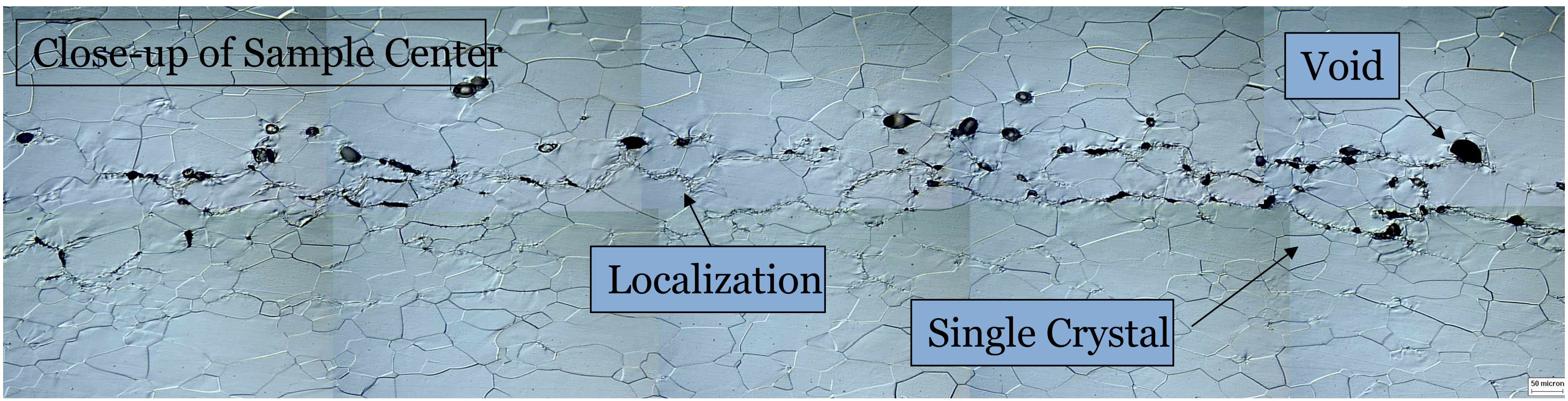
LA-UR-13-25368

Explosively Loaded Sample Demonstrates Ductile Damage and Failure Physics



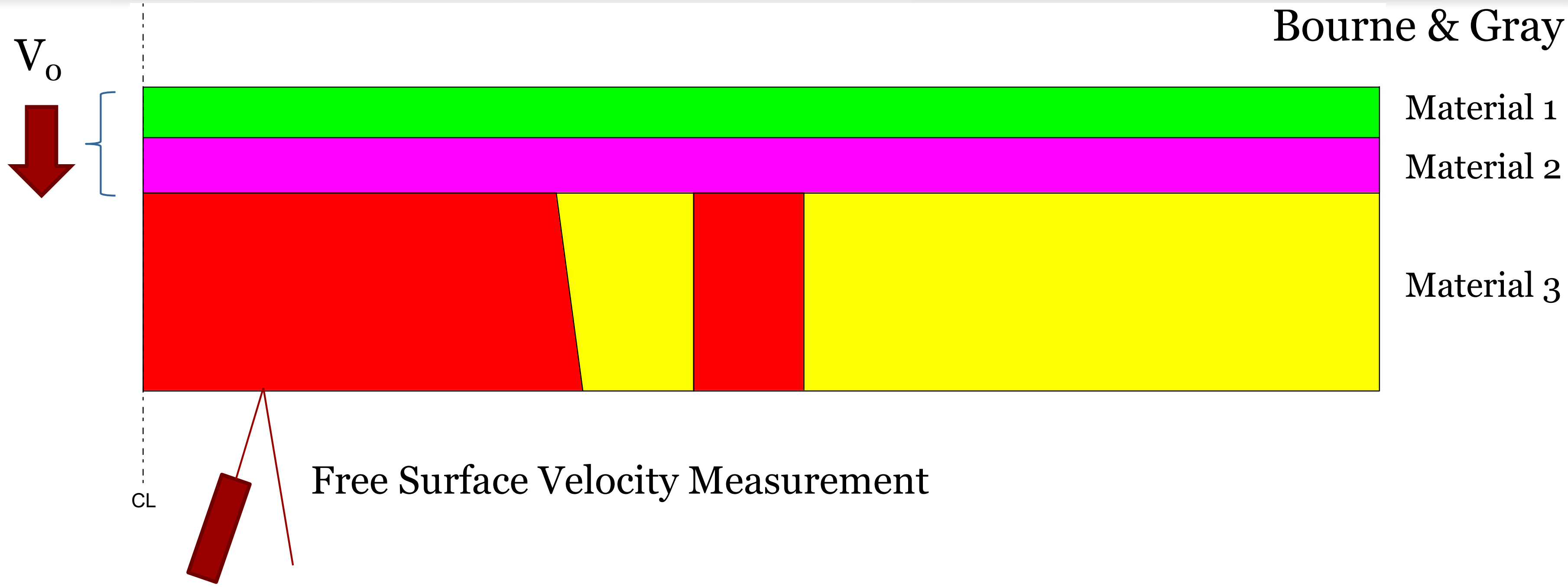
Explosively Loaded Tantalum Experiment
6 mm thick PETN Beneath Sample – Center Detonated
Soft Sample Recovery

Mason



Voids are forming along grain boundaries in the sample

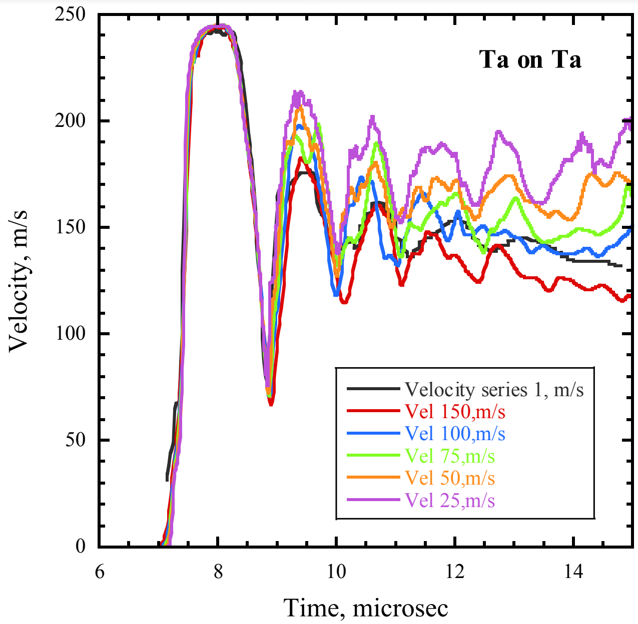
Ta Damage Modeling – Composite Flyer Experiments

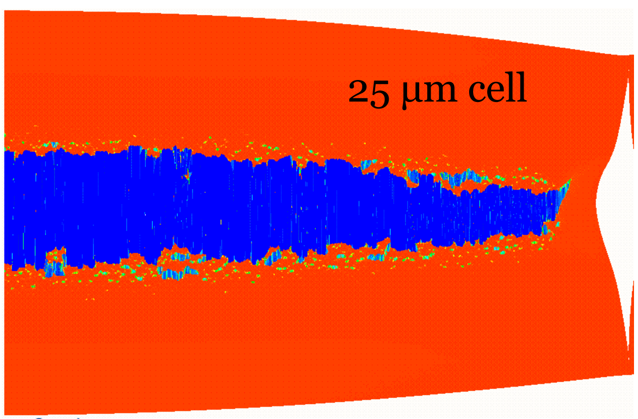


- Finite elasticity, equation of state, coupled energy.
- Rate/temperature dependent plasticity, Gurson-type porosity damage.
- Overstress and spatially variable flow stress for regularization.
- Nucleation not represented, only growth and coalescence.
- Fully implicit numerical integration scheme.
- EPIC 2006, DoD fully explicit code (transitioning to ABAQUS).

