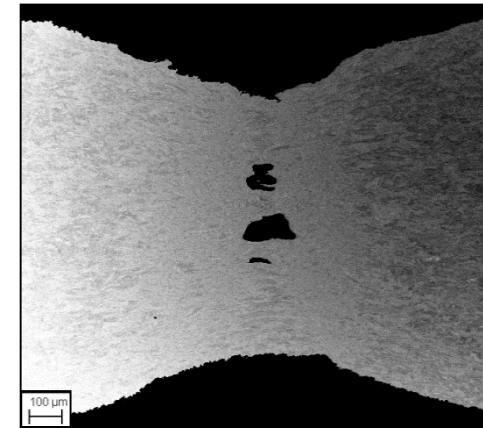
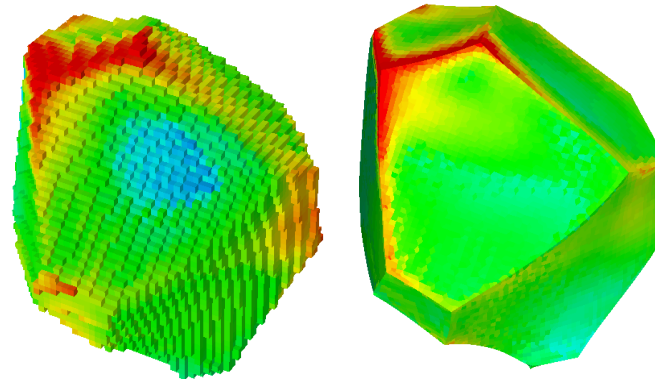
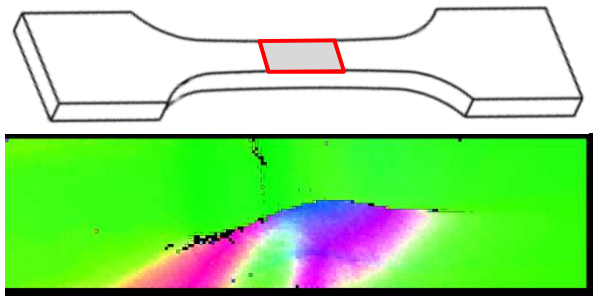


Exceptional service in the national interest



An Overview of Sandia's “Predicting Performance Margins” (PPM) Program

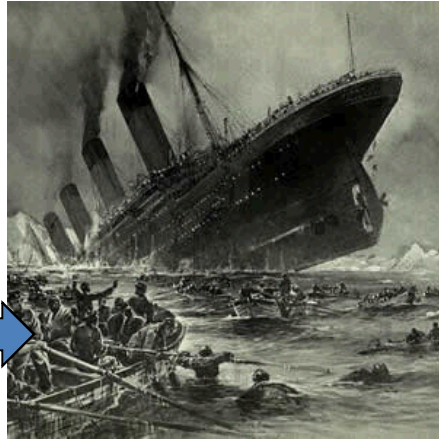
Brad L. Boyce

**Materials Science and Engineering Center
Sandia National Laboratories**

Most engineering disasters share a common thread: Deformation and Fracture



Chernobyl: power surge -> Reactor Vessel Rupture
Up to 4K near-term deaths
30K-1M premature cancer cases



Titanic: impact -> Hull rupture
p to 4K near-term deaths
1.5K deaths



Boston Molasses Disaster:
Rivet rupture
21 Deaths

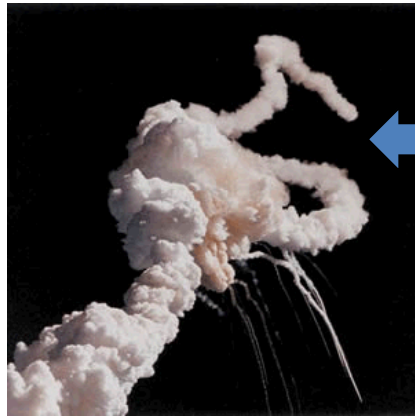


Space Shuttle Challenger: cold temperatures -> O-ring rupture
7 Deaths

96 separate airframe mechanical structural failures



Banquiao and Shimatan Reservoir Dams (1975): structural failure
50K – 150K deaths

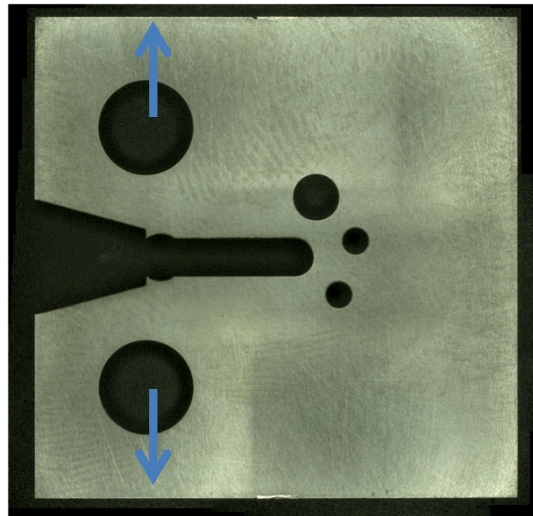


Tacoma Narrows Bridge:
twisting/resonance-> cable failure
1 Death

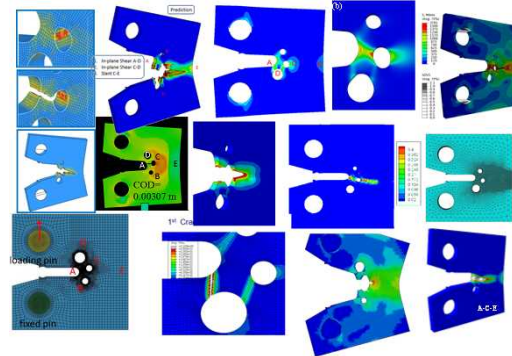


Sandia Fracture Challenge Reveals Shortcomings of Predictive Simulation for Even 'Simple' Scenarios

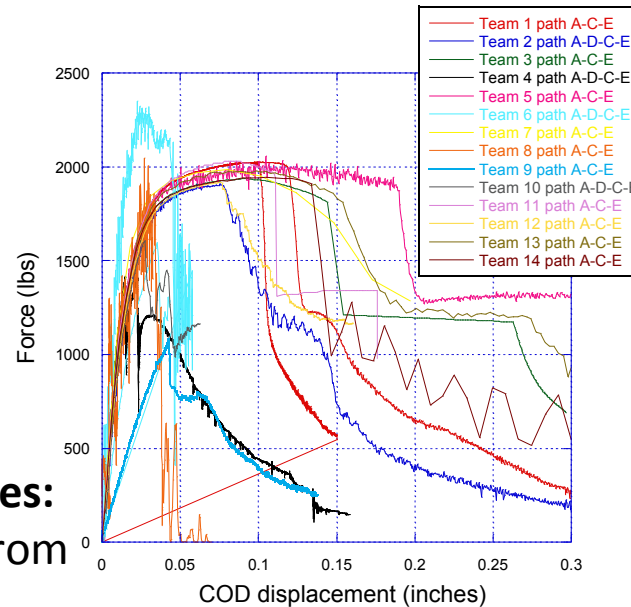
A 'simple' blind scenario:
What forces and displacements are required to cause fracture?



Assess international capabilities:
Engage Sandia and 13 teams from across the world.

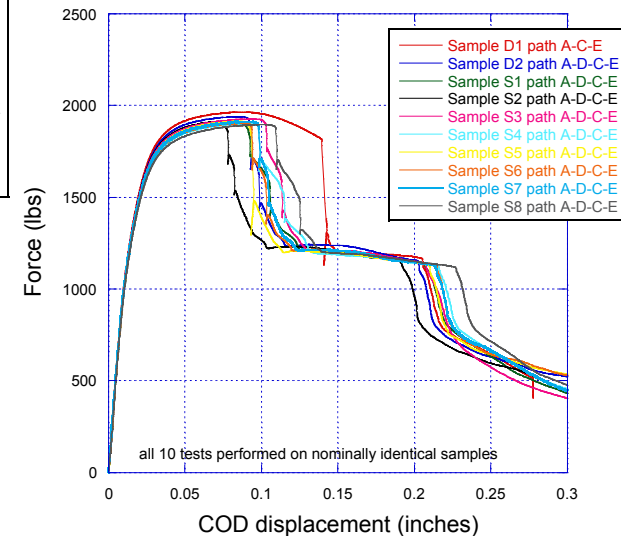


predictions - 14 institutions



- Among a consortium of leading computational mechanics groups, there was a wide breadth in the range of predictions.
- None of the teams predicted the experimentally observed scatter in response.

experiments - Sandia solid mechanics
Charlotte Kramer and Theresa Cordova



Boyce, et al. (50 authors), *Int. J. Fracture*, 2014

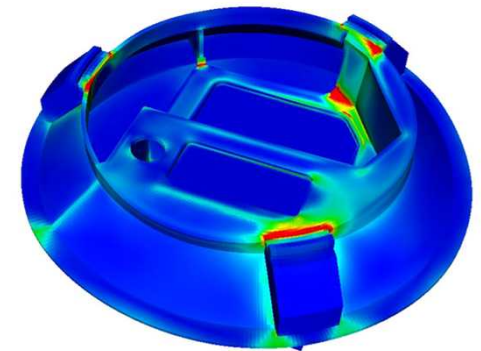
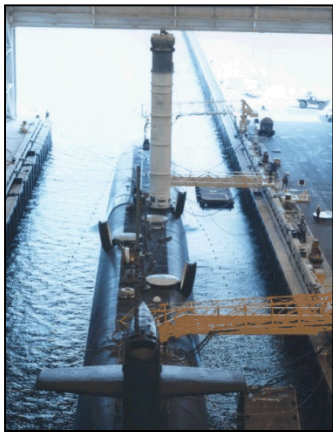
PPM's Overarching Objective

Materials behave stochastically, yet the micro- and nano-scale origins of performance variability are often unknown. The overarching goal of this project is to enhance the knowledge, tools, and capabilities to **evaluate and predict the stochastic reliability of structural metals** and alloys **due to materials variability**. This goal is achieved by integrating a scientific discovery process **at multiple length and time scales** to inform models that can be used by the weapons engineer to predict performance margins. As we achieve this goal, we will shift Sandia's existing modeling, design and analysis approach away from deterministic scalar properties and toward statistical properties that **capture realistic uncertainties and margins** that arise from the inherent variability in materials' structures and properties.

Transportation Crash



Loading Accident



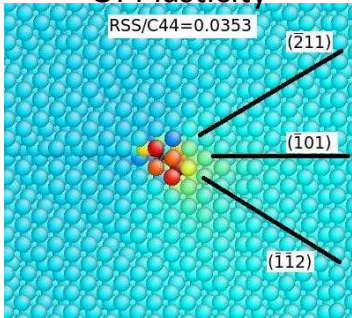
Housing/Cover
Failure Analysis



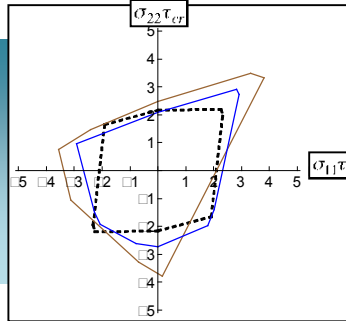
Broken Clip

Developing an experimentally validated model for grain scale deformation (crystal plasticity)

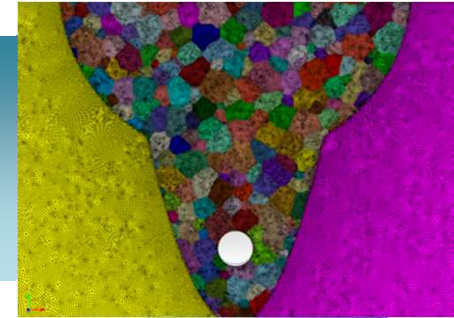
Atomic Mechanisms Of Plasticity



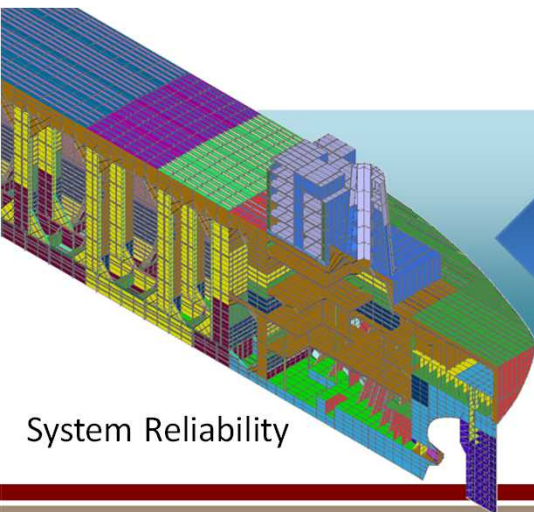
Single-Crystal Plasticity Models



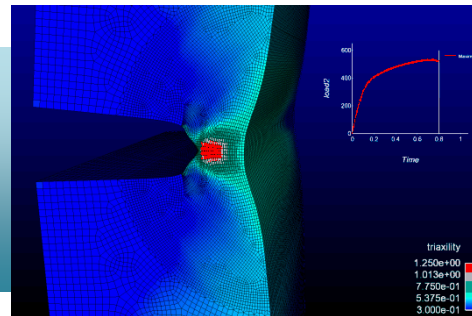
Polycrystalline Deformation Response



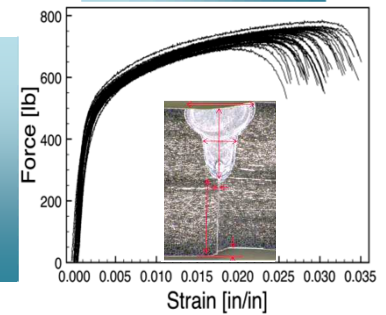
Goal: Provide a science-based foundation for design, analysis, and qualification capabilities that links mesoscopic/microscopic inhomogeneity to property variability.



