SAND2015-2756PE

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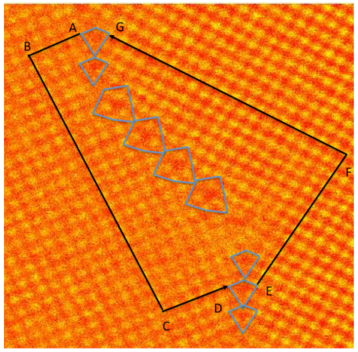
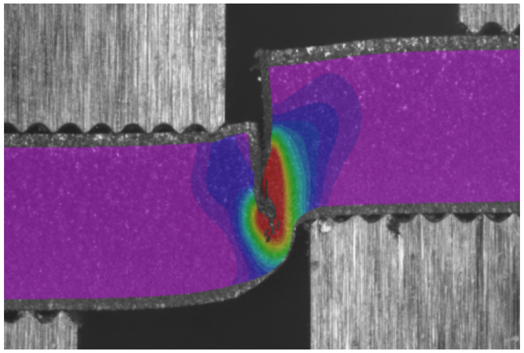
Sandia National Laboratories

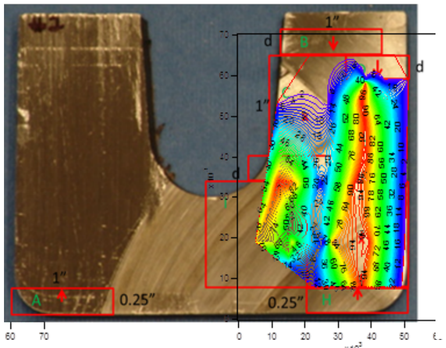
"Predicting Performance Margins" (PPM) Program



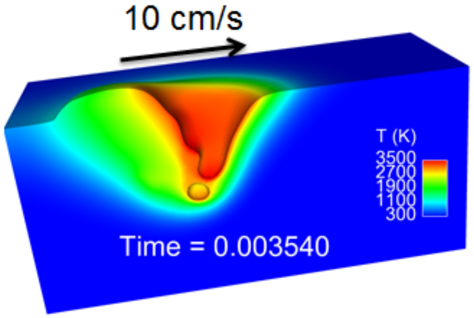
GB Structure



Weld Shear Testing



Property Mapping



Process Modeling

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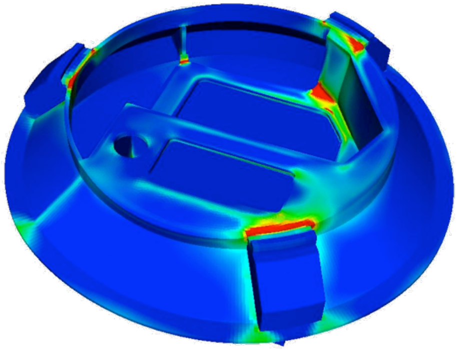
PPM's Goal and Motivation

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.

Loading Accidents

Transportation Safety

Broken Metal Retainer



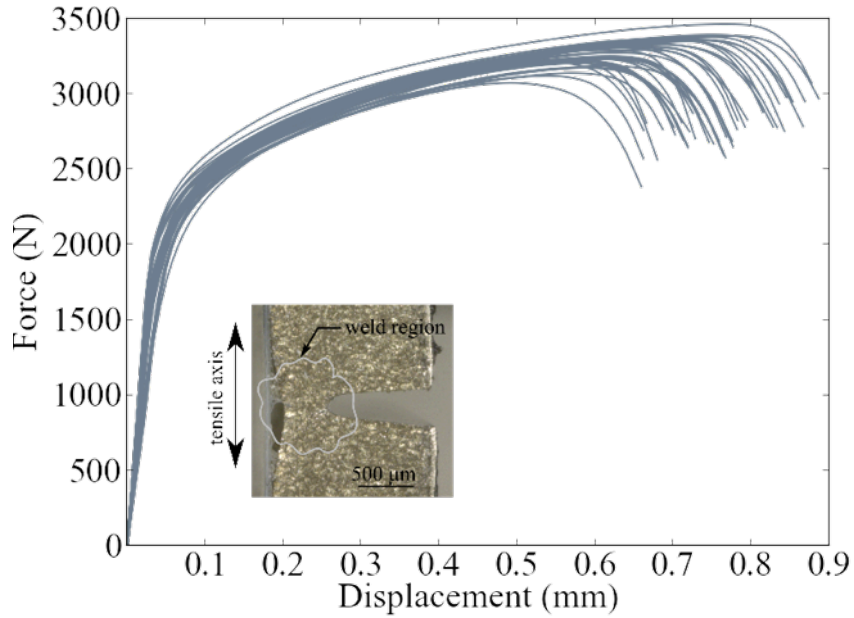
Engineering Analysis for Structural Failure Prevention

Variability in 304L PP Laser Welds

We care about laser welds: Laser welds are pervasive in engineering systems. Understanding the performance of laser welds enables designers to be better stewards.

We observe variability: The ductility of 304L laser welds varies from specimen to specimen. We observe both material and geometric variability.

We care about the impact of variability on performance: We need to develop methods that capture and propagate variability in a mathematically rigorous manner. *The tail of the distribution is what matters.*

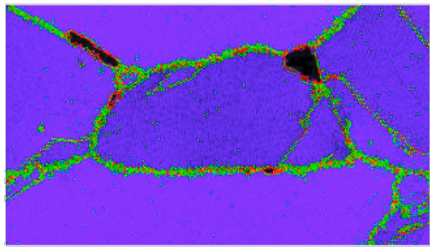


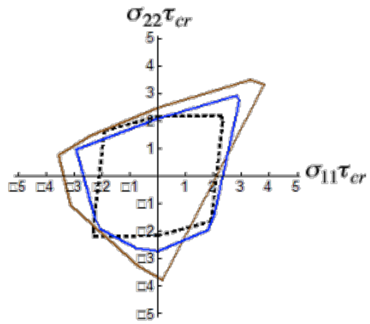
We seek the "rare" with limited computational resources: The only general approach to determine the tails of the output distribution is through repeated random sampling, Monte Carlo Simulation (MCS). We do not, however, have the computational resources to repeatedly sample component or system level finite element models. We need to be smarter in how we apply MCS.