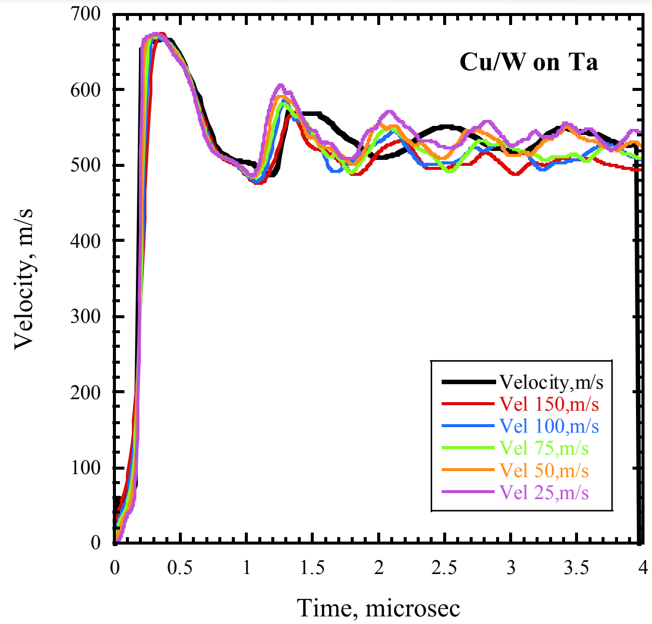
Ta Damage Modeling – Composite Flyer Experiments

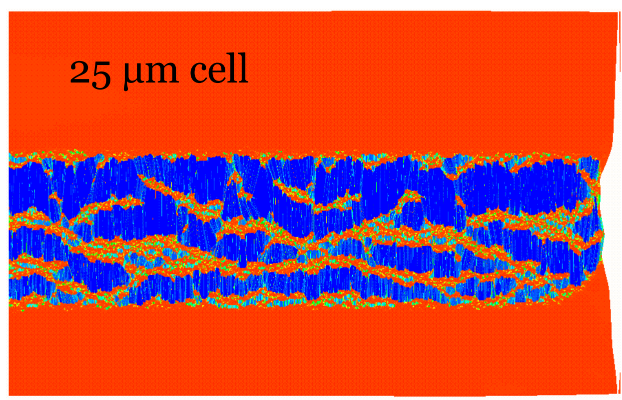
Ta Flyer



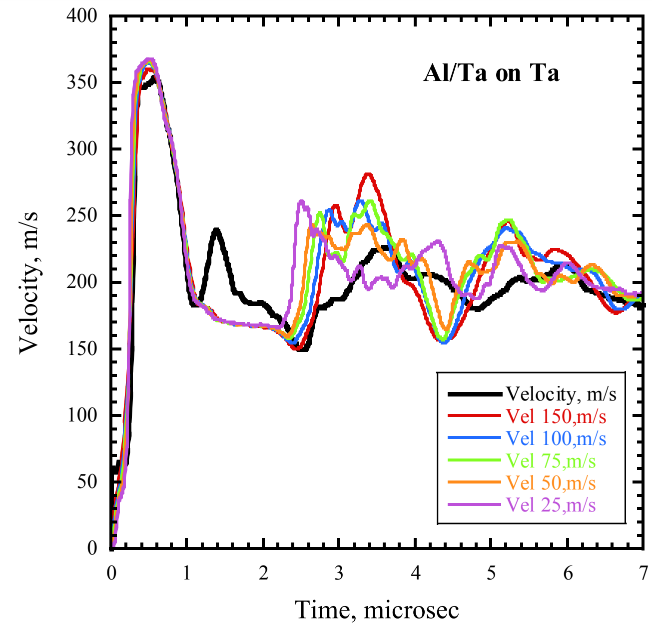


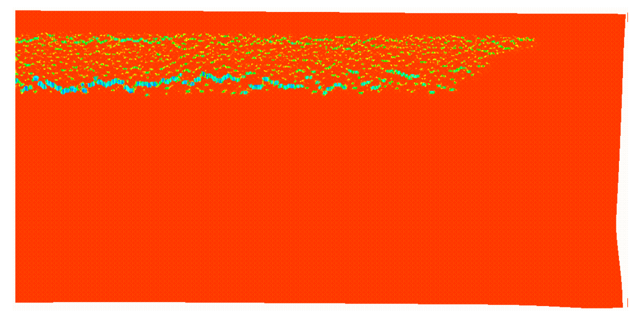
Cu + W Flyer





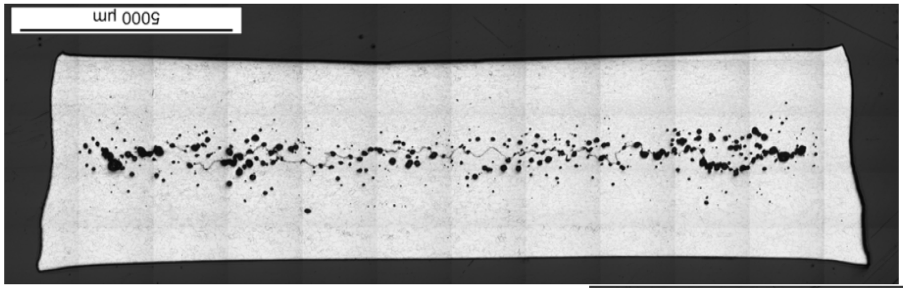
Ta + Al Flyer

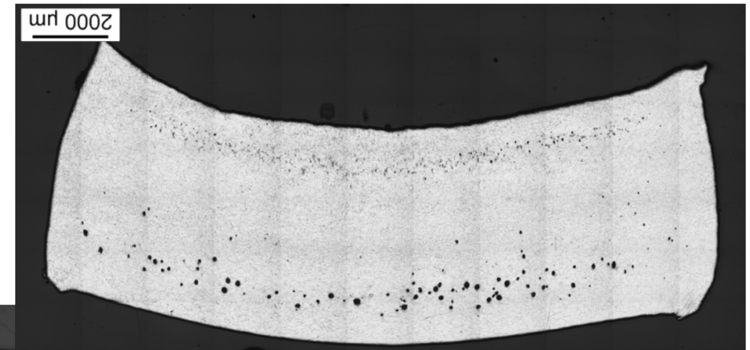


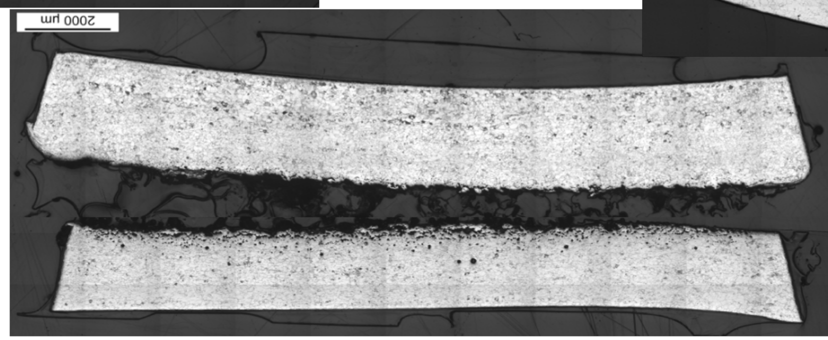


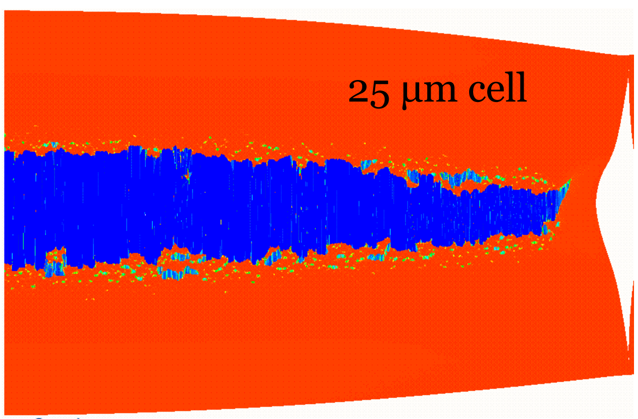
Ta Damage Modeling – Composite Flyer Experiments