System Reliability

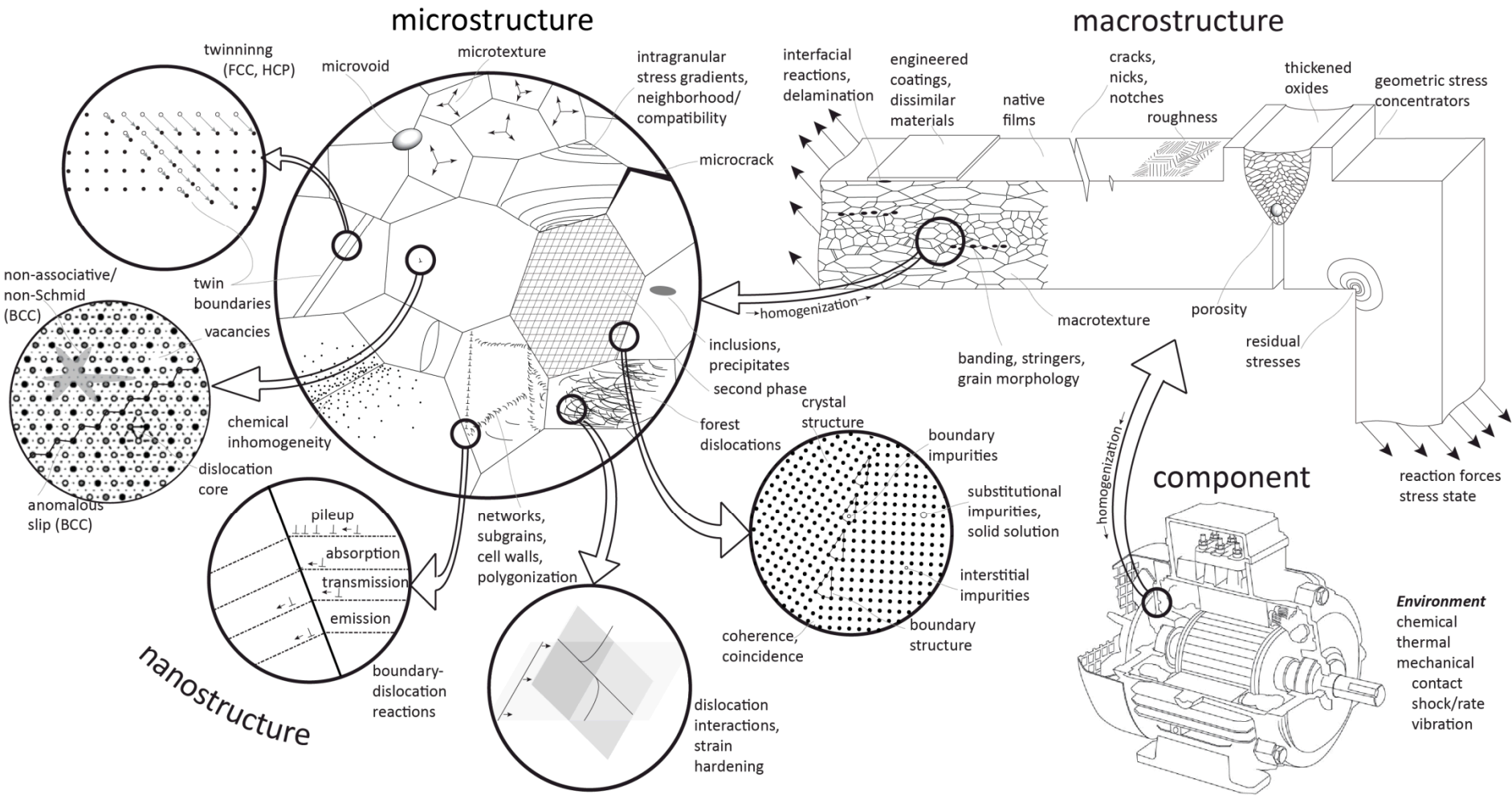


Reduced Order Modeling For Efficient Stochastic Computations



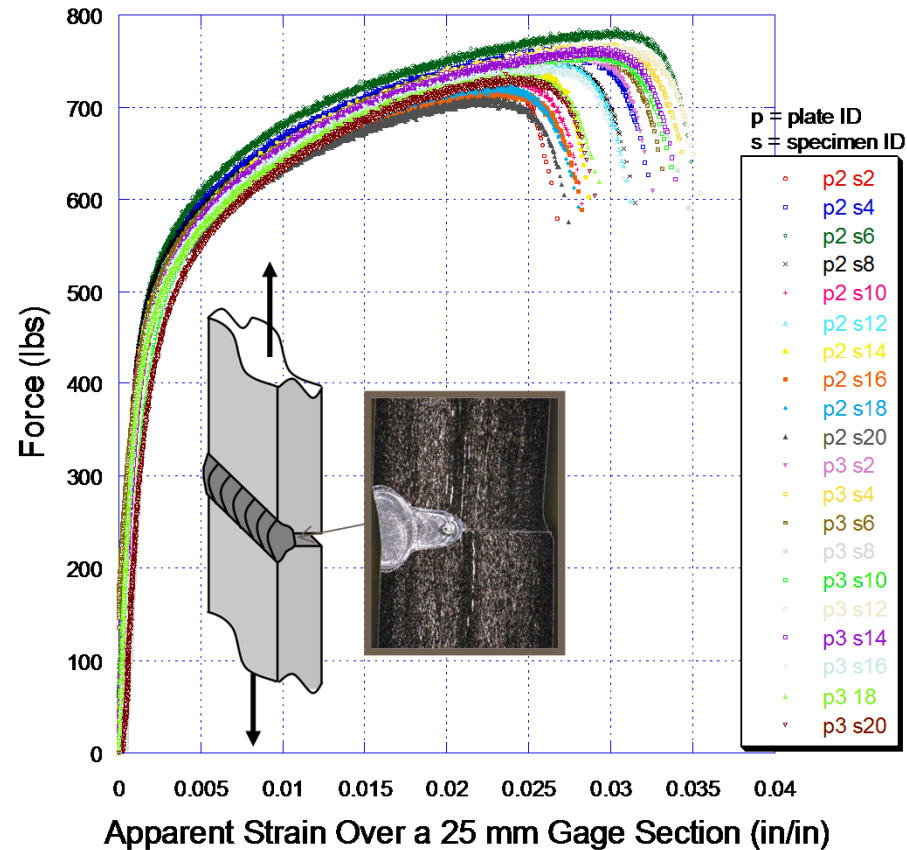
Stochastic Outcomes From Different Configurations

Material Complexity Roadmap for Deformation and Fracture



Computationally efficient algorithms to perform large-scale statistical sampling simulations

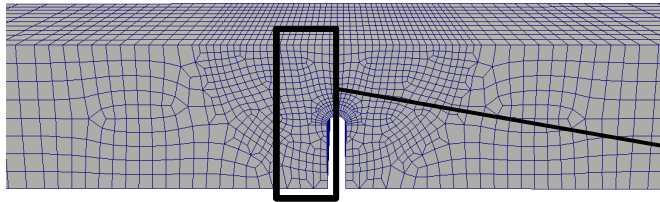
Variability in Tensile Performance of 20 Laser Butt Welds of 304L-to-304L



How do we use 20 test results to predict 1-in-1000 behavior?

Stochastic Reduced-Order Modeling (intelligent sampling)

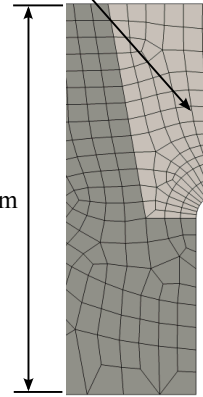
Weld FE model w/ idealized geometry



base sheet: deterministic
weld region: stochastic

WELD REGION

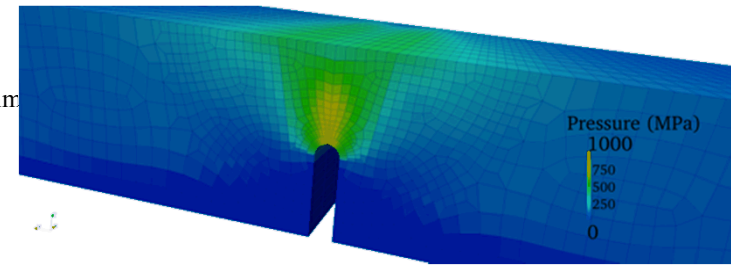
1.6 mm



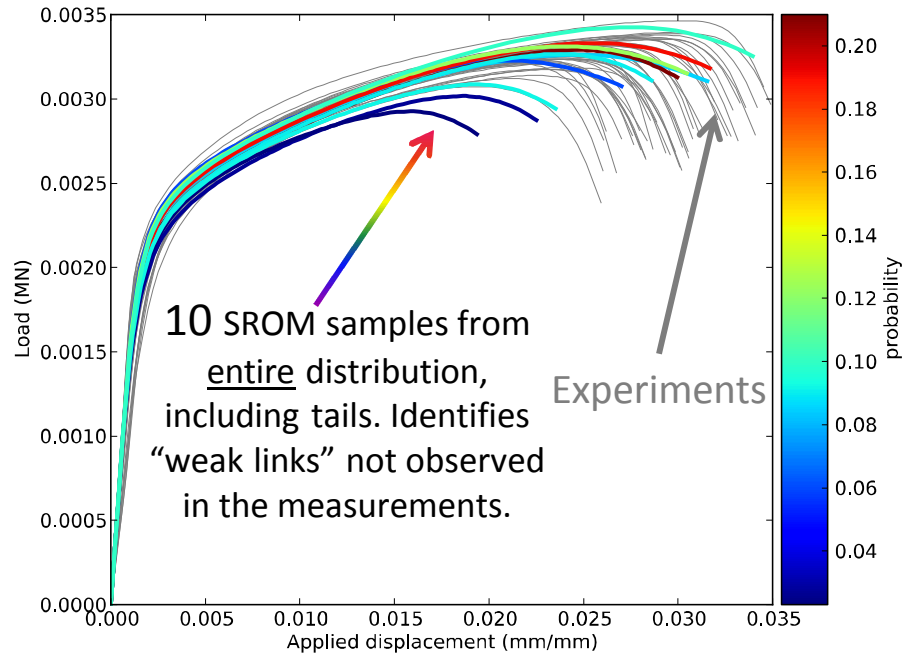
0.76 mm

NOTCH RADIUS

Simulated Pressure Map



Pressure (MPa)
1000
750
500
250
0



10 SROM samples from entire distribution, including tails. Identifies "weak links" not observed in the measurements.

Experiments

probability

initial yield stress

$$\sigma_y = Y + \kappa$$

hardening (linear)