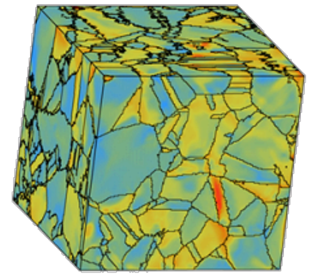
We need a framework that is flexible and extensible: We need to have the ability to incorporate new experiments and consider new physics. The analyst, not the framework, should dictate the path forward.

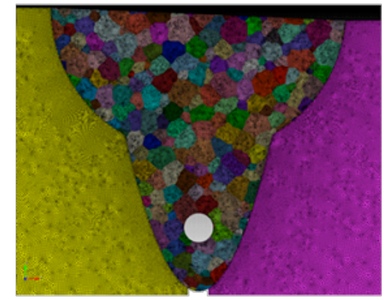
PPM's Approach to Multiscale

simulations

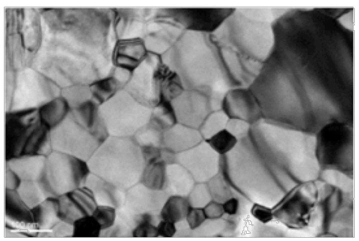


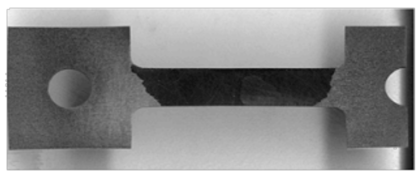


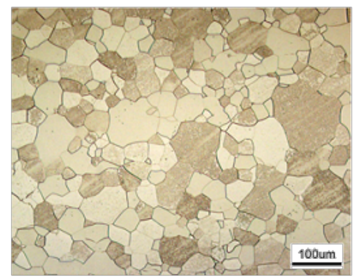


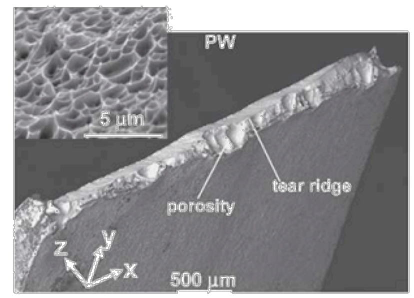


experiments









Atomic scale phenomena
10^{-9} m 10^{-9} s

Single crystal behavior
10^{-6} m 10^{0} s

Microstructural effects
10^{-3} m 10^{3} s

Material performance
10^{0} m 10^{6} s

Atoms-up: Develop physics-based models to provide scientific insight

Continuum-down: Augment engineering-scale models to provide improved fidelity

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Simulations of microstructure-induced uncertainty in metal deformation: Grain-scale notches in Ta

Hojun Lim[1], Corbett Battaile[1], Rémi Dingreville[2] and Lisa Deibler[3]

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[3]Materials Characterization & Performance
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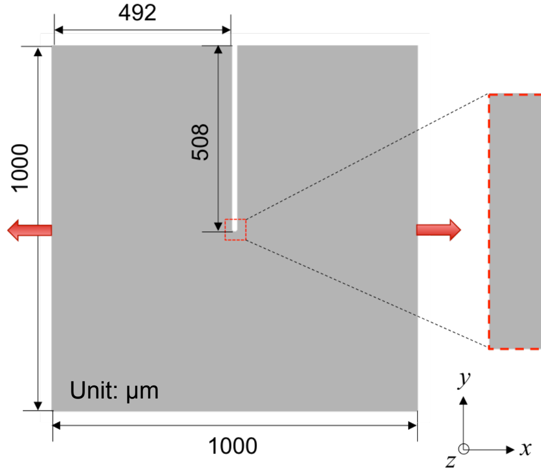
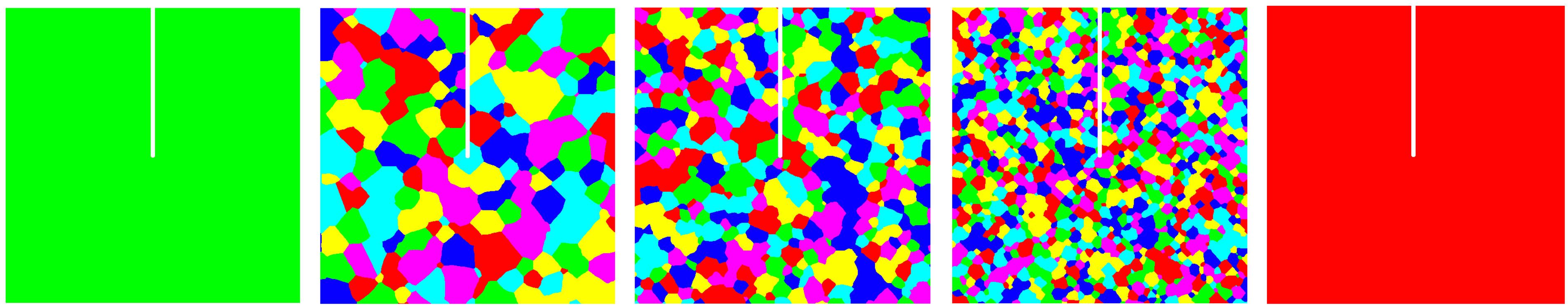
Simulation of Ta notch



- Mode I failure
- Single 3D hexahedral element through thickness
- BC: plane strain (no displacement in z dir.)
- Displacement control: $\dot{\varepsilon} = 10^{-4}\ s^{-1}$
- Strained up to 3%