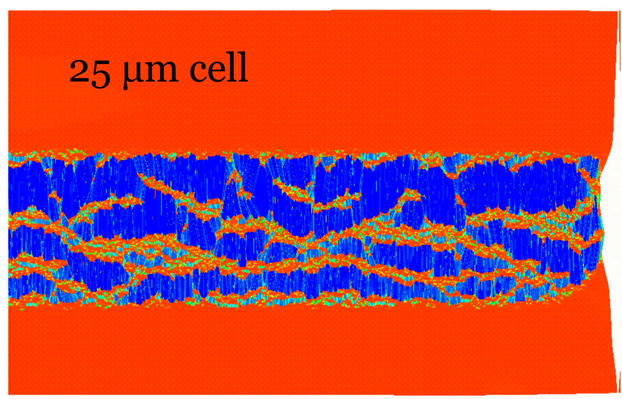
Ta Flyer | Cu + W Flyer | Ta + Al Flyer

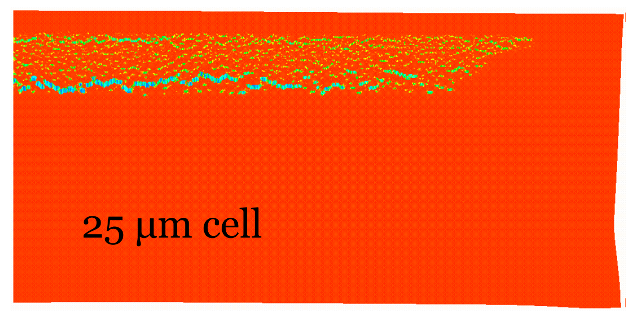












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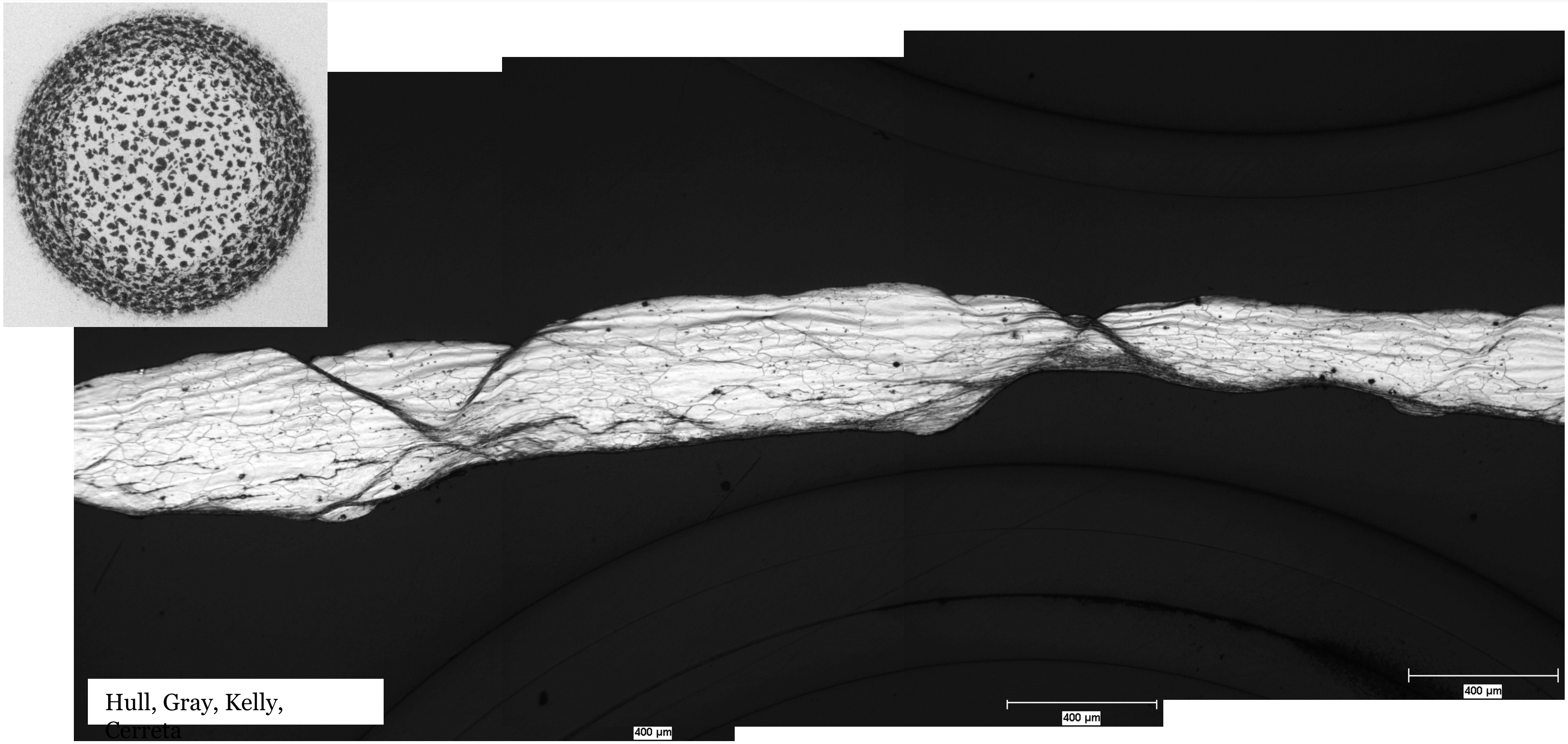
An explicit finite element formulation for dynamic strain localization and damage evolution in metals

H. M. Mourad, C. A. Bronkhorst, F. L. Addessio,
D. J. Luscher, E. K. Cerreta, J. F. Bingert

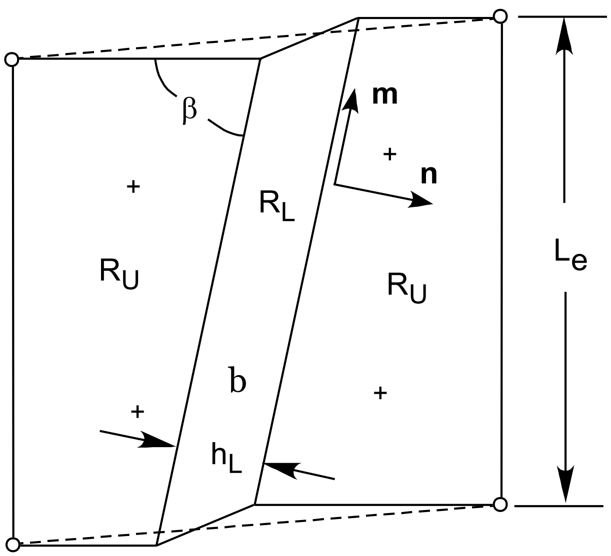
LA-UR-11-04195

Strain Localization in Fragmentation Problems



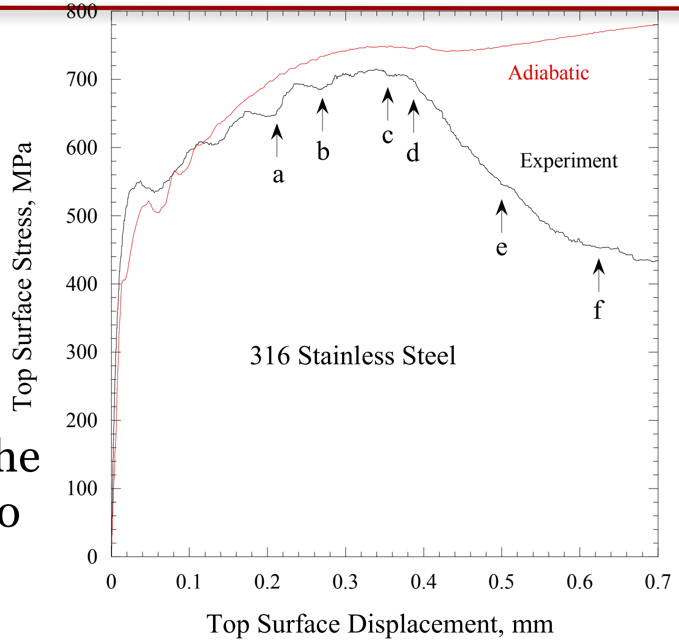
Cross-sectional metallography points to considerable amount of localized plastic work before failure.

Localization: Embedded-Localization Zone Approach



Technique allows for different material models to be used inside and outside the band.

Difference between the two curves believed to be due to dynamic recrystallization.



Sub-grid computational technique

- Allows part of the localization band to be embedded inside an element, obviating the need for excessive mesh refinement.
- Allows localization band width to be specified as a material parameter, instead of being dictated by the mesh size.
- Allows band orientation to be determined based on material stability analysis.
- Allows smooth transition from uniform to localized deformation.

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Micromechanics of Dynamic Solid-to-Solid Phase Transformations

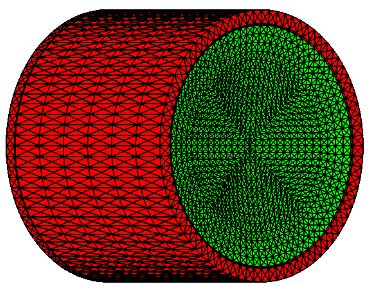
F. L. Addessio, T. Lookman, C. A. Bronkhorst, C. W. Greeff,
M. W. Schraad, D. W. Brown, E. K. Cerreta, P. A. Rigg, C. A. Bolme