$$\dot{\kappa} = [H - R\kappa] \dot{\epsilon}_p$$

$$\kappa(\epsilon_p) = \frac{H}{R} [1 - \exp(-R\epsilon_p)]$$

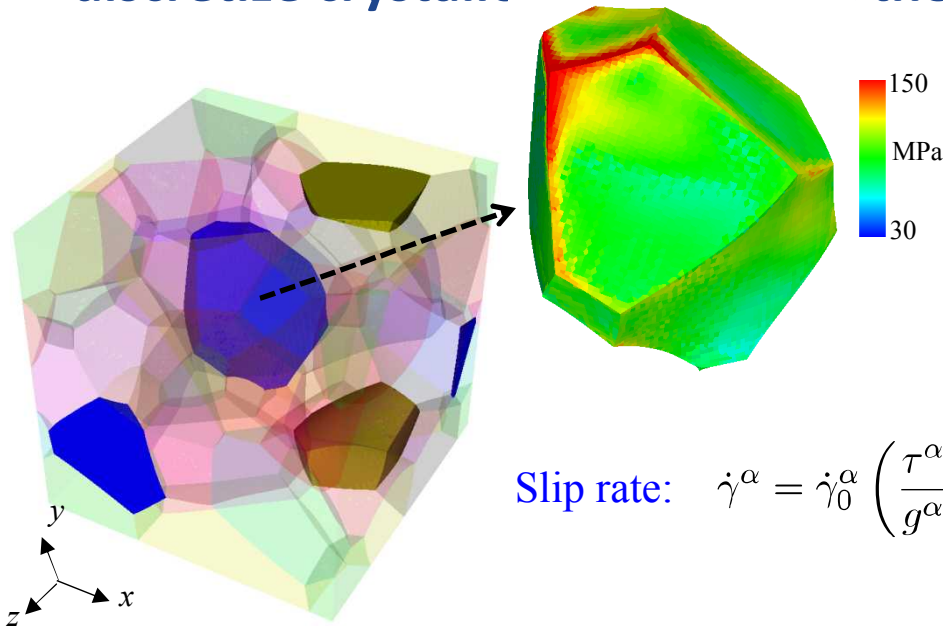
recovery coefficient

Material model w/ 3 stochastic parameters

Impact: An efficient path for NW analysis engineers when data on materials variability are limited and predictions of rare probability of failure events are required.

Computational speed up of >100X compared to conventional Monte Carlo methods.

Polycrystal plasticity employs finite element method to discretize crystallographic slip at the crystallographic-level.



Slip rate: $\dot{\gamma}^\alpha = \dot{\gamma}_0^\alpha \left(\frac{\tau^\alpha}{g^\alpha} \right)^{1/m}$ (Hutchinson, 1976) 24 $\langle 111 \rangle \{110\}$ slip systems

Slip resistance: $g^\alpha = \max(\tau_{\text{cr}}^\alpha - \tau_{\text{ns}}^\alpha, 0) + \tau_{\text{obs}}^\alpha$ (Weinberger, 2012)

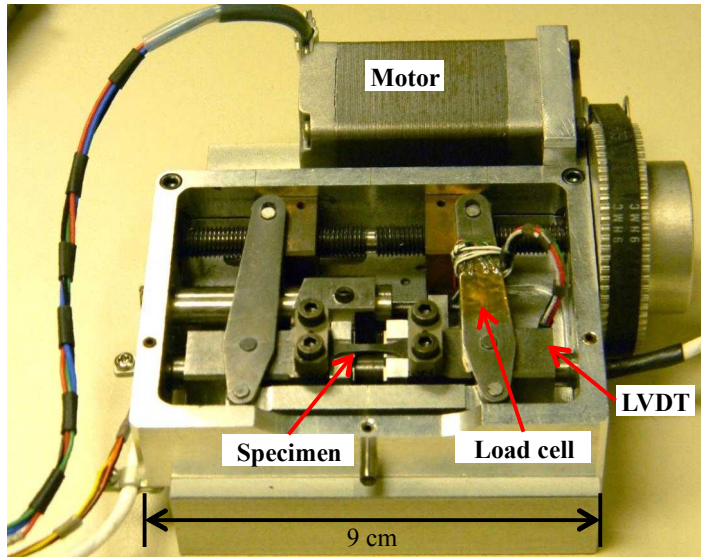
\swarrow Lattice friction \searrow Obstacle stress

Obstacle stress: $\tau_{\text{obs}}^\alpha = \alpha \mu b \sqrt{\sum_{\beta=1}^{NS} \rho^\beta}$ (Taylor, 1934)

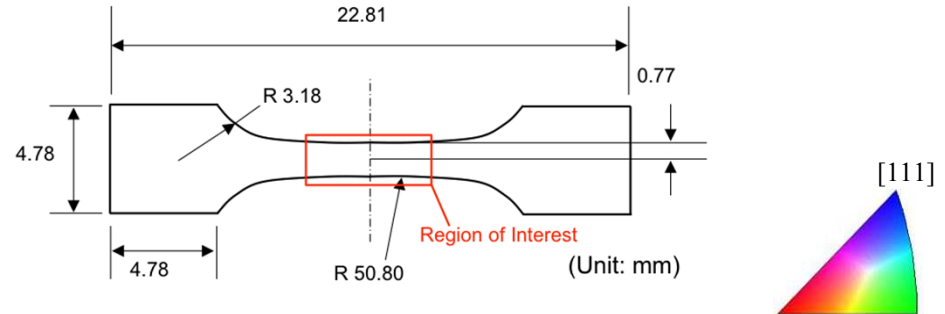
$$\rho^\alpha = \left(k_1 \sqrt{\sum_{\beta=1}^{NS} \rho^\beta} - k_2 \rho^\alpha \right) \cdot |\dot{\gamma}^\alpha| \quad (\text{Kocks, 1976})$$

Validated Multiscale Approach

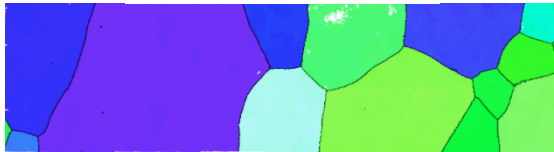
The 'oligocrystal' platform for *direct* comparison between experiments and simulations



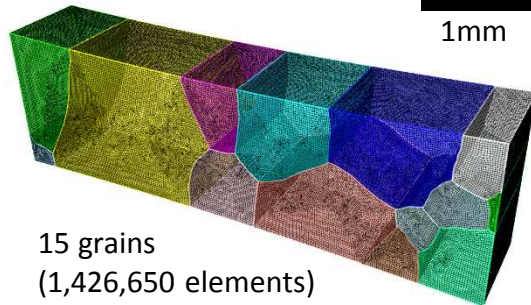
- Tantalum oligocrystals with mostly columnar 2D grain structure eliminate unknown subsurface grain morphology.
- *In-situ* load frame developed at Sandia
- HR-DIC (surface strain fields) and EBSD (crystal orientations) measurements at load inside SEM



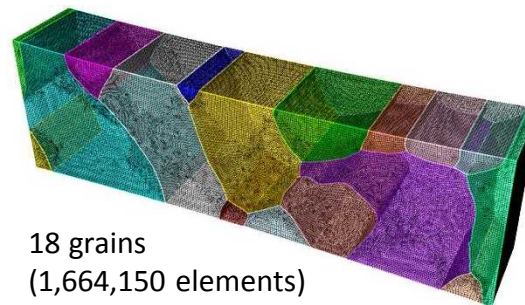
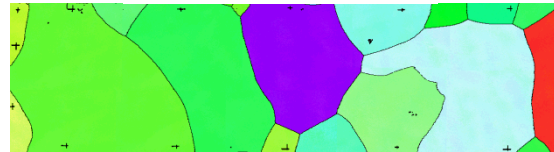
Specimen 1



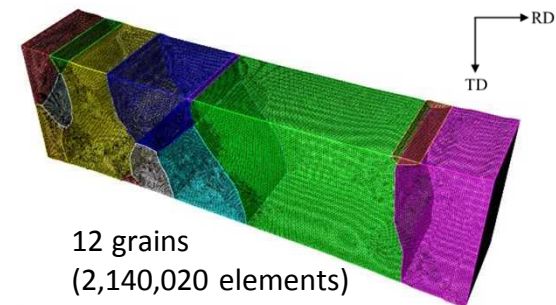
1mm



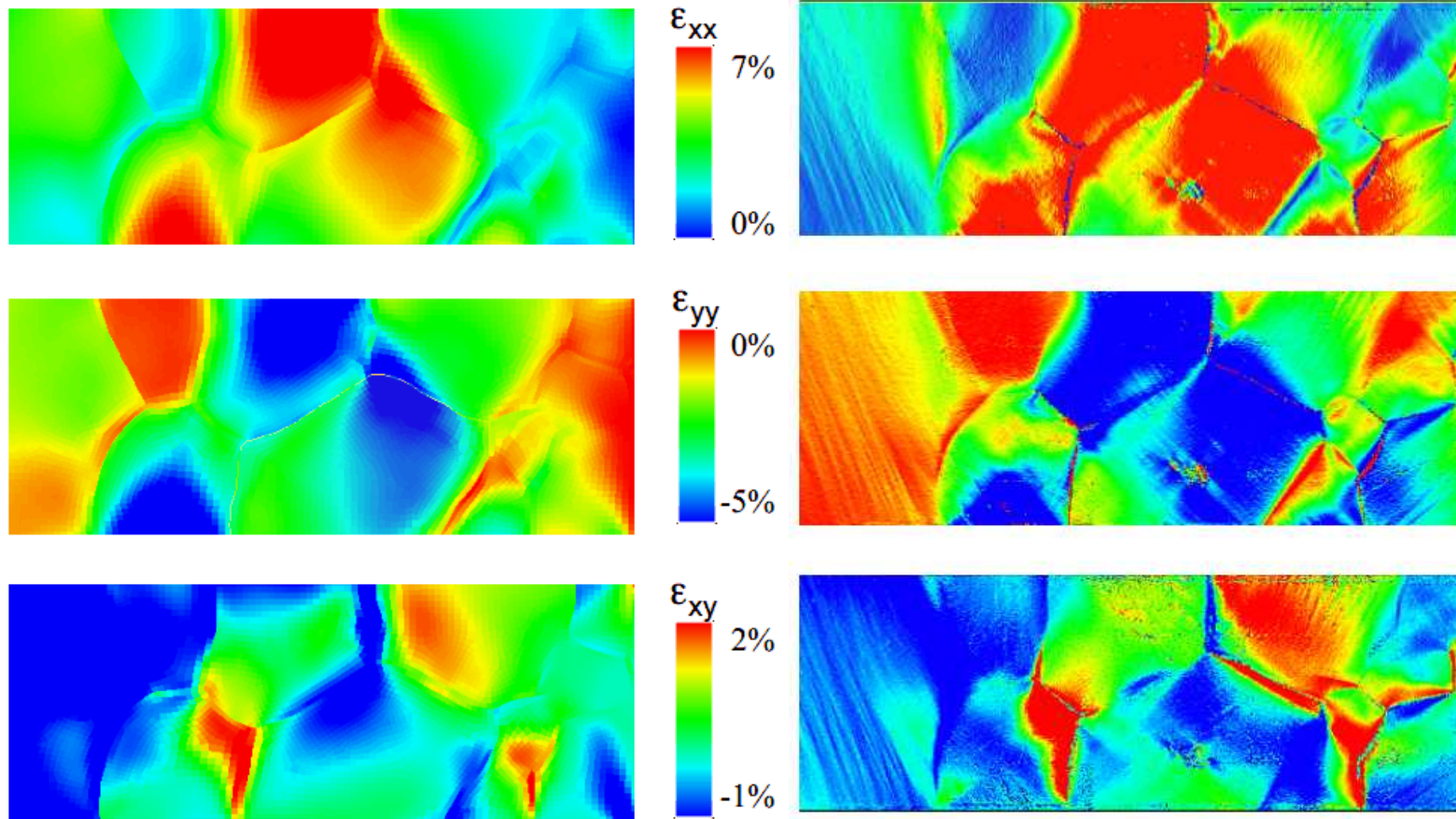
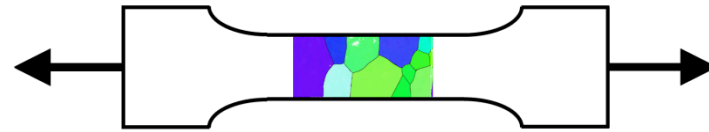
Specimen 2