CP-FEM: 1 grain
(111696 elements)
Grain size > 1 mm

CP-FEM: 204 grains
(115579 elements)
Grain size = 70 μm

CP-FEM: 482 grains
(111696 elements)
Grain size = 45 μm

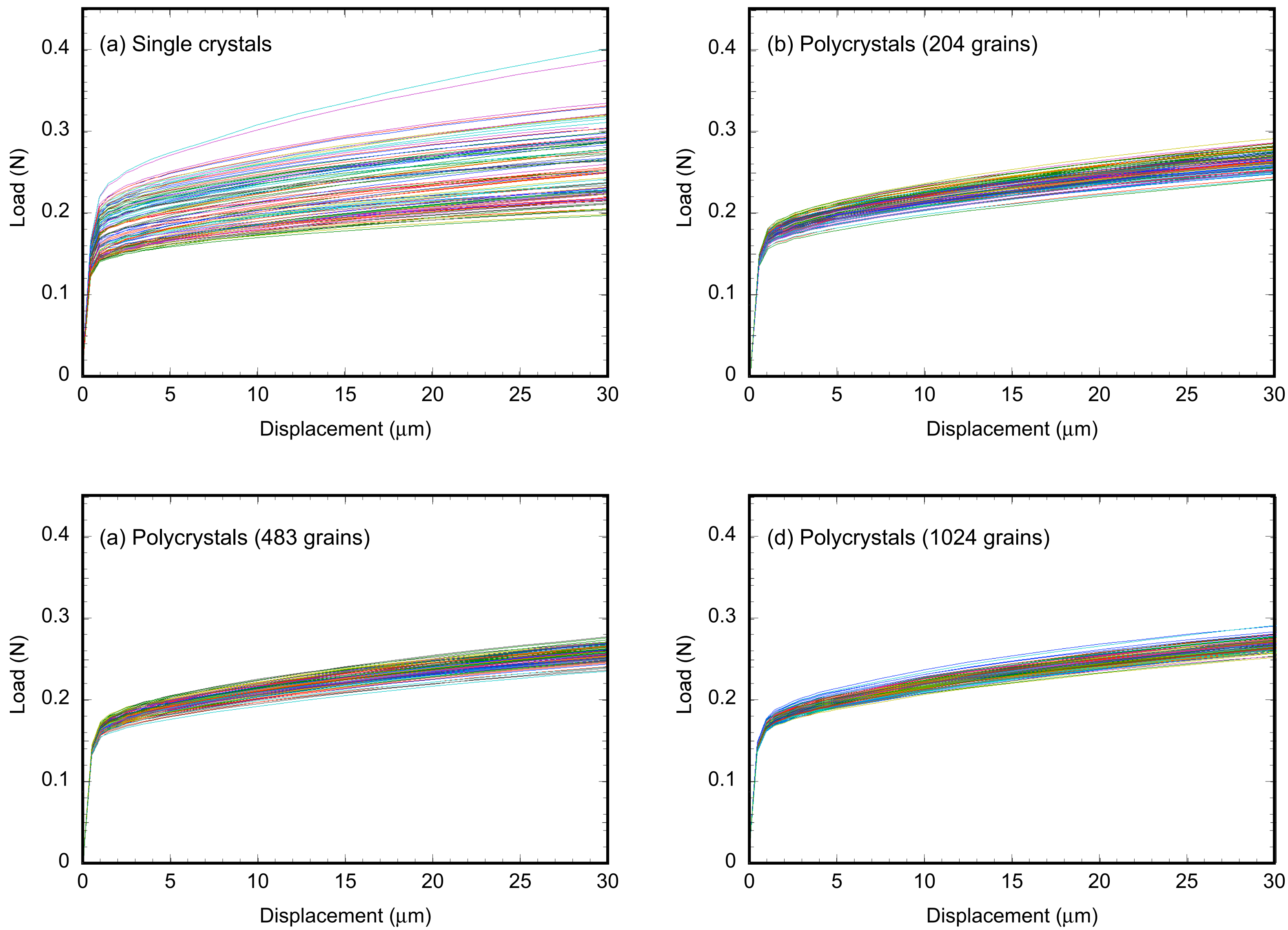
CP-FEM: 1184 grains
(83,657 elements)
Grain size = 30 μm

J2 FEM model
(83,386 elements)