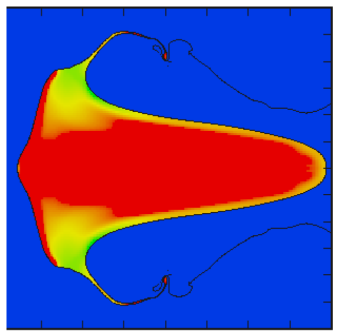
LA-UR-14-2092

Large Plastic Deformation with Phase Change

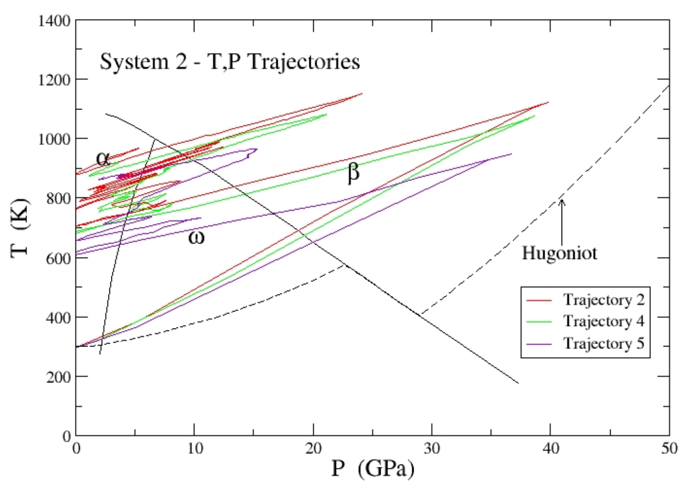
Complex Deformation History

- **Trajectory of deformation includes several potential phase changes**





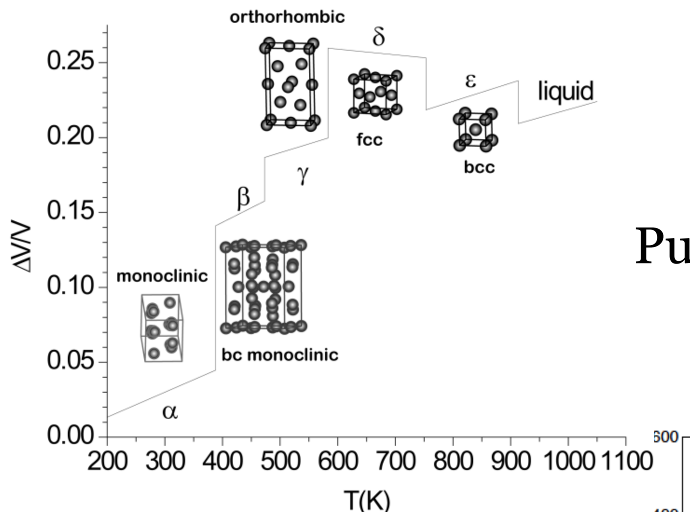
Explosively Formed Projectile (Zr)

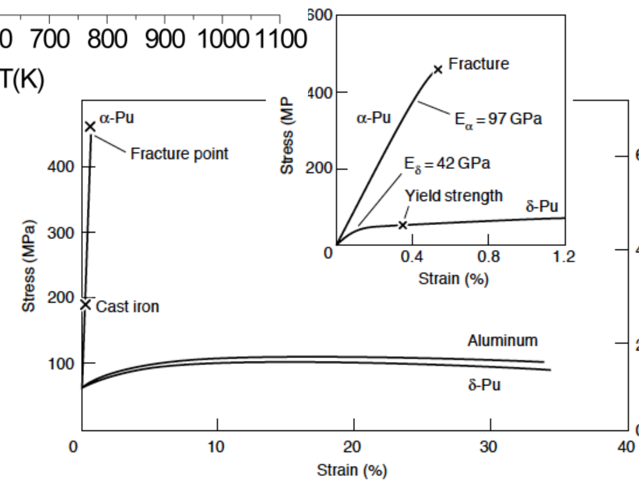


Zuo, Harstad, Addessio, Greeff, Modelling Simul. Mater. Sci. Eng. 14 (2006)

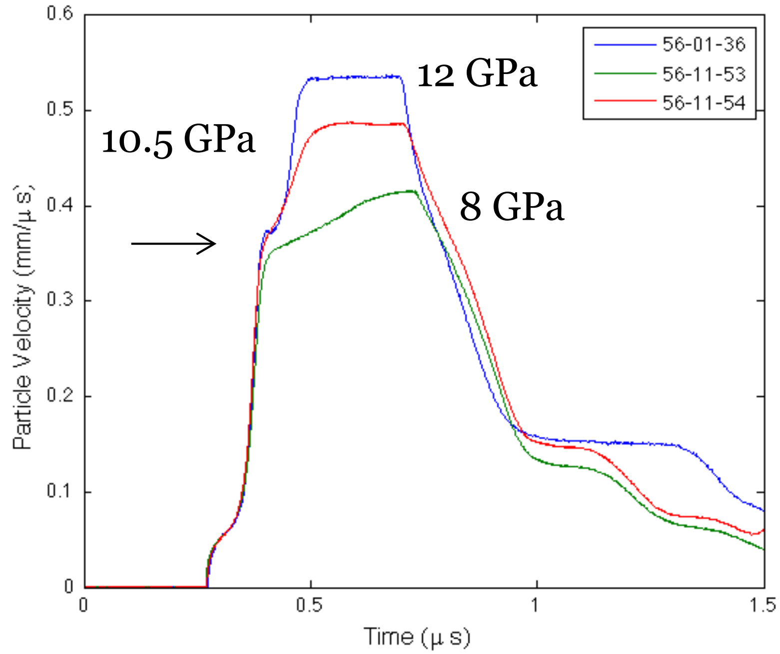
Complex Phase Behavior

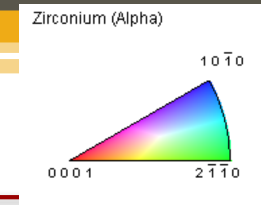
- **Different phases have very distinct properties**
- **Inheritance and evolution of plastic state is poorly understood**

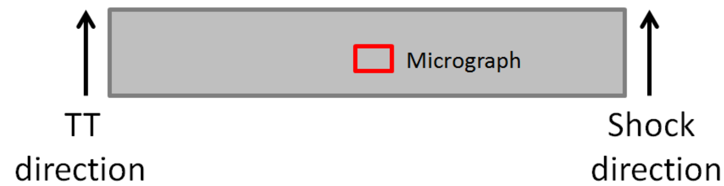


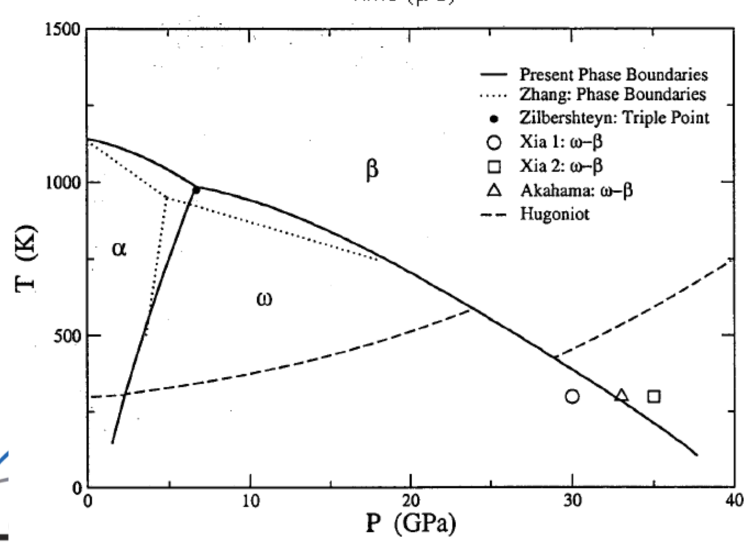


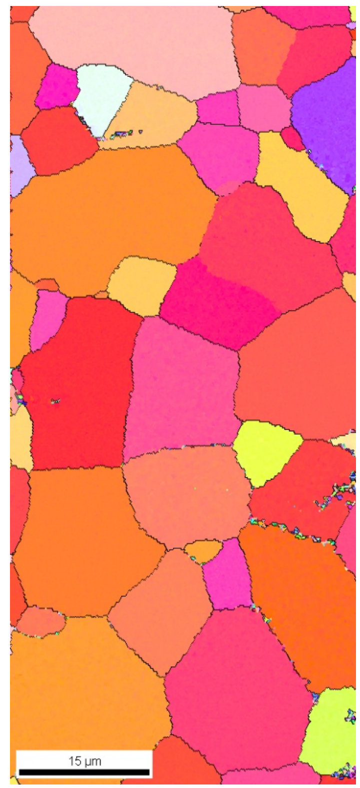
Shocked Polycrystal Zr (Ti, Hf) and the Retained Structure



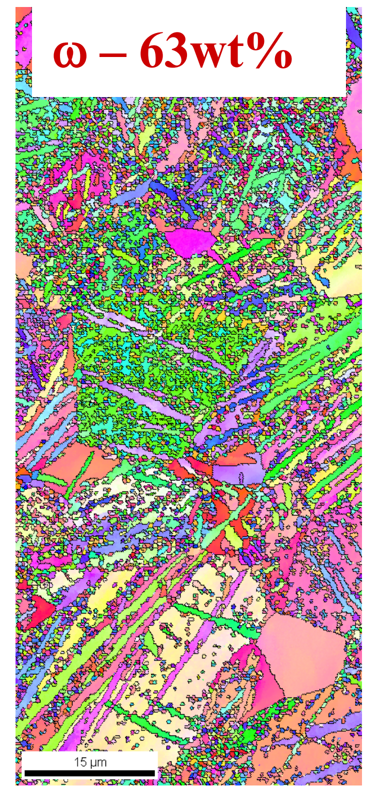








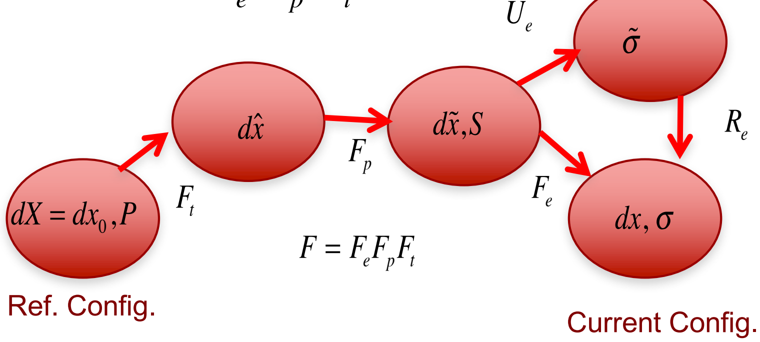
As-annealed



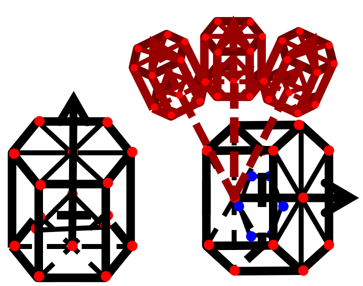
Shocked at 658m/s (8.0GPa)