Specimen 3



Experiments are needed at every length scale to develop models, calibrate parameters, and independently validate results

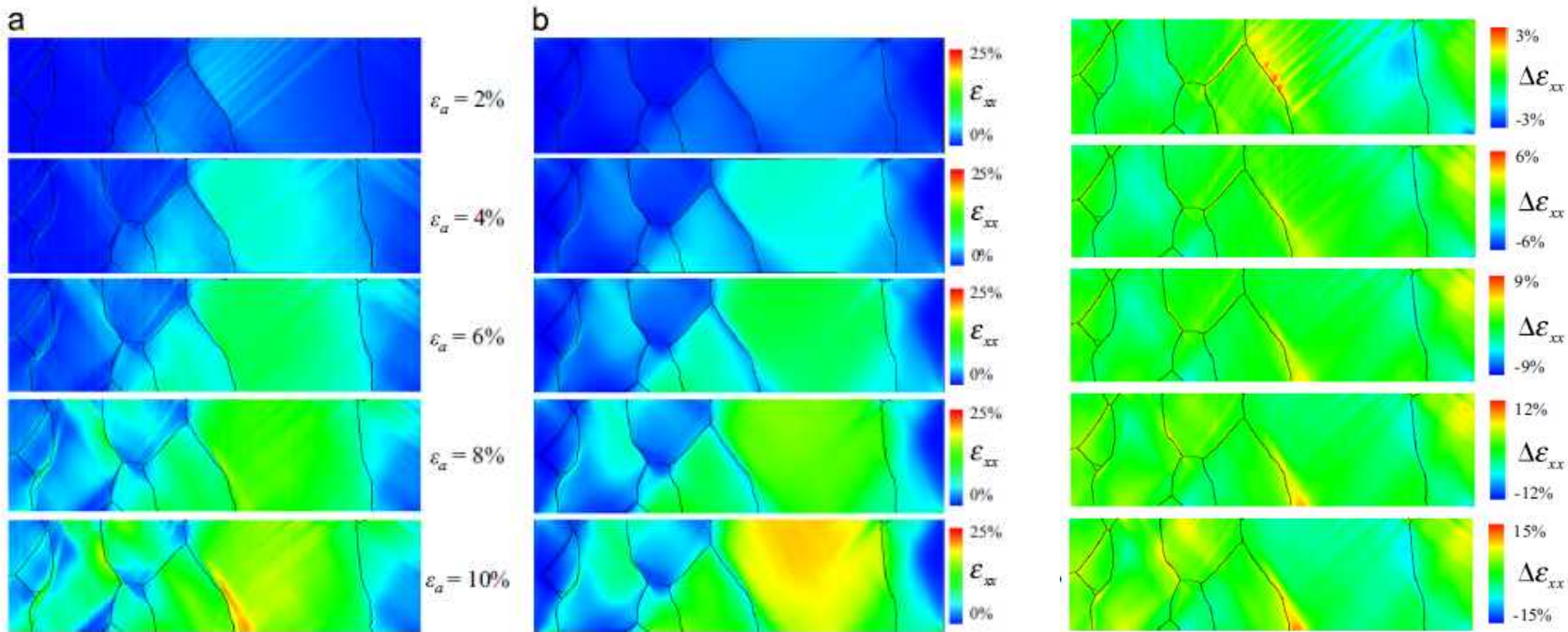


2D slice of a 3D simulation of strain inhomogeneity based on crystal plasticity finite element modeling.

Experimental measurement of strains within individual grains using SEM Digital Image Correlation

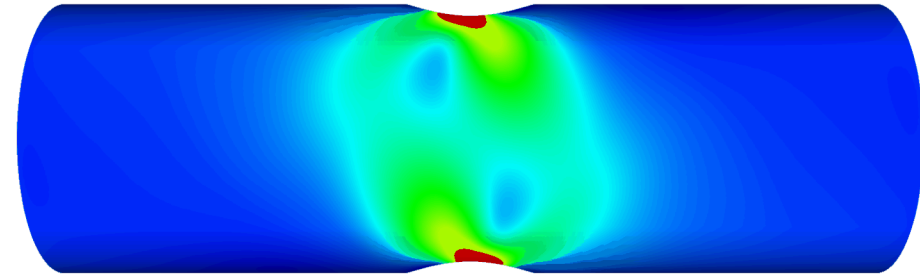
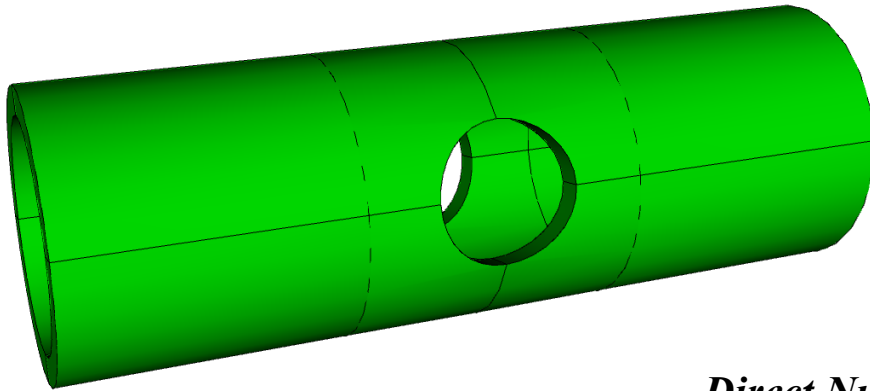
A Quantitative Model-Experiment Difference Map

$$\epsilon_{xx}^{DIC} - \epsilon_{xx}^{CPFEM} = \Delta\epsilon_{xx}$$



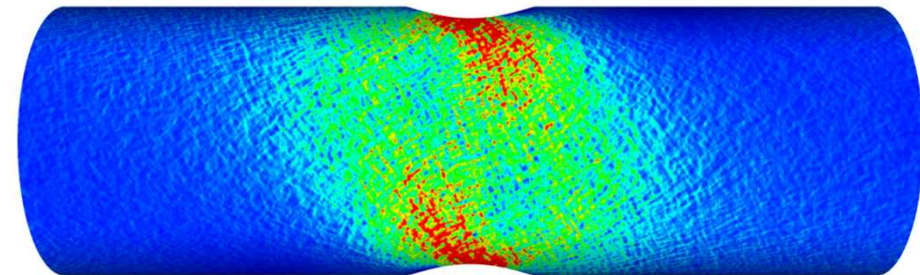
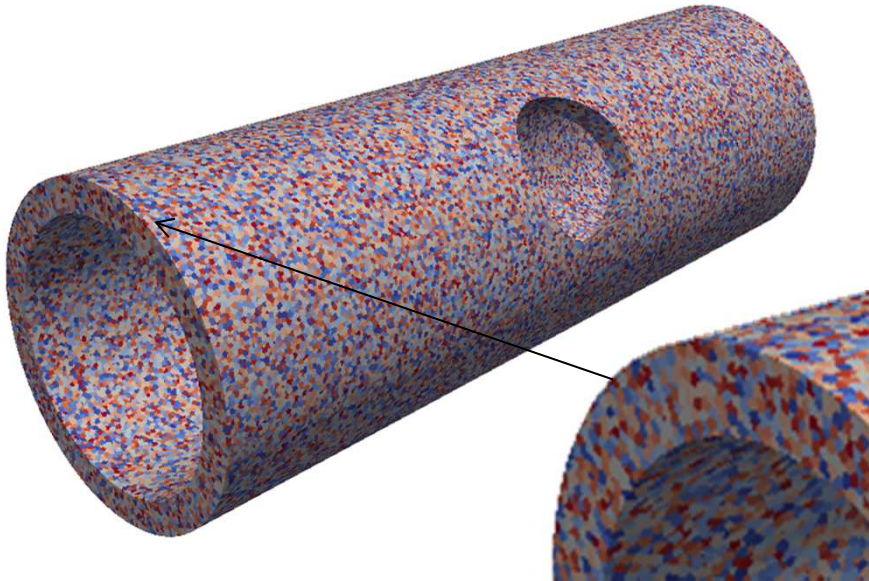
System-scale simulations with explicit microstructural representations.

Homogenization



8K elements

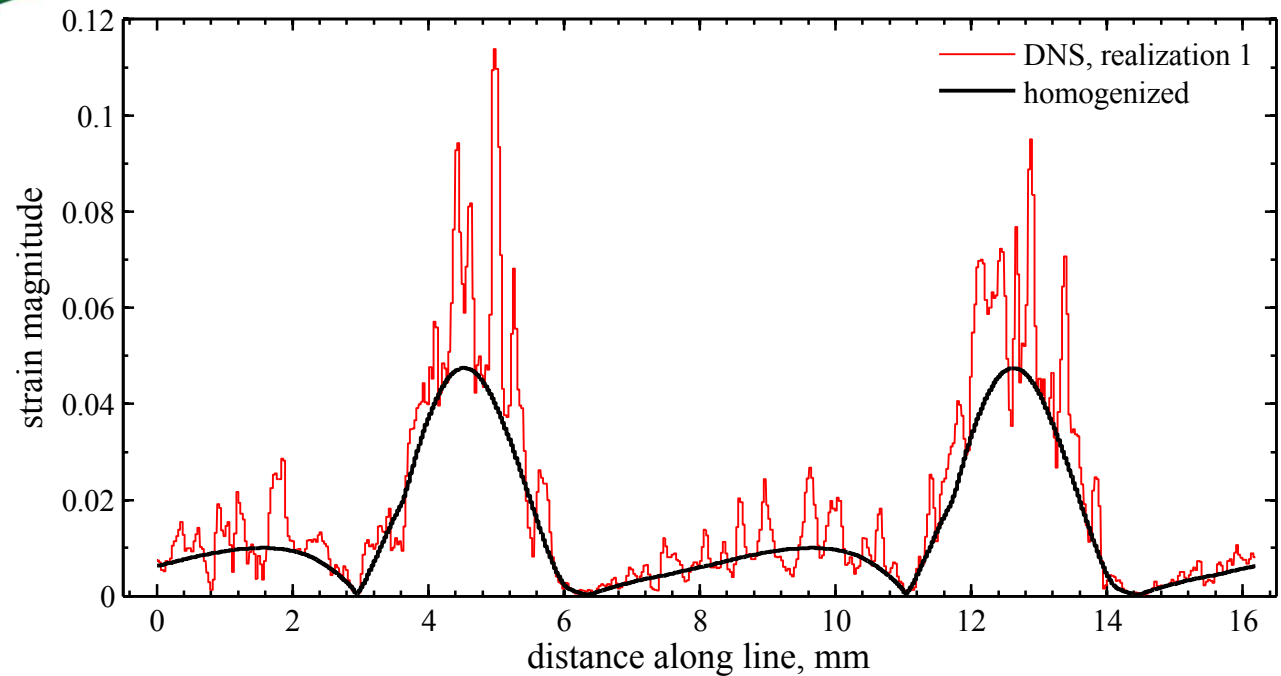
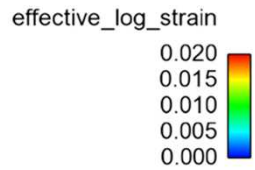
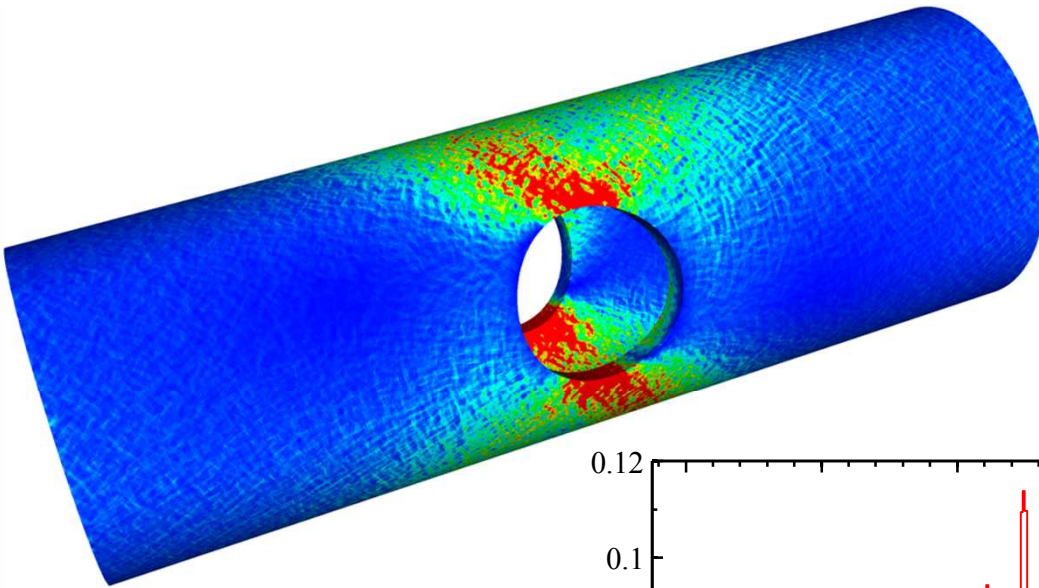
Direct Numerical Simulation