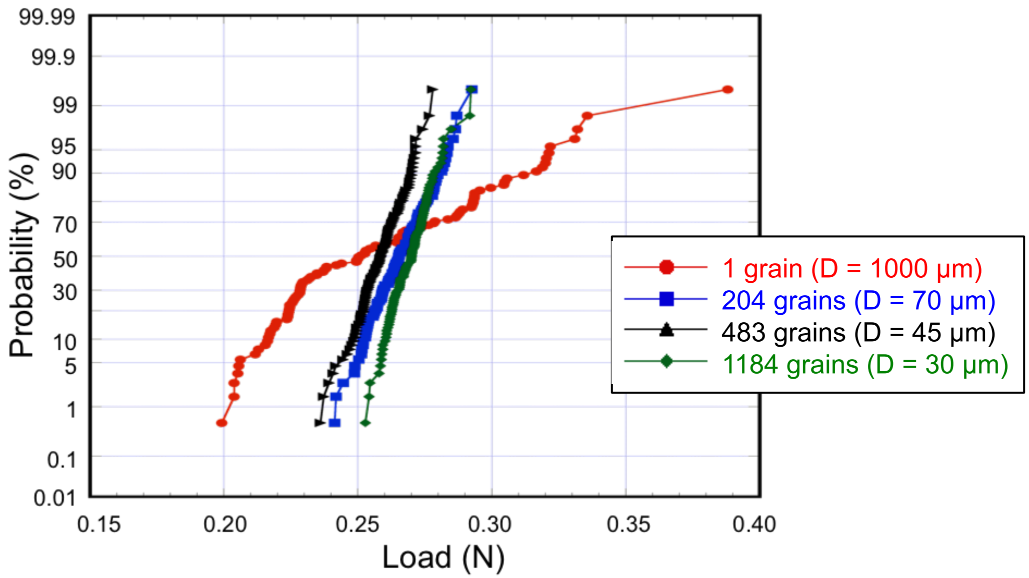
d: grain diameter l: notch length

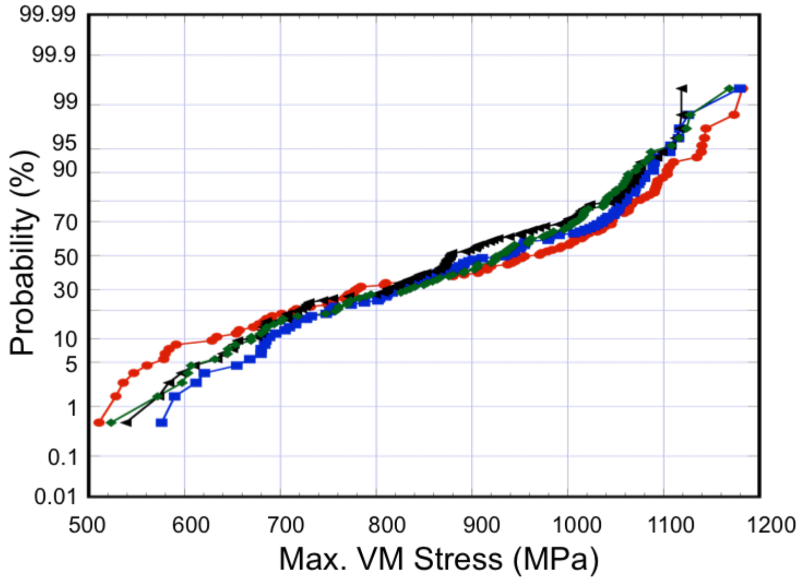
100 CP-FEM simulations with random texture (i.e. 100 microstructural realizations)