Thermodynamically Consistent Single Crystal Model

$$F = F_e \, F_p \, F_t$$

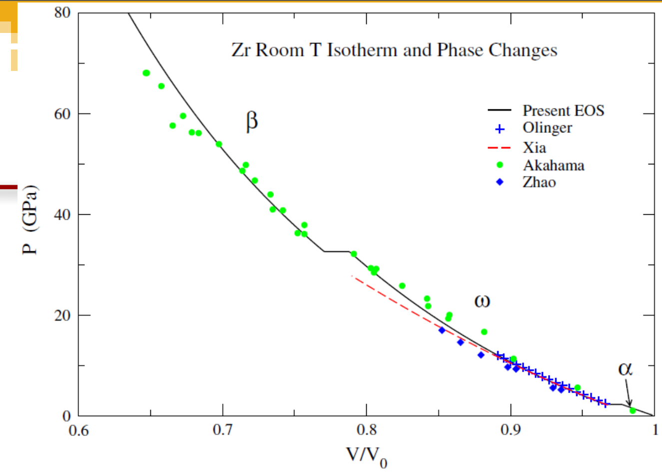


Large Deformation



Zr / Ti
(Silcock Mechanism)

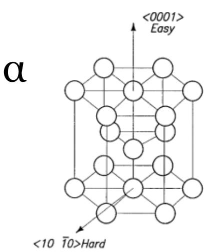
Phase Transformation



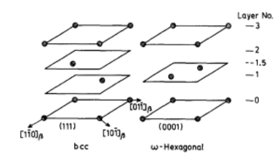
Finite Elasticity – Analytic EoS

Slip Crystallography

HCP - α



HEX - ω



Sikka et al, 1982

Prismatic
Pyramidal <c+a>

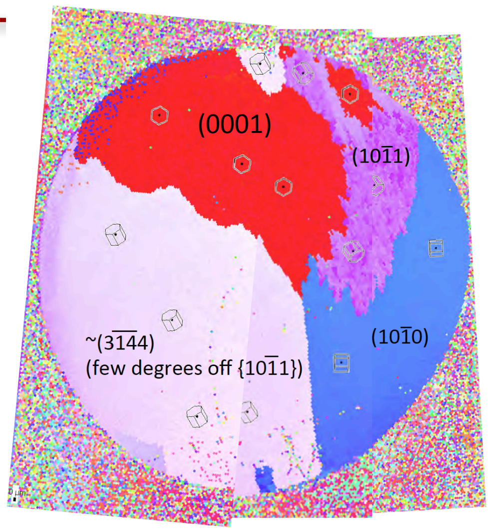
Basal (limited)
Prismatic (limited)

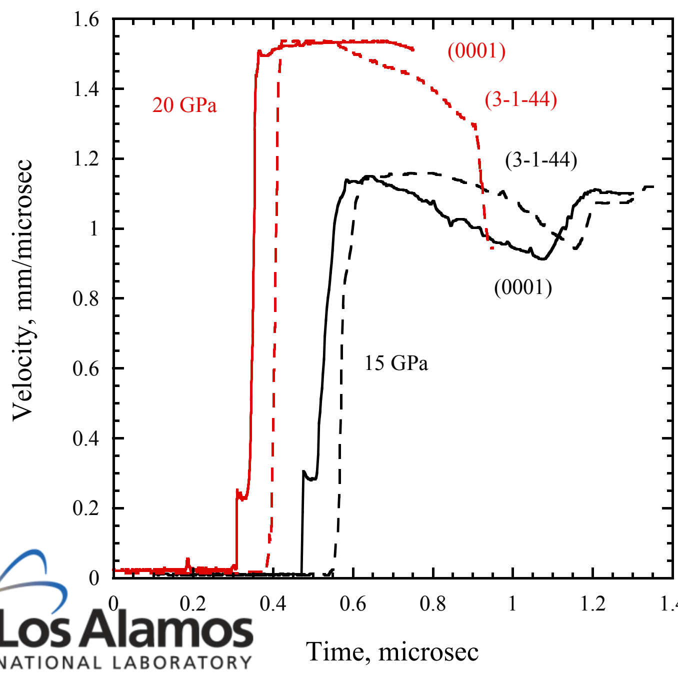
Twin Crystallography

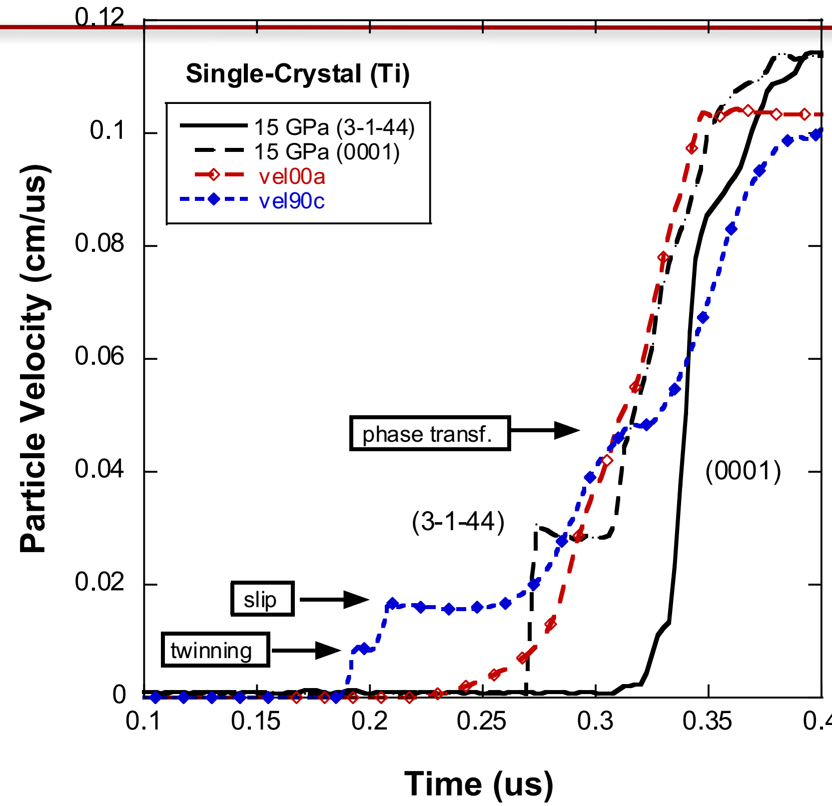
Tensile, Compressive

Plasticity – slip, twinning

Ti Tri-Crystal Experiments and Predictions







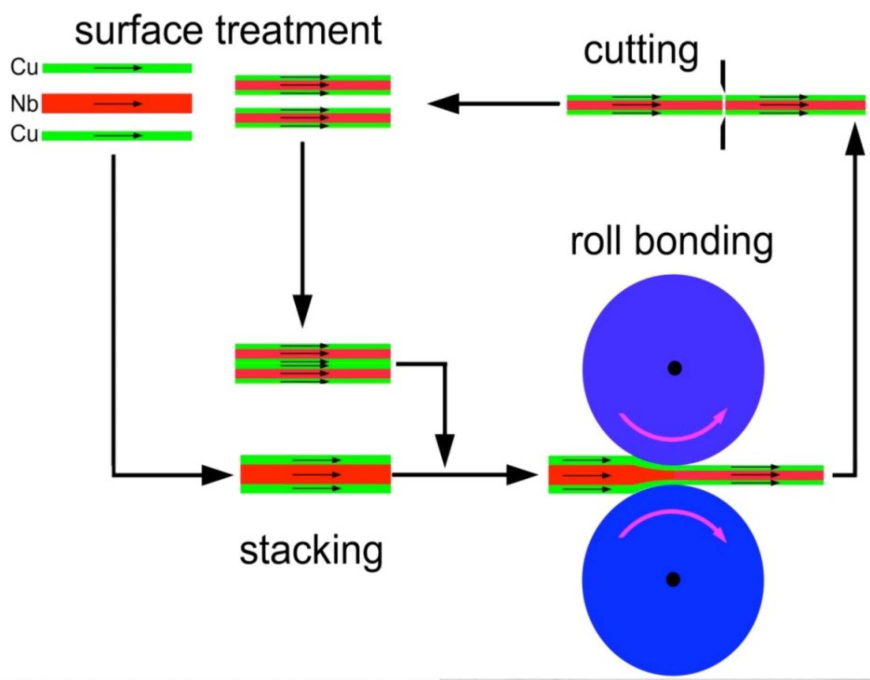
- Single crystal EoS development very important – coupled pressure and shear.
- Role of twinning/slip/transformation processes clear.
- Proper history dependent coupling will be a significant challenge.