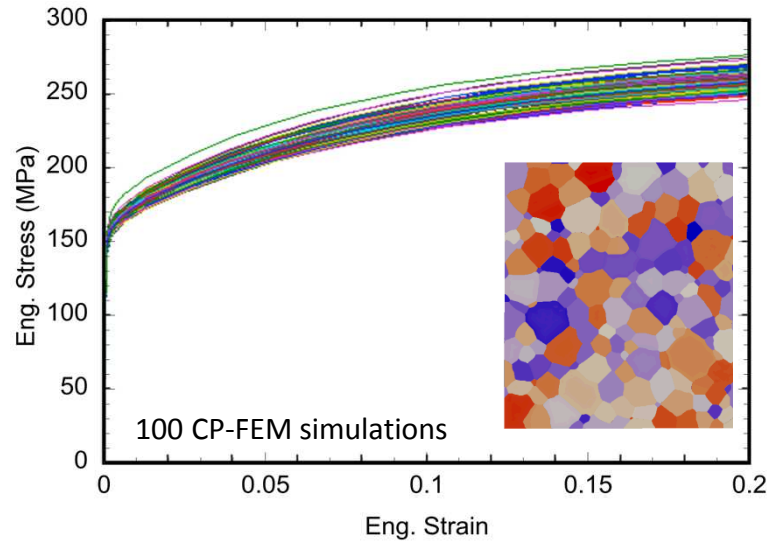
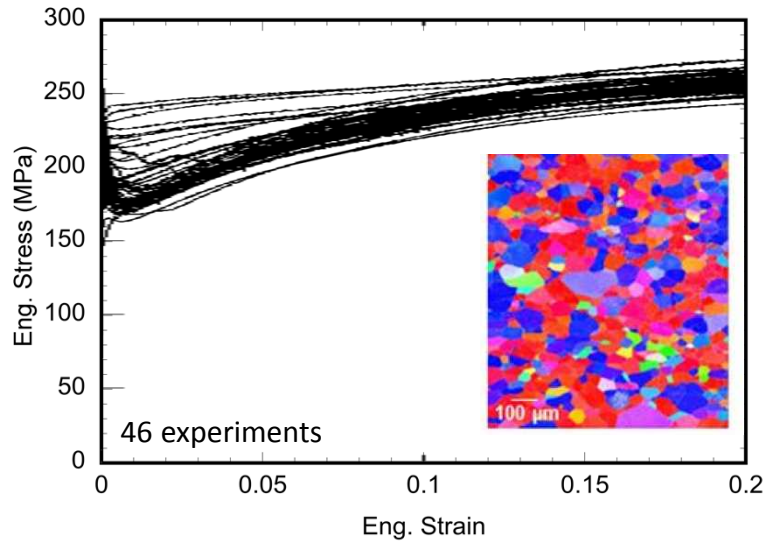
35M elements, 350K grains
2400 processors (Chama)

effective_log_strain
0.020
0.015
0.010
0.005
0.000

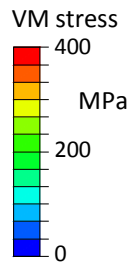
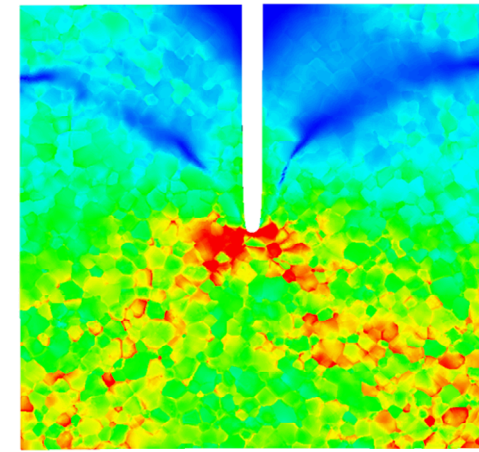
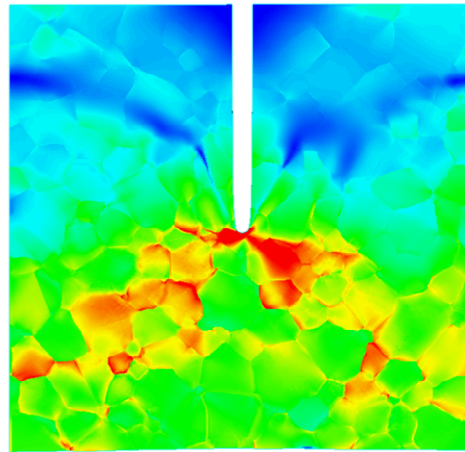
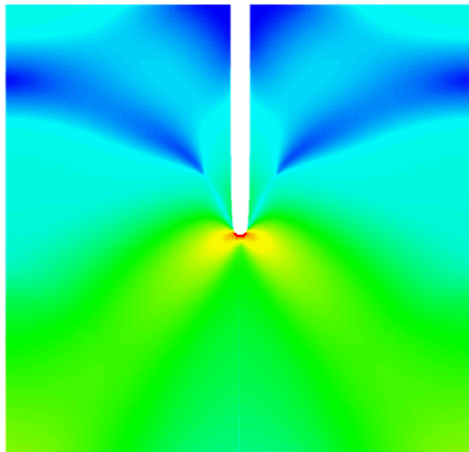
System-scale simulations with explicit microstructural representations.



Predicting Stochastic Behavior of Polycrystals



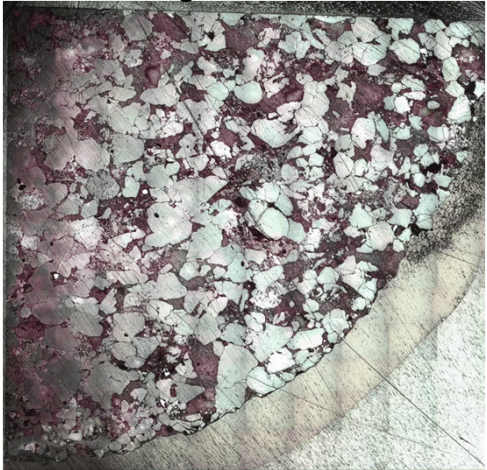
Grain-scale variability in macroscale response



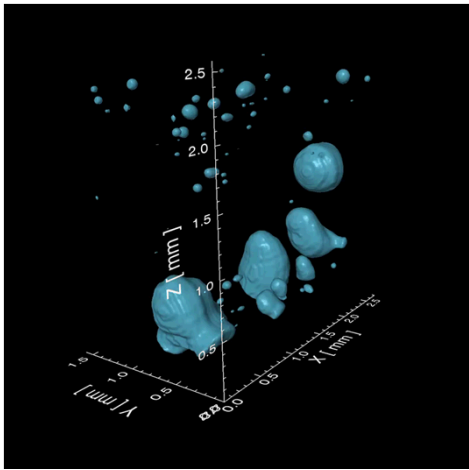
VM stress fields after 3% deformation

Emerging Capabilities: Modeling and Characterization of Realistic 3D Microstructures

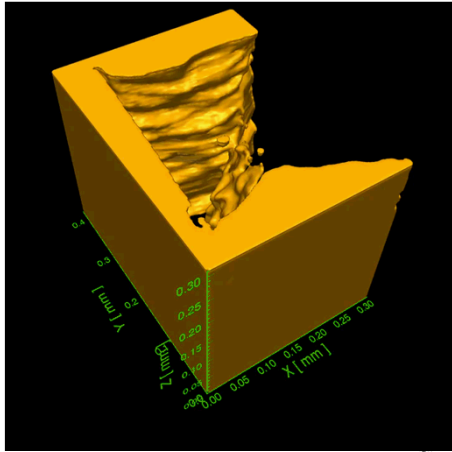
3D grain structure



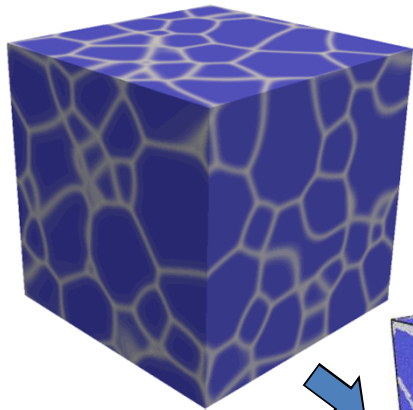
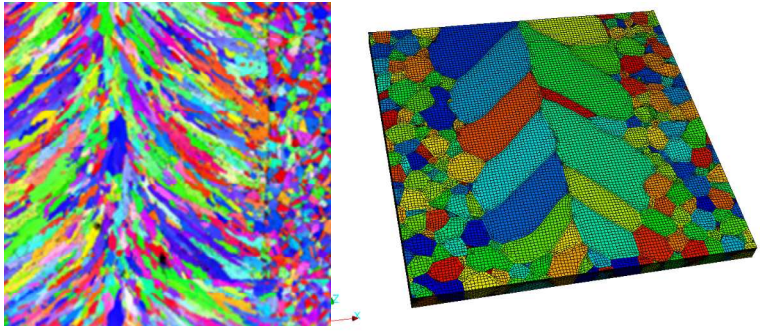
3D internal void distribution



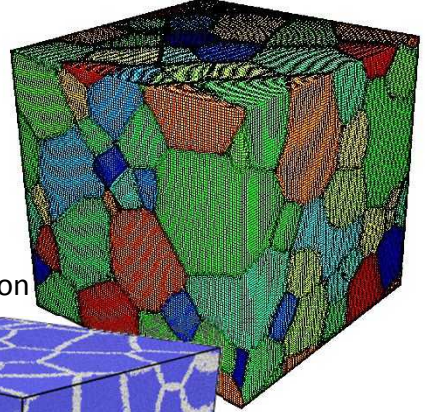
3D crack shape



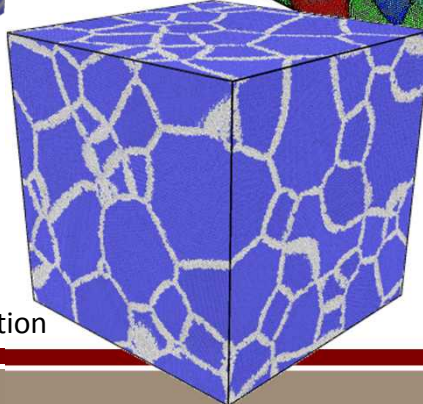
Realistic grain topologies



FEA simulation

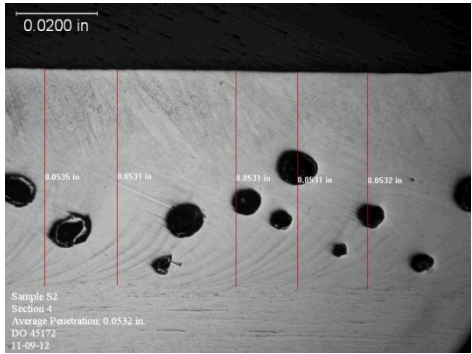


Phase field grain growth simulation



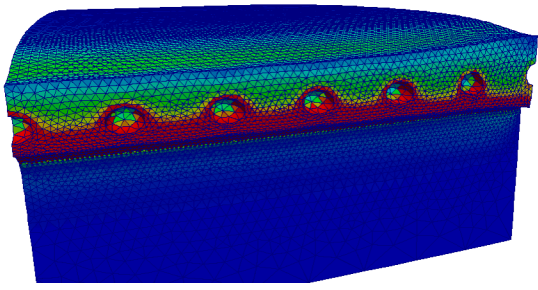
MD simulation

Making a weld deeper, doesn't always mean that it can hold more force... porosity factors in as well.