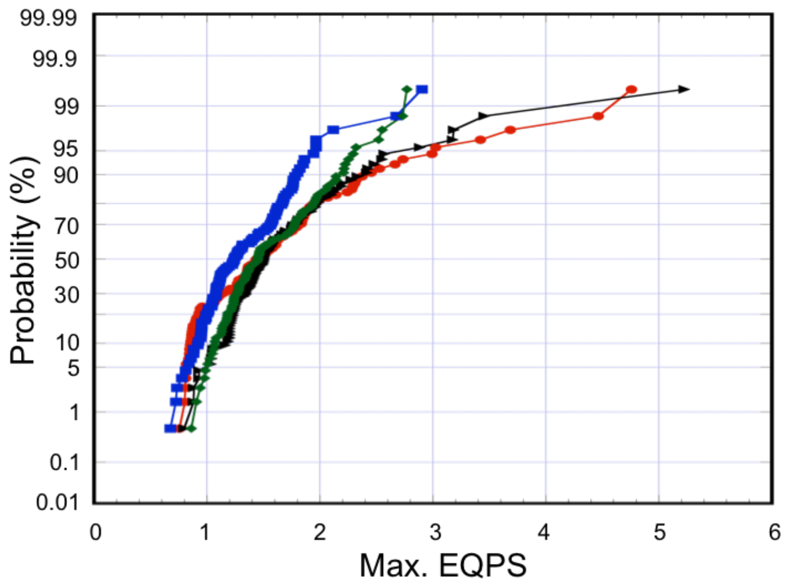
Load-Displacement



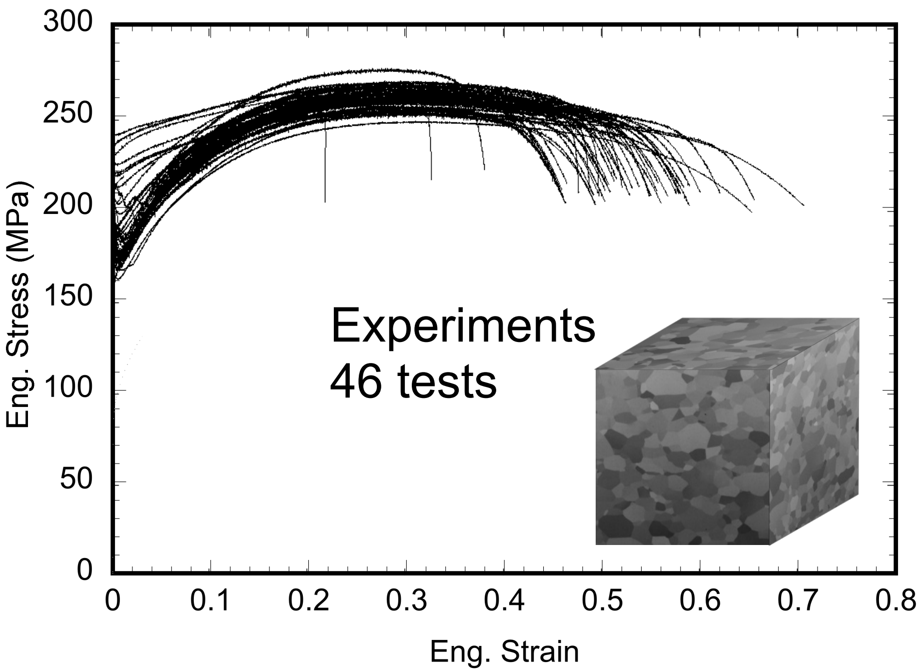
Probability: localized stress & strain

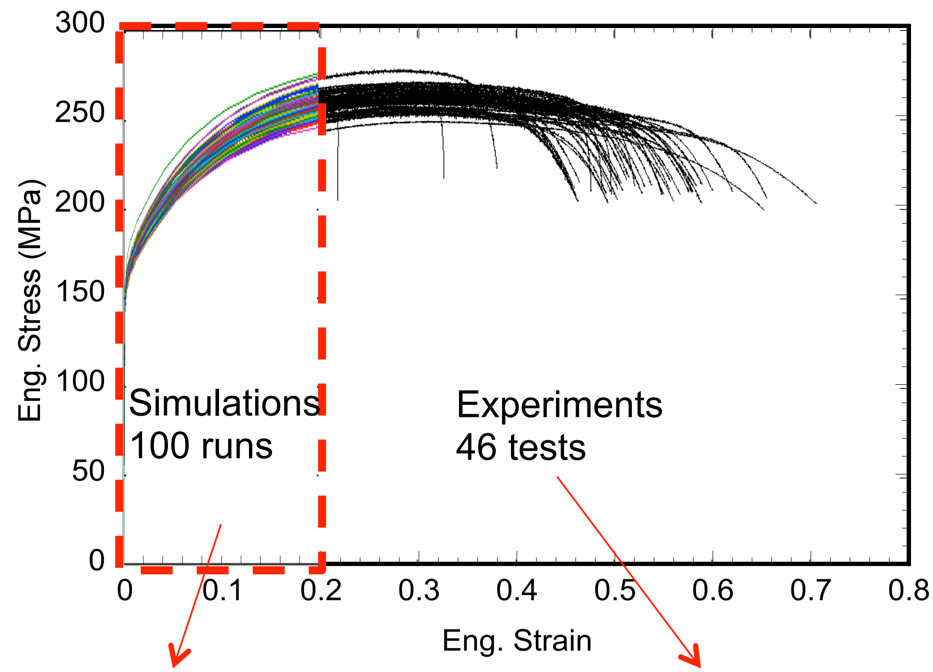


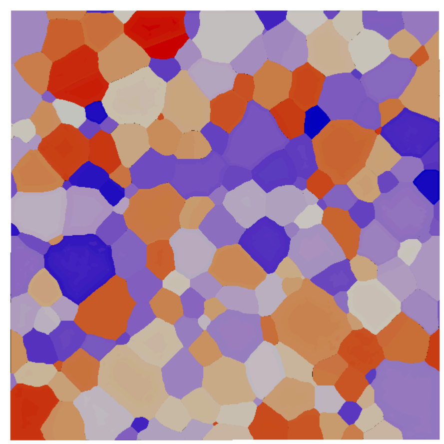




Comparisons with Ta tensile tests







Conformal hexahedral finite element meshing technology for 3D polycrystalline microstructures

Hojun Lim[1], Fadi Abdeljawad[1], Corbett Battaile[1], Steven Owen[2], Byron Hanks[2]

[1]Computational Materials & Data Science
[2]Simulation Modeling Sciences
Sandia National Laboratories

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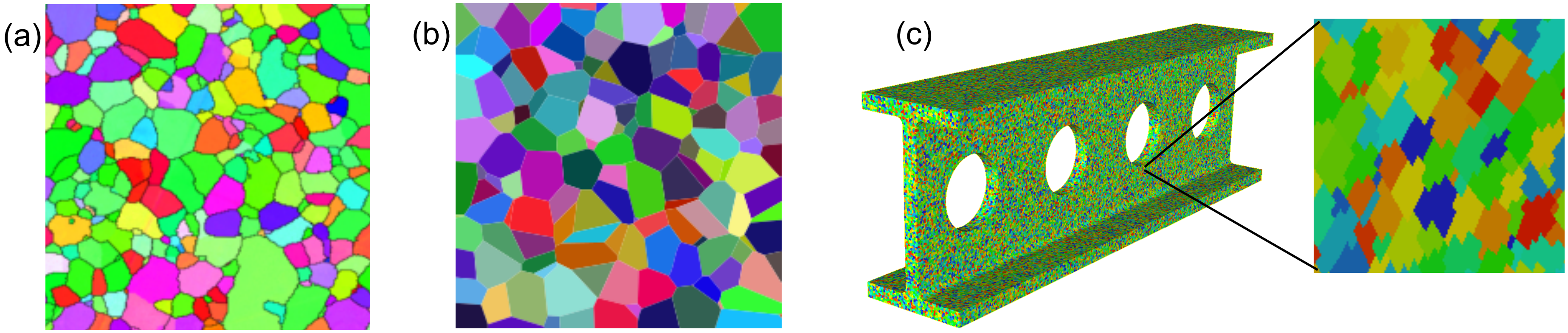
Motivation

Large-scale continuum simulations with microstructure fidelity are hindered by limited capabilities to model realistic 3D microstructures (Fig (a)).

- Most finite element based polycrystalline models use idealized grain shapes or Voronoi tesselations (Fig. (b)).
- 3D microstructures digitized from experiments conform to a uniform grid. (Fig. (c))

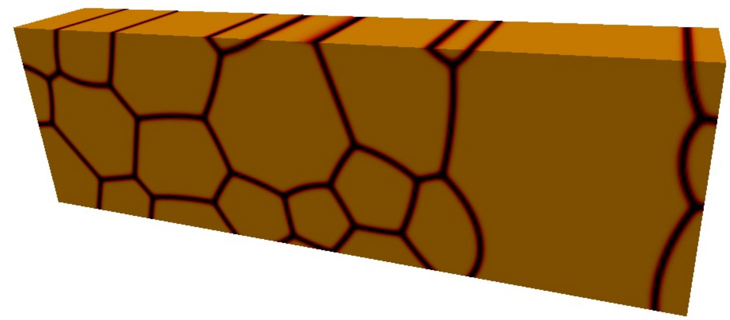


Microstructures from (a) electron back scatter diffraction, (b) Voronoi tesselation and (c) voxelated 3D structure of I-beam [Bishop et al., 2014].

Need a technique to create physically-based three-dimensional microstructures!