Modeling the Interface Formation within Cu/Nb Layered Composites by Accumulated Roll Bonding

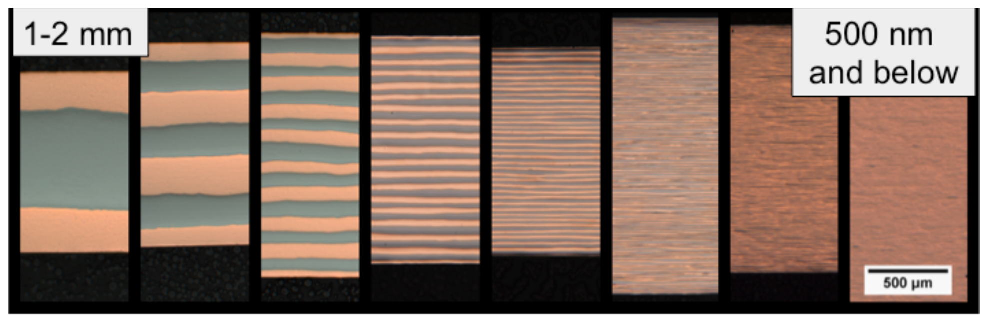
J. R. Mayeur, I. J. Beyerlein, H. M. Mourad, C. A. Bronkhorst,
J. S. Carpenter, R. J. McCabe, S. Pathak, N. A. Mara

LA-UR-14-20851

Cu/Nb Nano-Layered Composites by Severe Plastic Deformation



Tom Nizolek, UCSB summer PhD student



Metallic based multi-layered nano-composites are recognized for their increased plastic flow strength and indentation hardness, increased ductility, improved radiation damage resistance, improved electrical and magnetic properties, and enhanced fatigue failure resistance compared to conventional metallic materials.

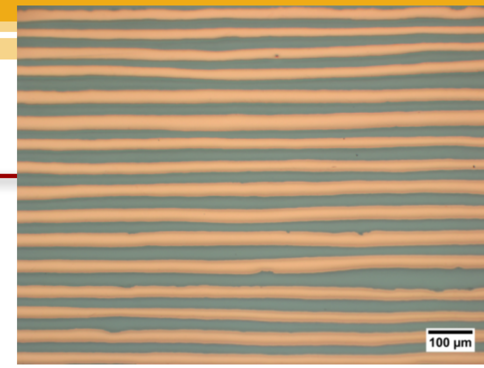
Texture and Interface Evolution

Layer thickness, h (nm)	Rolling Reduction, η (%)	Strain, ε
2,000,000	0	0
97000	95	3.03
45000	97.75	3.79
20600	98.9	4.58
7800	[illegible]	[illegible]
3500	[illegible]	[illegible]
1500	99.9	7.19
714	99.96	7.94
197	[illegible]	[illegible]
135	[illegible]	[illegible]
50	99.9975	10.60
31	[illegible]	[illegible]
20	99.999	11.51
10	99.9995	12.21

MICRON: Stable orientations – set 1

SUBMICRON: Stable orientations/interfaces – set 2

NANO: Stable orientations/interfaces – set 3



~60% rolling reduction per pass

1st Transition
1-2 grains thick Cu

2nd Transition
1-2 grains thick Nb

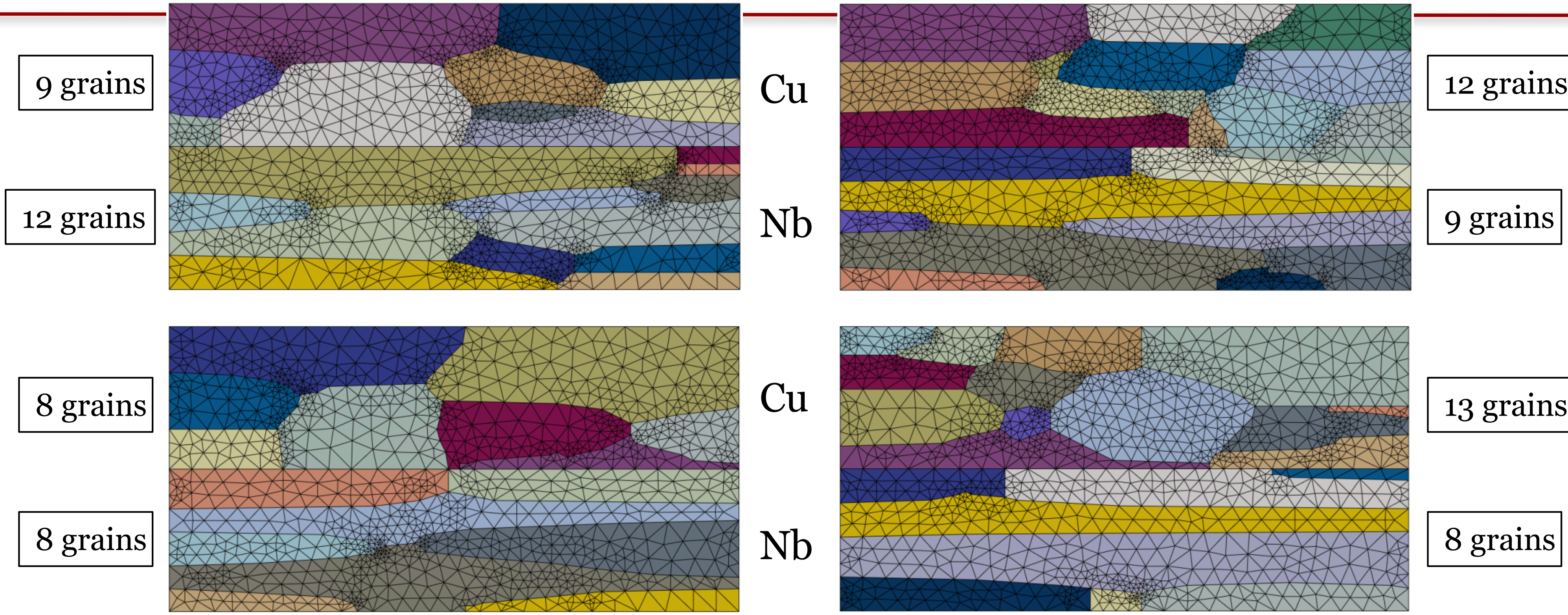
Hansen et al., 2013 Int. J. Plasticity 49(1), 71