Porosity in laser welds

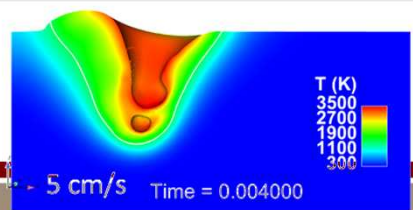
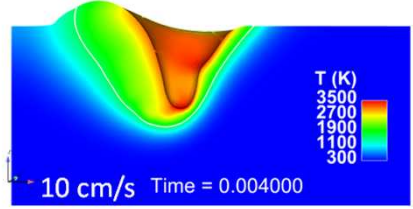
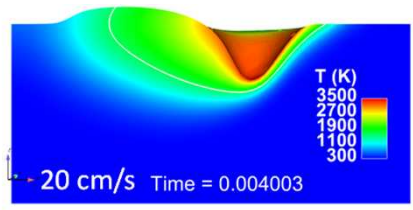
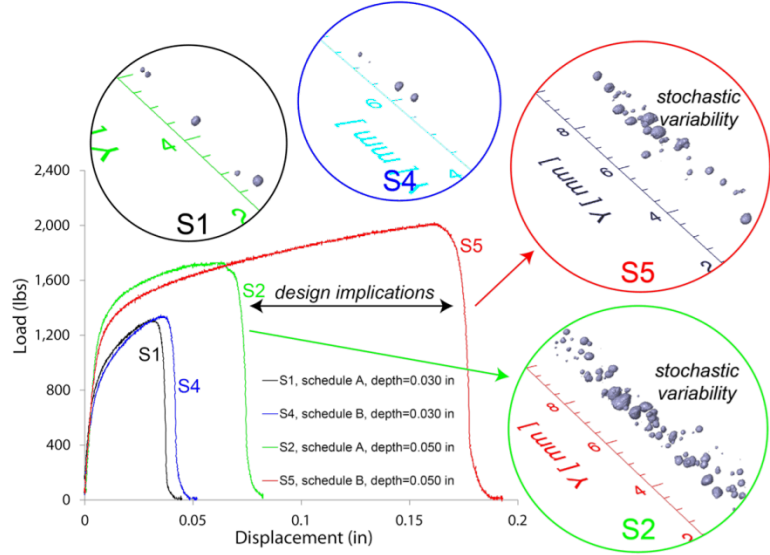
In laser welds of stainless steel, a common thread is the relationship between laser power, travel speed, porosity formation, and resulting properties.



Finite Element Representation of Porosity

A finite element model allows exploration of scenarios that may be difficult or time consuming to explore experimentally.

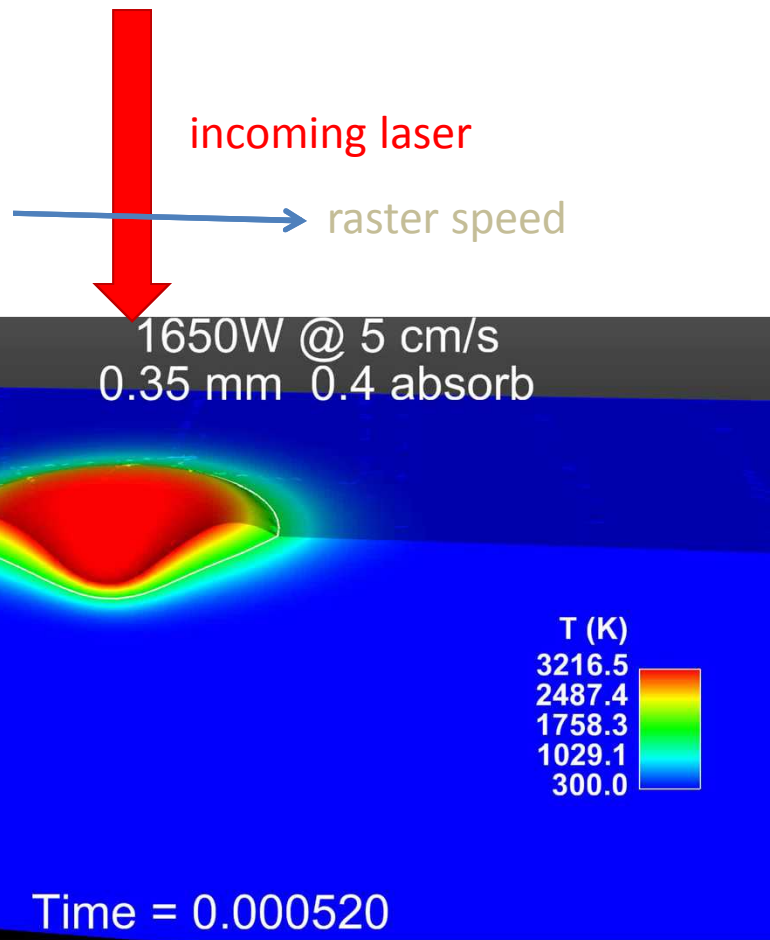
Weld Schedule exploration
Computed tomography images of weld porosity (circles) helps to interpret the effect of weld schedule on mechanical performance.



Weld process simulations

- *Surface tension & curvature
- *Maragoni Stresses
- *Energy loss:
 - Ablative
 - Radiative
 - Convective
- *Recoil pressure
- *Melting/solidification
- *Temp-dependent fluid properties $k(T)$, $C_p(T)$, $\mu(T)$

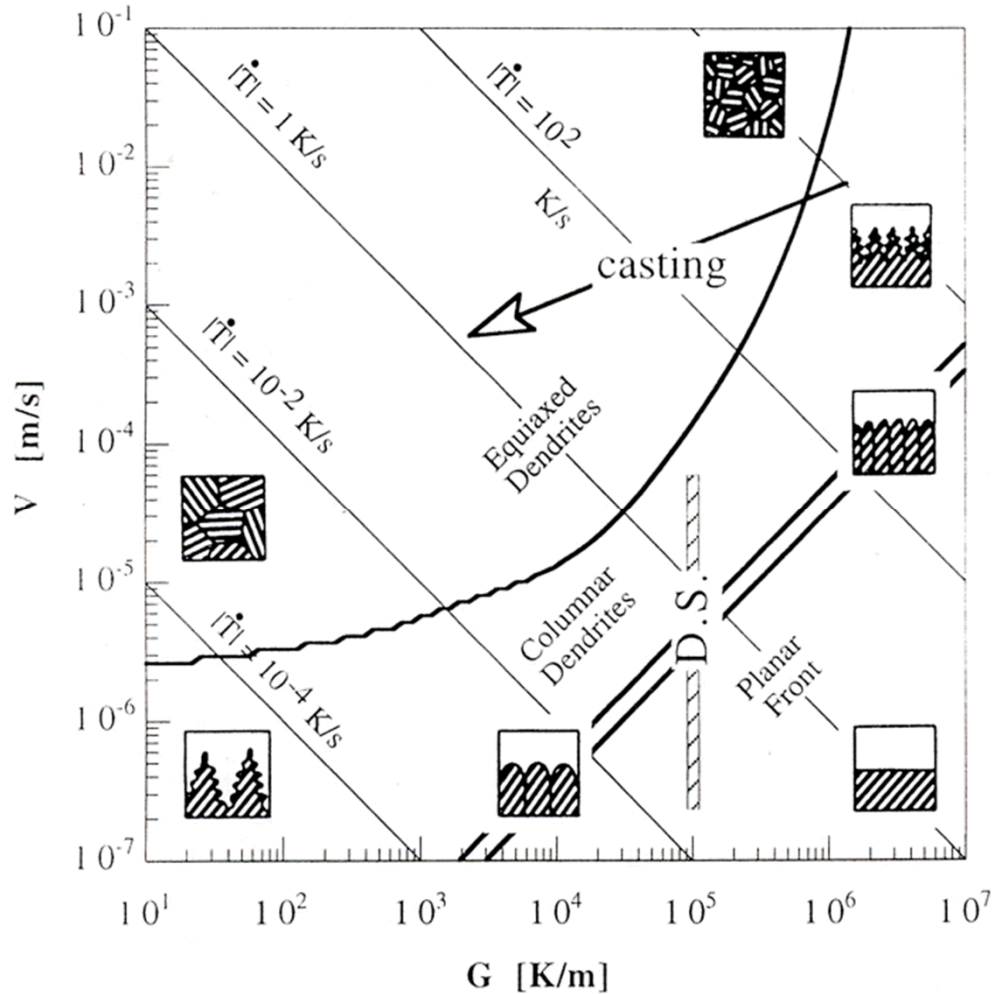
Laser Welding Simulation



For a complete picture, we need:

- Laser/plume interactions, raytracing
- Plasma fluid mechanics
- Radiation heat transfer
- Laser energy adsorption, radiation
- Thermal expansion
- Non-equilibrium vapor pressure
- Evaporation with latent heat
- Pressure-temperature relations
- T-dependent heat capacity
- Incompressible fluid dynamics
- Convective/conductive heat transfer
- Capillary forces
- Marangoni forces
- Hydrodynamic mixing
- Multicomponent liquid-solid diffusion
- Solidification macrosegregation
- Solidification shrinkage
- CTE thermal contraction
- Thermomechanical residual stress
- Solid-state diffusion
- Anisotropic crystallization
- Solid-state phase transformation

Can we predict solidification microstructure?

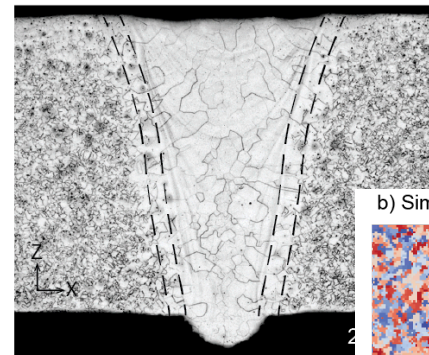


Potts Kinetic Monte Carlo

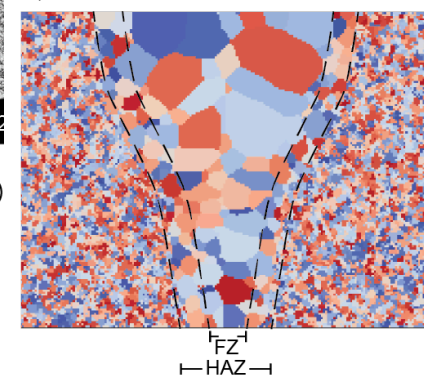
$$P = \begin{cases} \exp\left(\frac{-\Delta E}{k_B T_S}\right) & \text{if } \Delta E > 0 \\ 1 & \text{if } \Delta E \leq 0 \end{cases}$$

$$E = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^{26} (1 - \delta(q_i, q_j))$$

a) Experimental



b) Simulated



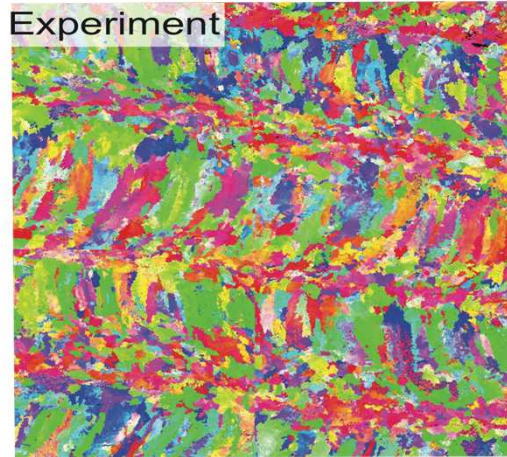
FZ
HAZ

FZ
HAZ

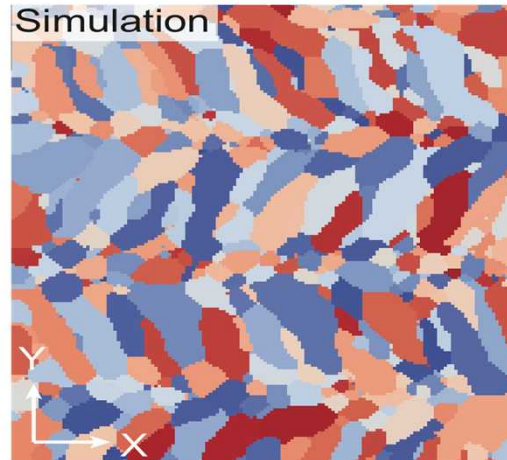
Capturing complex solidification Microstructure in Additive Manufacturing