Approach

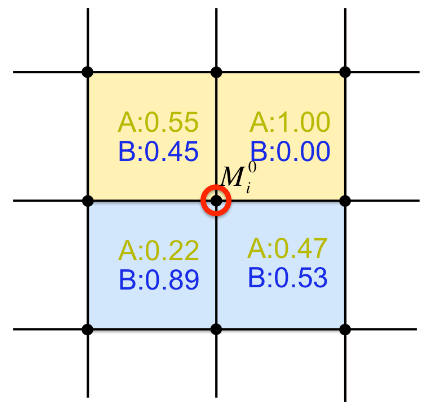
PHASE FIELD GRAIN GROWTH SIMULATIONS

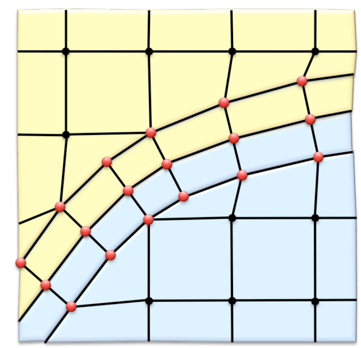


INPUT: (x, y, z, Φ(i))

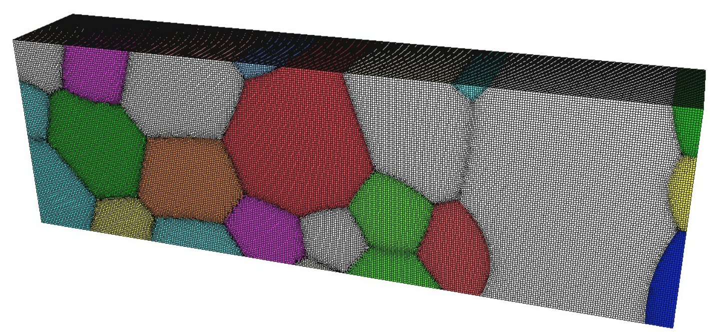
CUBIT 'SCULPT' TECHNOLOGY

OUTPUT: Exodus mesh



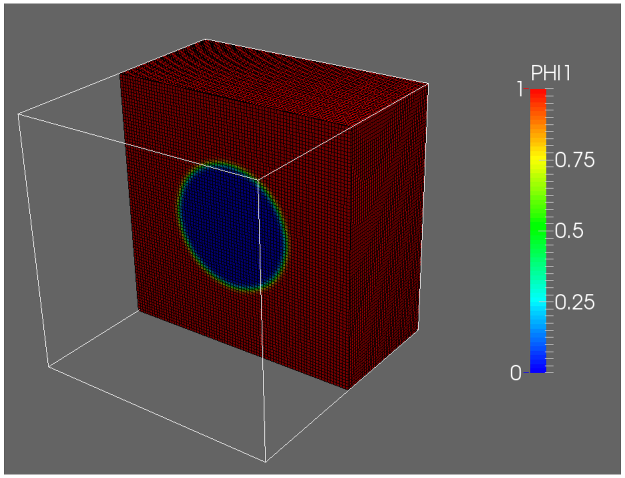


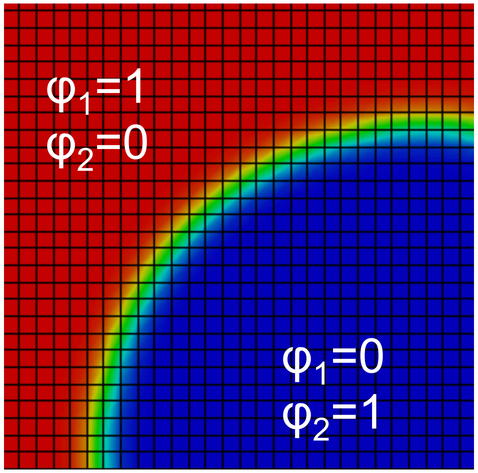