Mayeur et al., 2014, Materials 7(1), 302

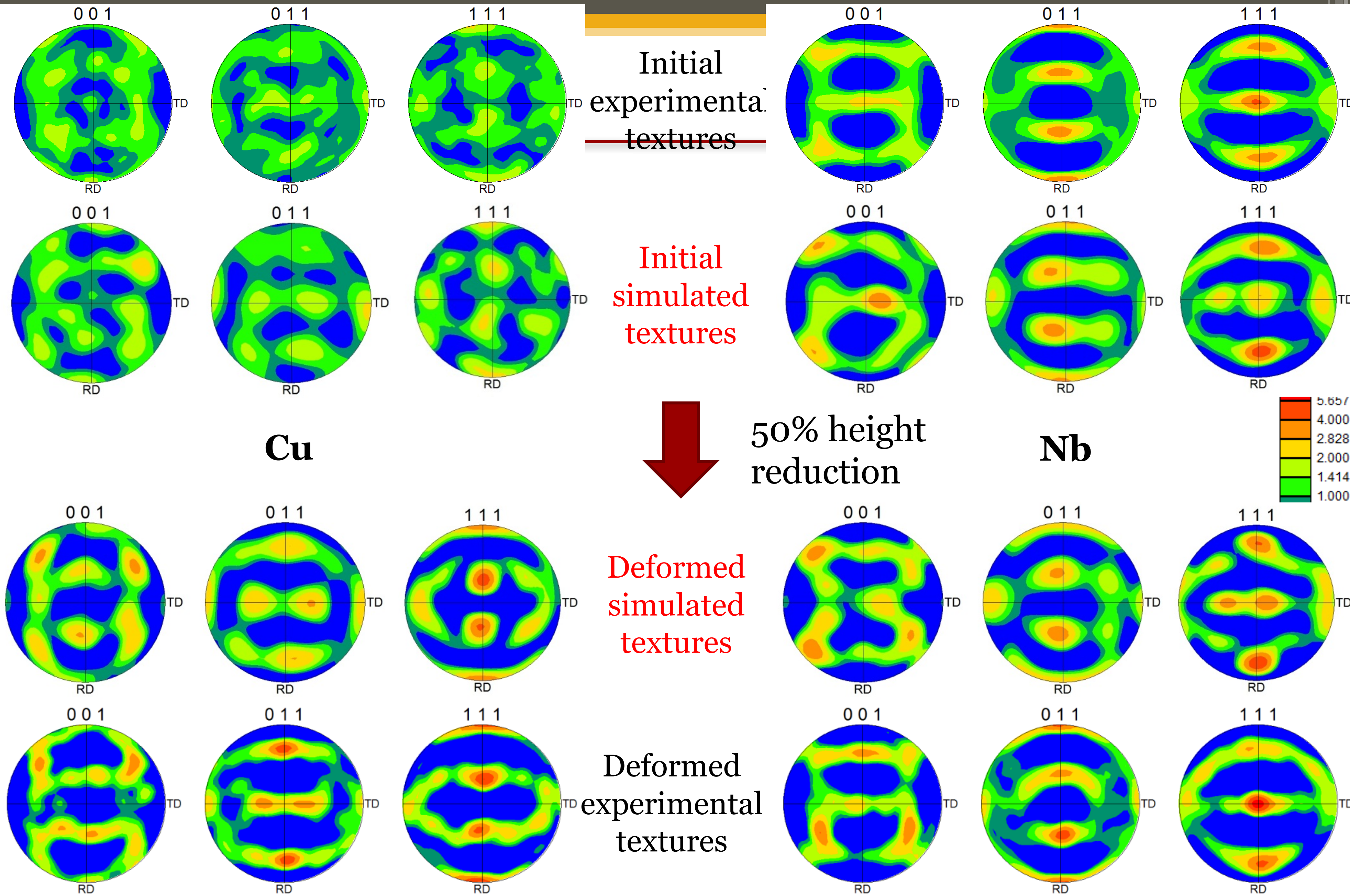
Bronkhorst et al., 2013, JOM 65(3), 431

Mayeur et al., 2013, Int. J. Plasticity 48,72

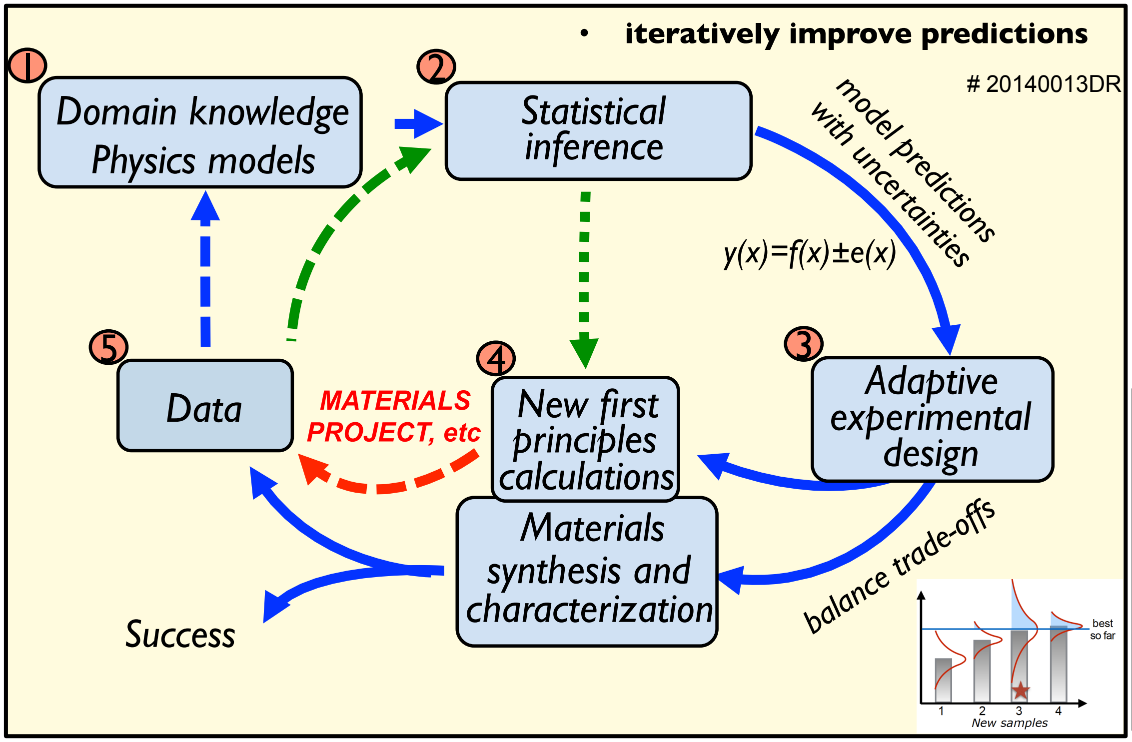
Single Pass Plane Strain Compression + 4 more



- Eight geometric realizations – 84 Cu grains, 79 Nb grains.
- Five crystallographic realizations for each – 420 Cu grains, 395 Nb grains.
- Multi-point constraint linking top surface to both sides to preserve area.
- Temperature constant at 298K.
- No degrees of freedom at the bi-material interface.


Initial experimental textures
Initial simulated textures
50% height reduction
Cu
Nb
Deformed simulated textures
Deformed experimental textures
0 0 1
0 1 1
1 1 1
TD
RD
5.657
4.000
2.828
2.000
1.414
1.000

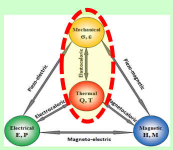
Accelerated Materials Discovery via Adaptive Design



Goal:
Optimal learning of materials with targeted properties by guided experiments and calculations

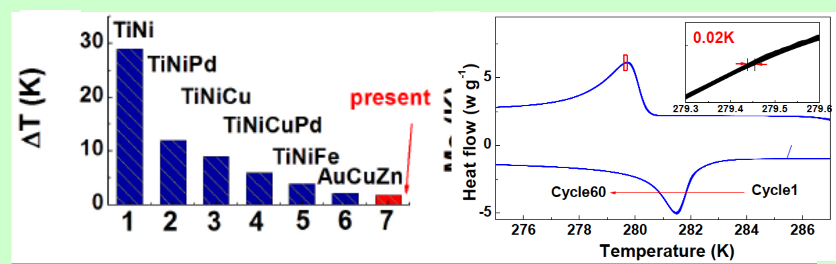
Approach:

- **'Exploit vs Explore' high dimensional search space of possible candidates via global optimization**



Findings: New ultra low dissipation smart alloys

9 prediction/synthesis/characterization iterations
(batch mode: 4 predictions/experiments at a time)
14 alloys better than the best in training data
(p value<.001)



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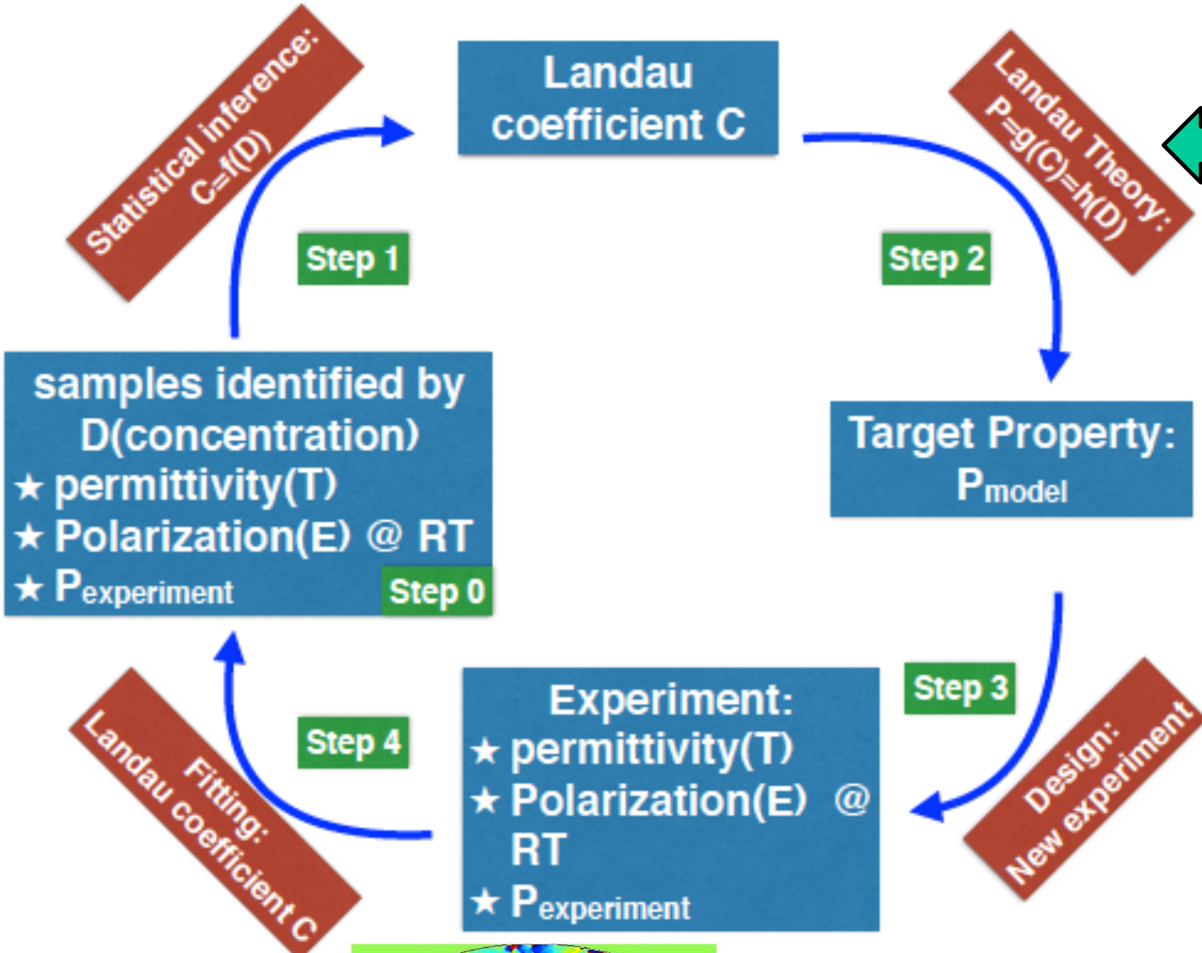
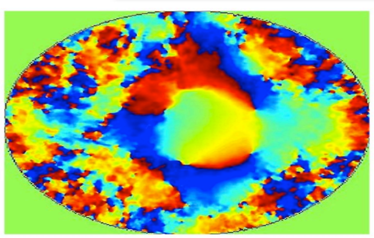
Predictive Mesoscale Models and Simulations via Informatics, Synthesis and *in situ* Characterization