Comparison with
3.8 kW EBSD results

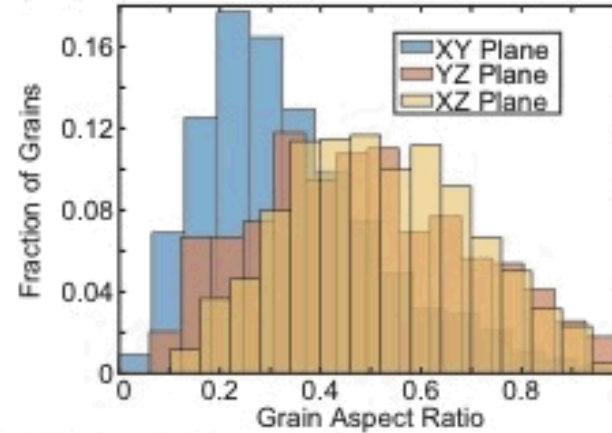
XY Plane



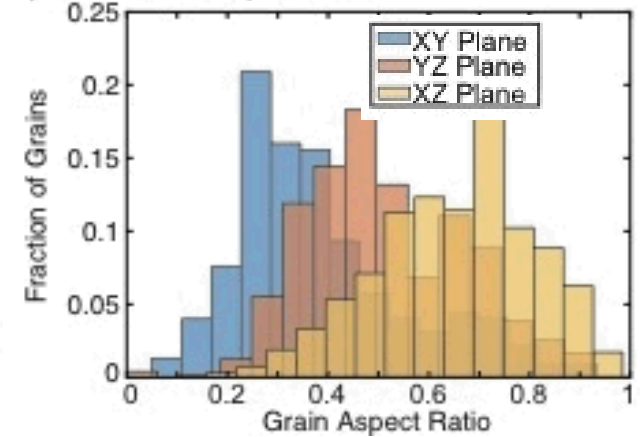
1.0 mm



a) Experimental 2D aspect ratios



b) Simulated 2D aspect ratios



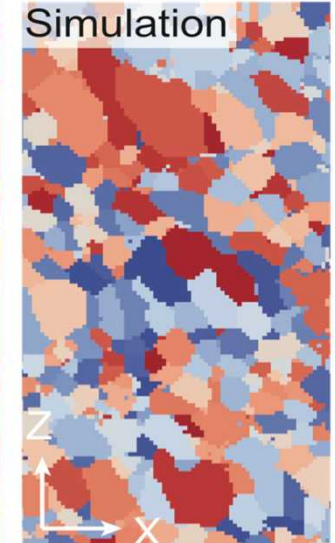
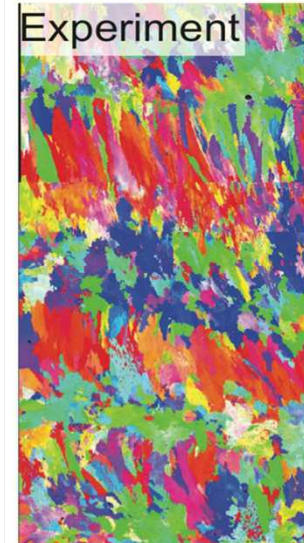
YZ Plane