CRYSTAL PLASTICITY FINITE ELEMENT SIMULATIONS



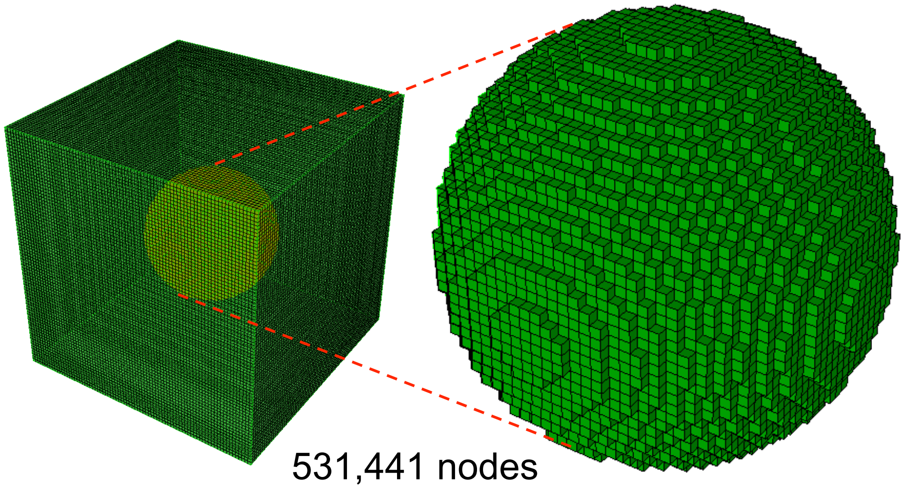
Initial mesh: Case 1

Phase field



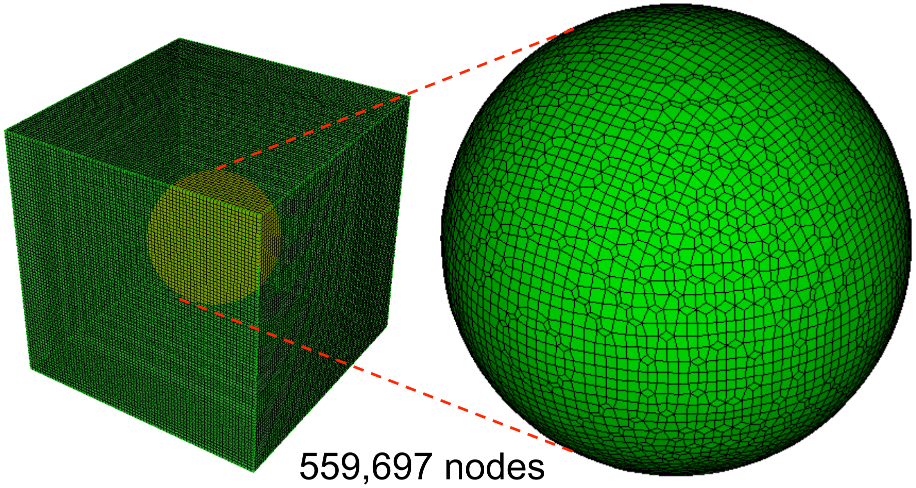


Voxelated FE mesh



531,441 nodes
512,000 elements

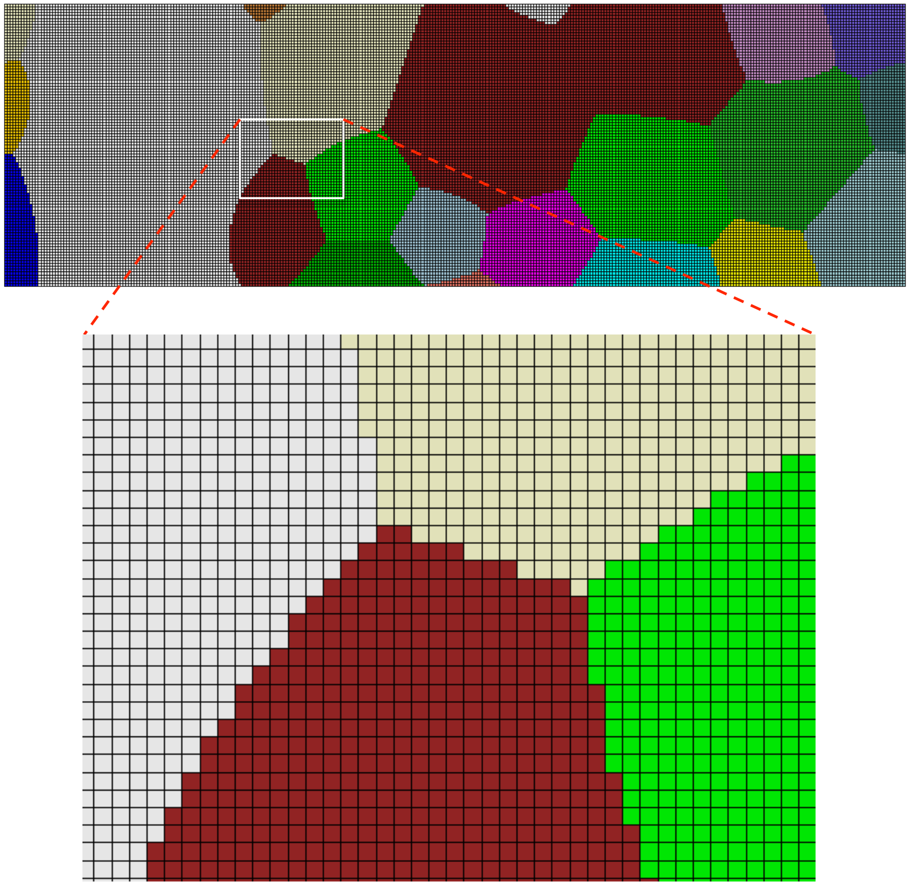
Conformal FE mesh



559,697 nodes
540,248 elements