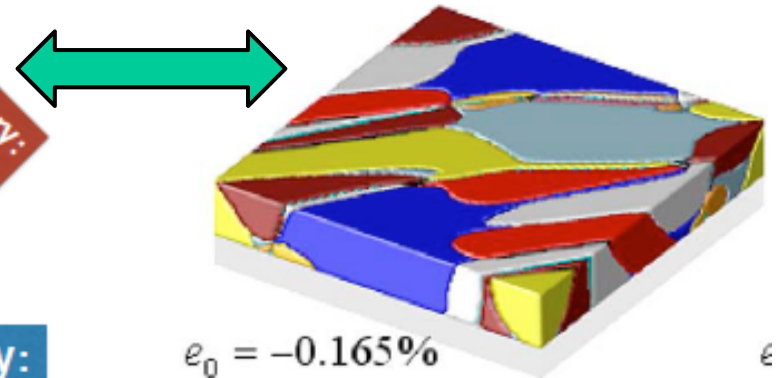


In situ @ LCLS

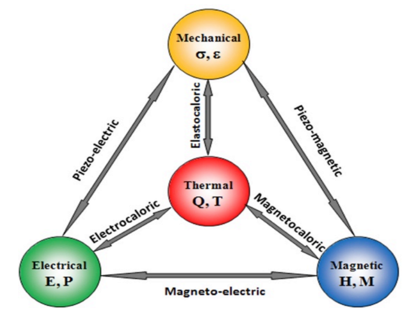
Image maps

Polarization

Distortion

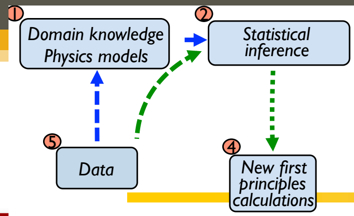


Phase field simulations



Applications to energy harvesting materials

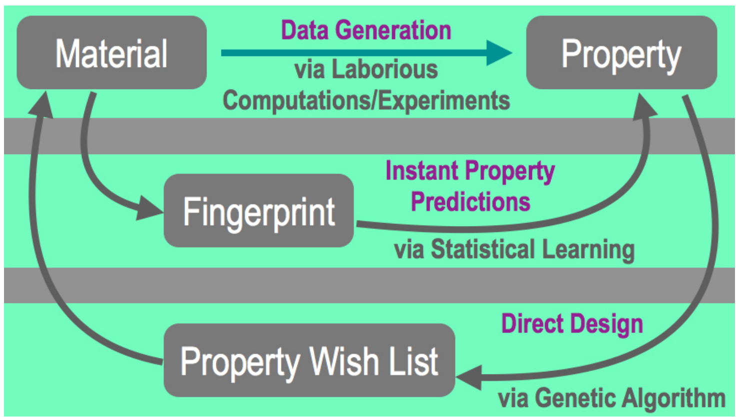
- ferroelectrics
- electrocalorics
- magnetocalorics

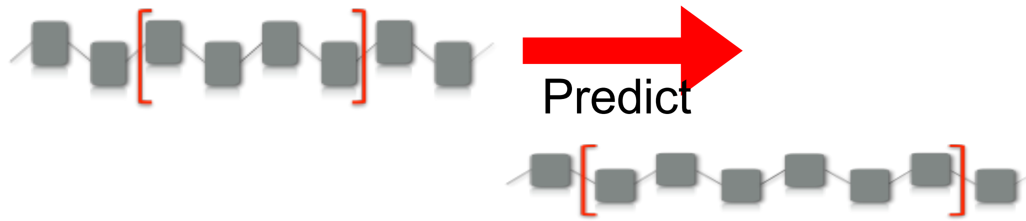


Predictions via machine learning

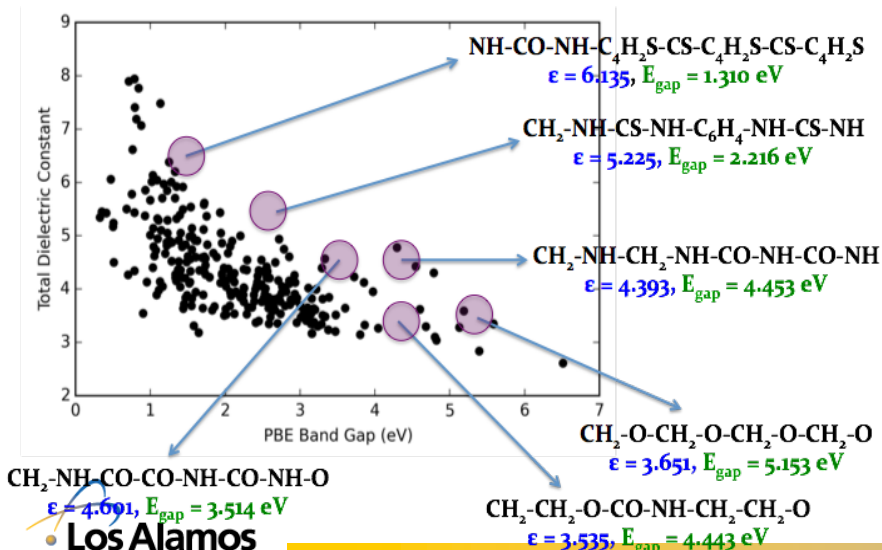
Goal: Polymers for high energy density capacitors and release: large wide band gap & dielectric constant

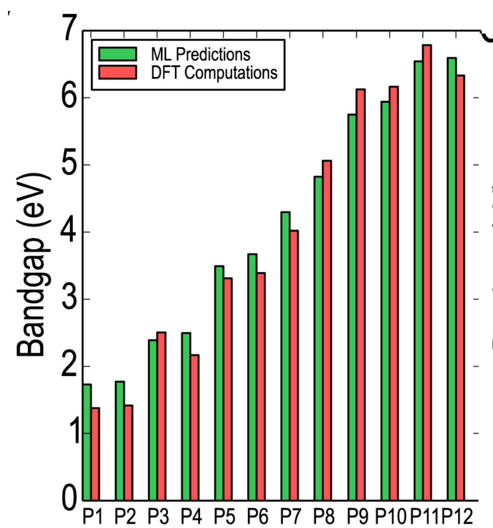
$$\text{Maximum Energy Density } \alpha \ \varepsilon E_{bd}^2$$

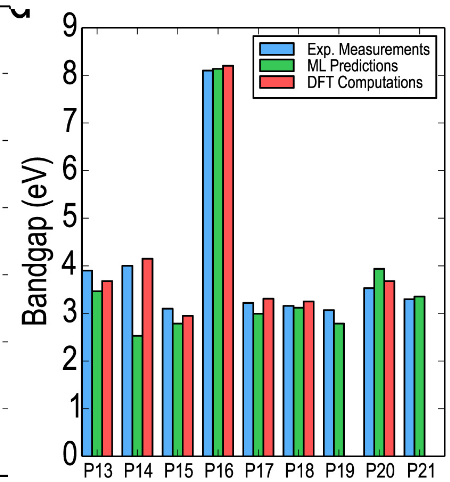




- **Learn from polymers with small repeat units to predict response for large repeat unit polymers**







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