1.0 mm

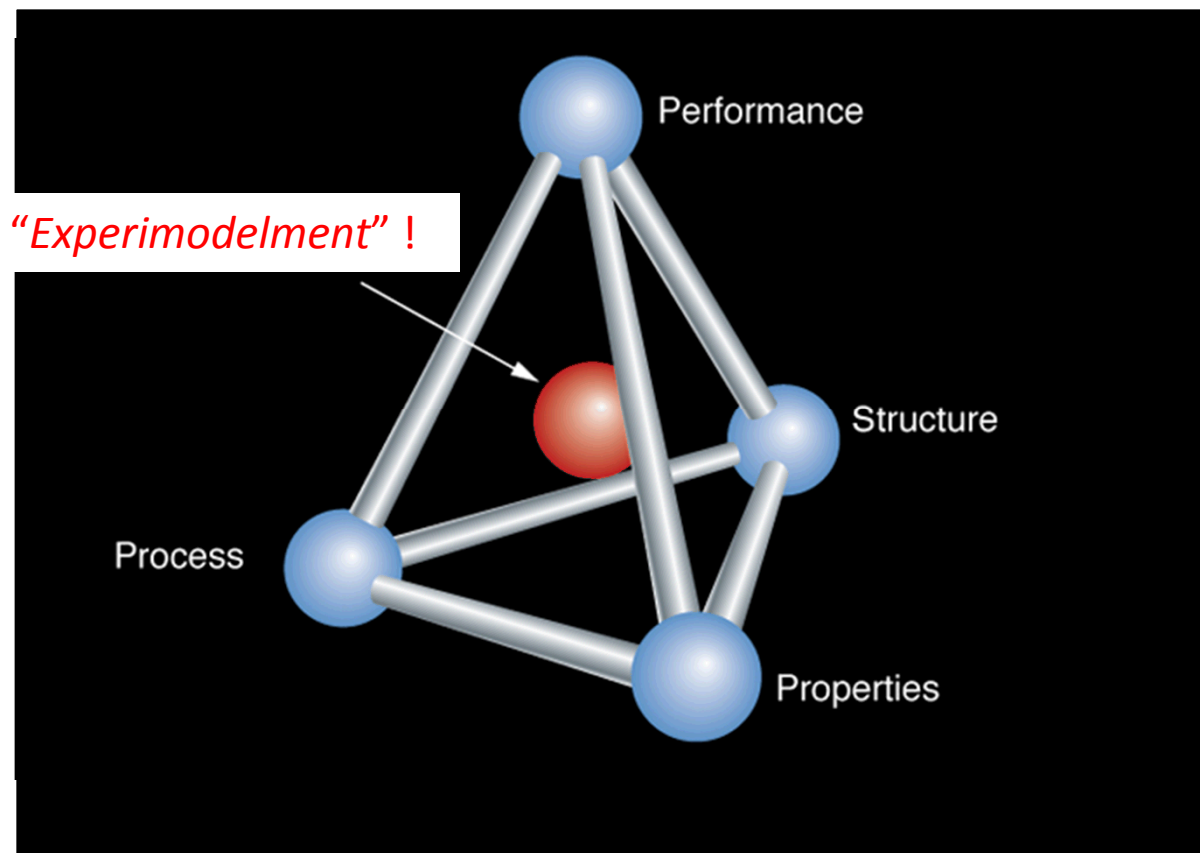


XZ Plane



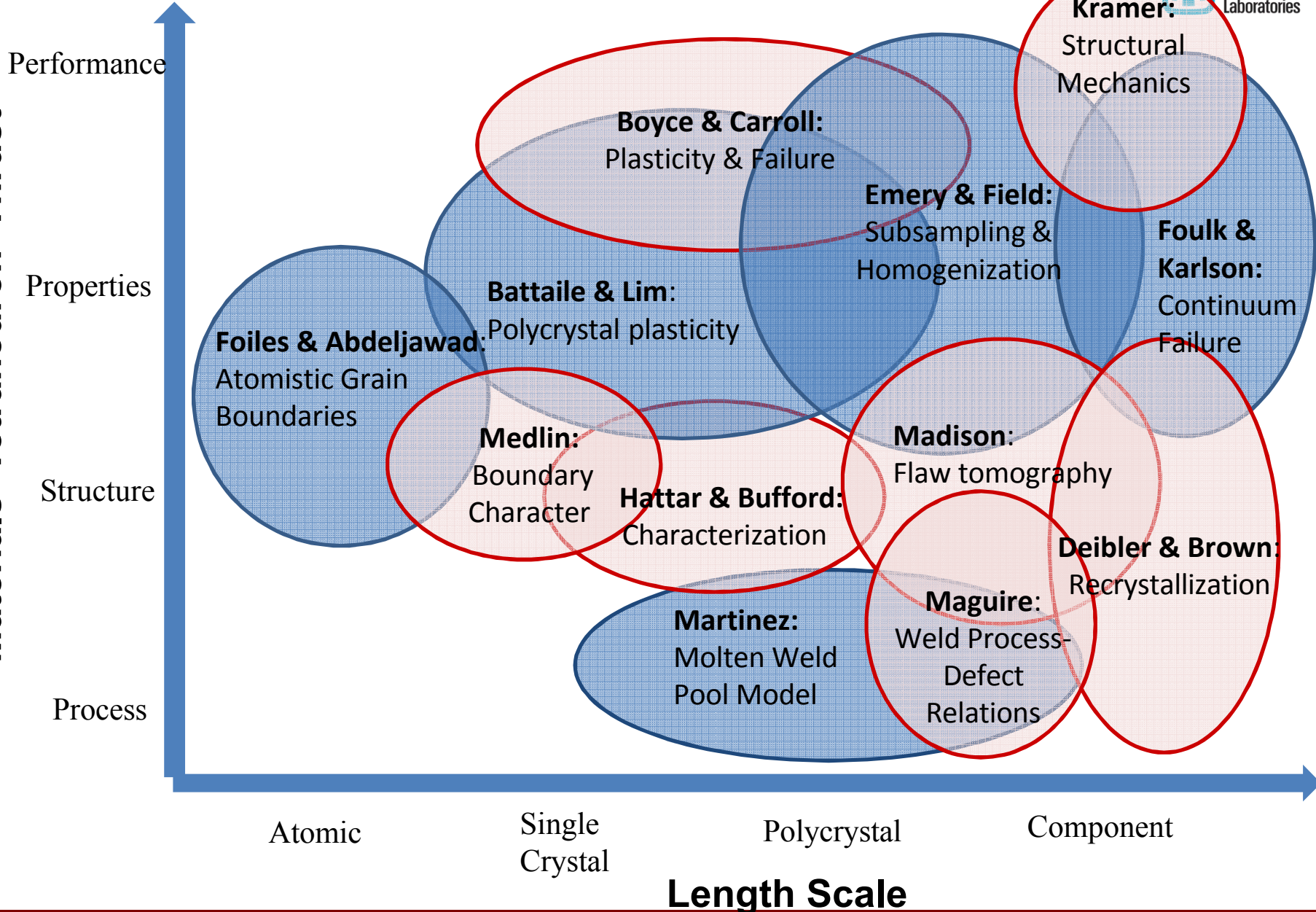
1.0 mm

Summary: Living the Materials Science Tetrahedron



Summary: The PPM Team

Materials 'Tetrahedron' Thrust



1. T.E. Buchheit, C.C. Battaile, C.R. Weinberger, and E.A. Holm, "Multi-scale modeling of low-temperature deformation in B.C.C. metals", JOM, 63, p. 33-36, 2011.
2. C.R. Weinberger, C.C. Battaile, T.E. Buchheit, and E.A. Holm, "Incorporating atomistic data of lattice friction into BCC crystal plasticity models", International Journal of Plasticity, 37, p. 16-30, 2012.
3. J.D. Carroll, W.Z. Abuzaid, J. Lambros, and H. Sehitoglu, "High resolution digital image correlation measurements of strain accumulation in fatigue crack growth", International Journal of Fatigue, 2012.
4. J.D. Carroll, L.N. Brewer, C.C. Battaile, B.L. Boyce, J.M. Emery, "The effect of grain size on local deformation near a void-like stress concentration", International Journal of Plasticity, 39, p. 46-60, 2012.
5. J. Madison, L. K. Aagesen, "Quantitative Characterization of Porosity in Laser Welds of Stainless Steel", Scripta Materialia, 67(9), p. 783-786, 2012.
6. J. Madison and L.K. Aagesen. "Porosity in Millimeter-Scale Welds of Stainless Steel: Three-Dimensional Characterization", 2012. SAND2012-4474.
7. Lim, H., Battaile, C. C., Weinberger, C. R. "Simulating dislocation plasticity in BCC metals by integrating fundamental concepts with macroscale models," book chapter in Integrated Computational Materials Engineering (ICME) for metals: Case Studies, Mark Horstemeyer (Ed.), John Wiley & Sons, 2012
8. C.R. Weinberger, B.L. Boyce, and C.C. Battaile, "Slip planes in BCC transition metals", International Materials Reviews, 58(5), p.296-314, 2013.
9. B.L. Boyce, B.G. Clark, P. Lu, J.D. Carroll, and C.R. Weinberger, "The morphology of tensile failure in tantalum", Metallurgical and Materials Transactions A, 44(10), p. 4567-4580, 2013
10. J.D. Carroll, W.Z. Abuzaid, J. Lambros, and H. Sehitoglu, "On the interactions between strain accumulation, microstructure, and fatigue crack behavior," International Journal of Fracture, 180(2), p. 223-241, 2013.
11. H. Lim, C. R. Weinberger, C. C. Battaile, T. E. Buchheit, "Application of generalized non-Schmid yield law to low temperature plasticity in BCC transition metals", Modeling and Simulation in Materials Science and Engineering, 21, p. 145015, 2013.
12. C.R. Weinberger, G.J. Tucker, and S.M. Foiles, "The Peierls potential of screw dislocations in BCC transition metals: predictions from density functional theory", Phys. Rev. B, 87, p. 054114, 2013.
13. J.D. Carroll, B.G. Clark, T.E. Buchheit, B.L. Boyce, C.R. Weinberger, "An experimental statistical analysis of stress projection factors in BCC tantalum", Materials Science and Engineering A, 581, p. 108, 2013.
14. L. Deibler, A. Brown, J. Puskar, "Modeling and experiments to design a softening heat treatment for 304L stainless steel", submitted to Modeling and Simulation in Materials Science and Engineering, October 2013.
15. J. Madison, L.K. Aagesen, C.C. Battaile, J.M. Rodelas, T.K.C.S. Payton, "Coupling 3D quantitative interrogation of weld microstructure with 3D models of mechanical response", Metall. Microstruct., Anal., 2, p. 359-363, 2013.
16. T. E. Buchheit, J. D. Carroll, B. G. Clark, B. L. Boyce, "Evaluating absolute rotation in a polycrystal during in-situ tensile deformation using EBSD", Microscopy and Microanalysis, 2015, doi:10.1017/S1431927615000677.
17. T.R. Bieler, S.C. Sutton, B.E. Dunlap, Z.A. Keith, P. Eisenlohr, M.A. Crimp, B.L. Boyce, "Grain boundary responses to heterogeneous deformation in tantalum polycrystals", JOM, 66, p. 121-128, 2014.
18. H. Lim, S. Subedi, D. T. Fullwood, B. L. Adams, R. H. Wagoner, "A Practical Meso-Scale Polycrystal Model to Predict Dislocation Densities and the Hall-Petch Effect", Materials Transactions, 55 (1), p. 35-38, 2014.
19. N. A. Pedrazas, T. E. Buchheit, E. A. Holm, E. M. Taleff, "Dynamic Abnormal Grain Growth in Tantalum", Mater. Sci. Eng. A, 610, p. 76-84, 2014.
20. J.D. Madison, L.K. Aagesen, V.W.L. Chan, K. Thornton, "Advancing Quantitative Description of Porosity in Autogeneous Laser-Welds of 304L Stainless Steel, Integrating Materials and Manufacturing Innovation, vol. 3, 2014.
21. L.M. Hale, J.A. Zimmerman and C.R. Weinberger, "Simulations of bcc tantalum screw dislocations: why classical inter-atomic potentials predict [112] slip", Comp. Mater. Sci., 90, p. 106 (2014)
22. J.A. Zimmerman, A.S. Sabau, M. Asle Zaeem, M.A. Tschopp and D.E. Spearot, "Algorithm Development in Computational Materials Science", JOM, 66, p. 397 (2014)
23. T.R. Bieler, P. Eisenlohr, C.Zhang, H. Phukan, M.A. Crimp, "Grain Boundaries and Interfaces in Slip Transfer", Current Opinion in Solid State & Materials Science, 18, p. 212-226, 2014.
24. L. Smith, J.A. Zimmerman, L.M. Hale, and D. Farkas, "Molecular Dynamics Study of Deformation and Fracture in a Tantalum Nano-Crystalline Thin Film", Mod. Sim. Mater. Sci. Eng., 22, p. 045010, 2014.
25. H. Lim, J.D. Carroll, C.C. Battaile, T.E. Buchheit, B.L. Boyce, and C.R. Weinberger, "Grain-scale Experimental Validation of Crystal Plasticity Finite Element Simulations of Tantalum Oligocrystals," Int. J. Plasticity, 60, p. 1-18, 2014.
26. C.M. Barr, L. Barnard, J.E. Nathaniel, K.Hattar, K.A. Unocic, I. Szlurska, D. Morgan, and M.L. Taheri, "Grain boundary character dependence of radiation induced segregation in a model Ni-Cr alloy," J. Mater. Res., 30 (9), p. 1290-1299, 2014.
27. C.M. Barr, G.A. Vetterick, K.A. Unocic, K. Hattar, X.-M. Bai, and M.L. Taheri, "Anisotropic radiation-induced segregation in 316L austenitic stainless steel with grain boundary character," Acta Mater. 67 (2014) 145-155.
28. H. Lim, L.M. Hale, J.A. Zimmerman, C.C. Battaile, and C.R. Weinberger, "A multi-scale model of dislocation plasticity in a Fe: incorporating temperature, strain rate and non-schmid effects", Int. J. Plasticity, 73 (2015) 100-118.
29. C.C. Battaile, J.M. Emery, L.N. Brewer, and B.L. Boyce, "Crystal Plasticity Simulations of Microstructure-Induced Variability in the Deformation Behavior at Void-Like Defects in Polycrystalline Brass," Philosophical Magazine, 2015.
30. H. Lim, C. R. Weinberger, C. C. Battaile, J. D. Carroll, B. L. Boyce, "A physically based temperature and strain rate dependent crystal plasticity model for BCC metals," J. Mech. Phys. Sol., 74, p. 80-96, 2015.
31. J. M. Emery, R. V. Field, Jr., J. W. Foulk, III, K. N. Karlson, and M. Grigoriu, "Predicting laser weld reliability with stochastic reduced-order models", International Journal for Numerical Methods in Engineering, 103, 914-936, 2015.
32. J. Bishop, J. Emery, R. Field, C. Weinberger, D. Littlewood, "Direct numerical simulations in solid mechanics for understanding the macroscale effects of microscale material variability", Comp. Meth. App. Mech. Eng., 287, 262-289, 2015.
33. L.M. Hale, H. Lim, J.A. Zimmerman, C.C. Battaile, and C.R. Weinberger, "Insights on Activation Enthalpy for Non-Schmid Slip in BCC Metals," Scripta Mater., 99,p. 89-92, 2015.
34. M.T. Janish, P.G. Kotula, B.L. Boyce, and C.B. Carter, "The observation of fcc and hcp tantalum," J. Mater Sci., v. 50 (2015) 3706-3715.
35. H. Lim, J.D. Carroll, C.C. Battaile, C.R. Weinberger, and B.L. Boyce, "Quantitative comparison between experimental measurements and CP-FEM predictions of plastic deformation in a tantalum oligocrystal," Int. J. Mech. Sci., v92, 98-108, 2015.
36. R. V. Field, Jr., M. Grigoriu, and J. M. Emery, "On the efficacy of stochastic collocation, stochastic Galerkin, and stochastic reduced order models for solving stochastic problems", Probabilistic Engineering Mechanics, 40, 60-72, 2015.
37. J. Wang, Z. Zeng, C.R. Weinberger, Z. Zhang, T. Zhu, S.X. Mao, "In situ atomic-scale observation of twinning dominated deformation in nanoscale body-centred cubic tungsten", Nature Materials, DOI: 10.1038/NMAT4228.
38. D.F. Susan, T.B. Crenshaw, J.S. Gearhart, "The effects of casting porosity on the tensile behavior of investment cast 17-4PH stainless steel", Journal of Materials Engineering and Performance, 24, 2917-2923, 2015.
39. F. Abdeljawad, and J. A. Zimmerman, "Screw dislocation glide in tantalum: Atomistic studies using the spectral neighbor analysis potential (SNAP)," 2015. SAND2015-7906
40. J.M. Emery, M.D. Grigoriu, and R.V. Field Jr., "Bayesian methods for characterizing unknown parameters of material models," Applied Mathematical Modelling, (2016) available online. doi:10.1016/j.apm.2016.01.046
41. J.E. Bishop, J.M. Emery, R.V. Field Jr., C.R. Weinberger, and D.J. Littlewood, "Direct numerical simulations in solid mechanics with comparisons to homogenization theory," Comp. Meth. App. Mech. Eng., Volume 287, April 2015, pp. 262–289. doi:10.1016/j.cma.2015.01.017
42. H. Lim, S. Owen, F. Abdeljawad, B. Hanks and C. C. Battaile, "Creating physically-based three-dimensional microstructures: Bridging phase field and crystal plasticity models," 2015. SAND2015-7870
43. A.A. Brown, L.A. Deibler, L.L. Beghini, T.D. Kostka, B.R. Antoun, "Process modeling and experiments for forging and welding," book chapter in Challenges in Mechanics of Time Dependent Materials, B. Antoun (Ed.), Springer, vol. 2, p. 19-25, 2016.
44. R. Jones, J. Templeton and J. Zimmerman, "Principles of Coarse-graining and Coupling using the Atom-to-Continuum (AtC) Method" for Multiscale Modeling for Nanomechanics, Edited by C. Weinberger and G. Tucker (In Preparation)
45. J. Madison, H. Jin, J. Foulk, S. Murawski, C. Robino, "New Microstructural Insights to the Constitutive Behavior of Laser-Welds in 304L Stainless Steel –I." (In preparation), Met. Trans. A.
46. J.T. Ostien, J.W. Foulk III, A. Mota, M.G. Veilleux, "A 10-Node Composite Tetrahedral Finite Element for Solid Mechanics," (In preparation) Computational Mechanics.
47. J.W. Foulk III, M.G. Veilleux, J.M. Emery, A. Mota, S.E. Leon, J.T. Ostien, "Capturing finite deformations in metallic structures through robust remeshing and mapping of internal state variables," (In Preparation) International Journal of Numerical Methods in Engineering.
48. H. Lim, R. Dingreville, L.A. Deibler, T.E. Buchheit, C.C. Battaile. "Investigation of grain-scale microstructural variability in tantalum using crystal plasticity-finite element simulations," Comp. Mater. Sci. 117 (2016) 437-444
49. F. Abdeljawad, D. L. Medlin, J. A. Zimmerman, S. M. Foiles, and K. Hattar, "A non-local regularized diffuse interface model of grain boundary faceting," (In preparation) Journal of Applied Physics.
50. D. L. Medlin, K. Hattar, J. A. Zimmerman, F. Abdeljawad, and S. M. Foiles, "Defect character at grain boundary facet junctions: Analysis of an asymmetric $\Sigma=5$ grain boundary in BCC Fe," (In preparation) Acta Materialia.
51. H. Lim, H., Abdeljawad, F., Owen, S.J., Hanks, B.W., Foulk, J.W., Battaile, C.C., "Incorporating physically-based microstructures in materials modeling: Bridging phase field and crystal plasticity frameworks," Model. Simul. Mater. Sci. Eng., (2016), In press.
52. J.E. Bishop, J.M. Emery, R.V. Field Jr., D.J. Littlewood, and A.J. Baines, "Direct numerical simulations in solid mechanics for quantifying the macroscale effects of microstructure and material-model form error," JOM, (2016), in press.
53. S. Welsh, M. Kapoor, O. Underwood, R.L. Martens, G.B. Thompson, J.L. Evans, "Influence of Grain Boundary Character and Annealing Time on Segregation in Commercially Pure Nickel," J. Mater. (2016) pp. 1-15
54. J. Madison, "Integrated Computational Materials Engineering: Tools, Simulations and New Applications," JOM, vol. 68, no. 5, (2016) pp. 1376-1377