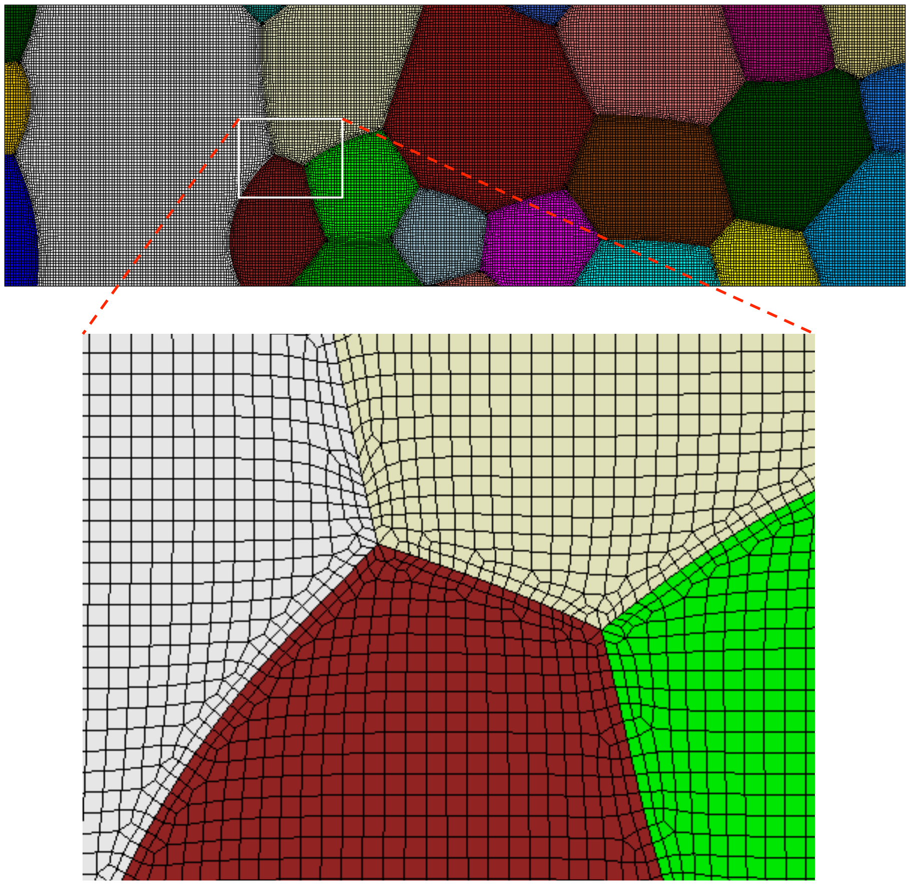
Initial mesh: Case 2

Voxelated FE mesh



1,653,471 nodes
1,600,000 elements

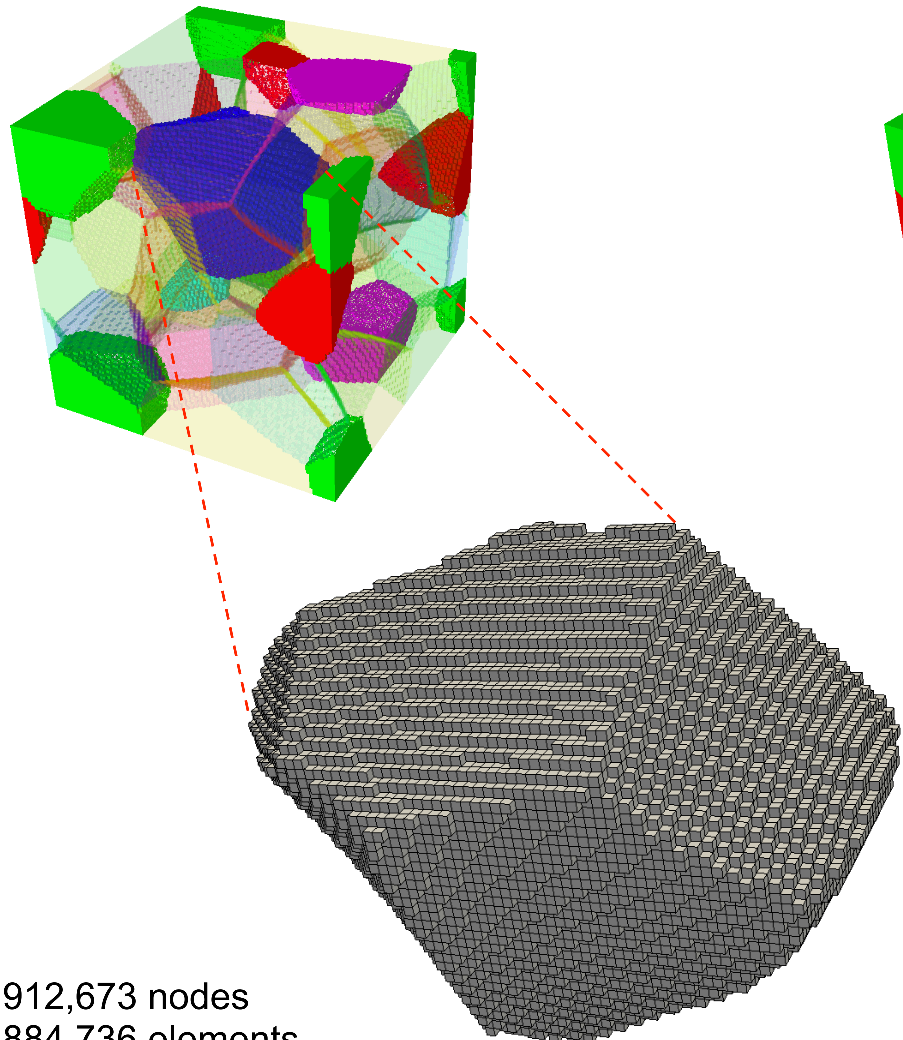
Conformal FE mesh



1,940,295 nodes
1,879,100 elements

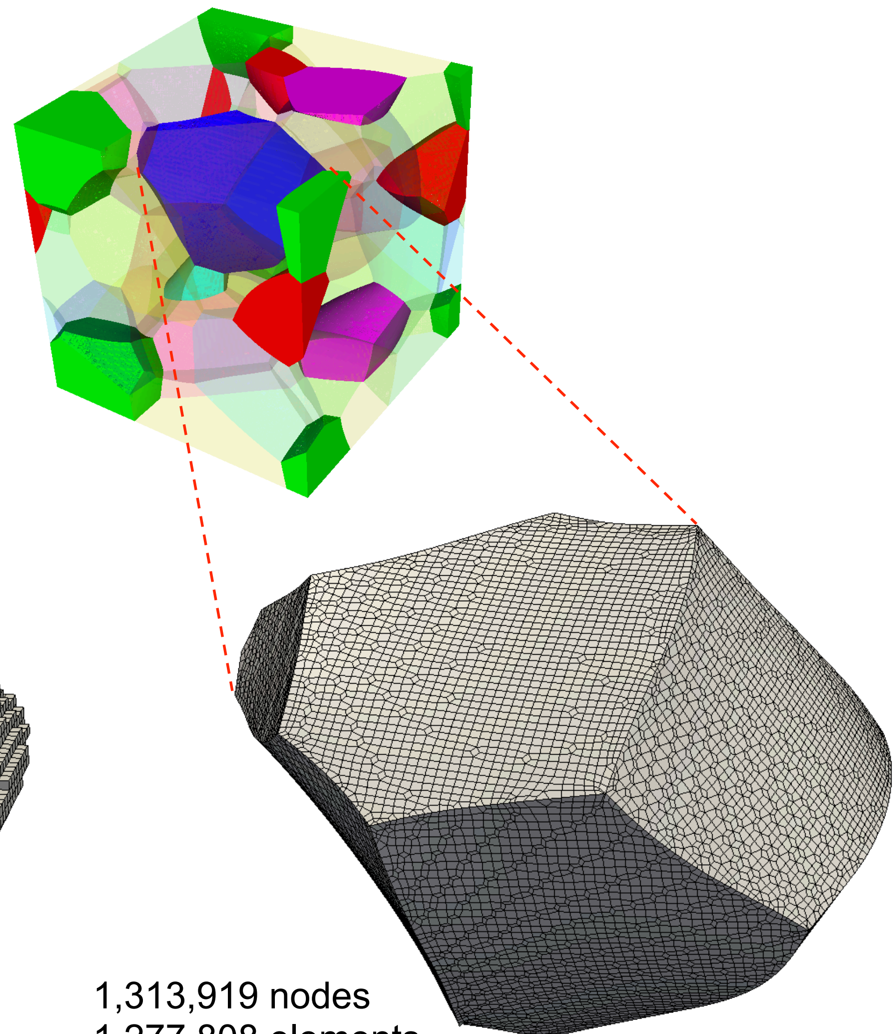
Initial mesh: Case 3

Voxelated FE mesh



912,673 nodes
884,736 elements

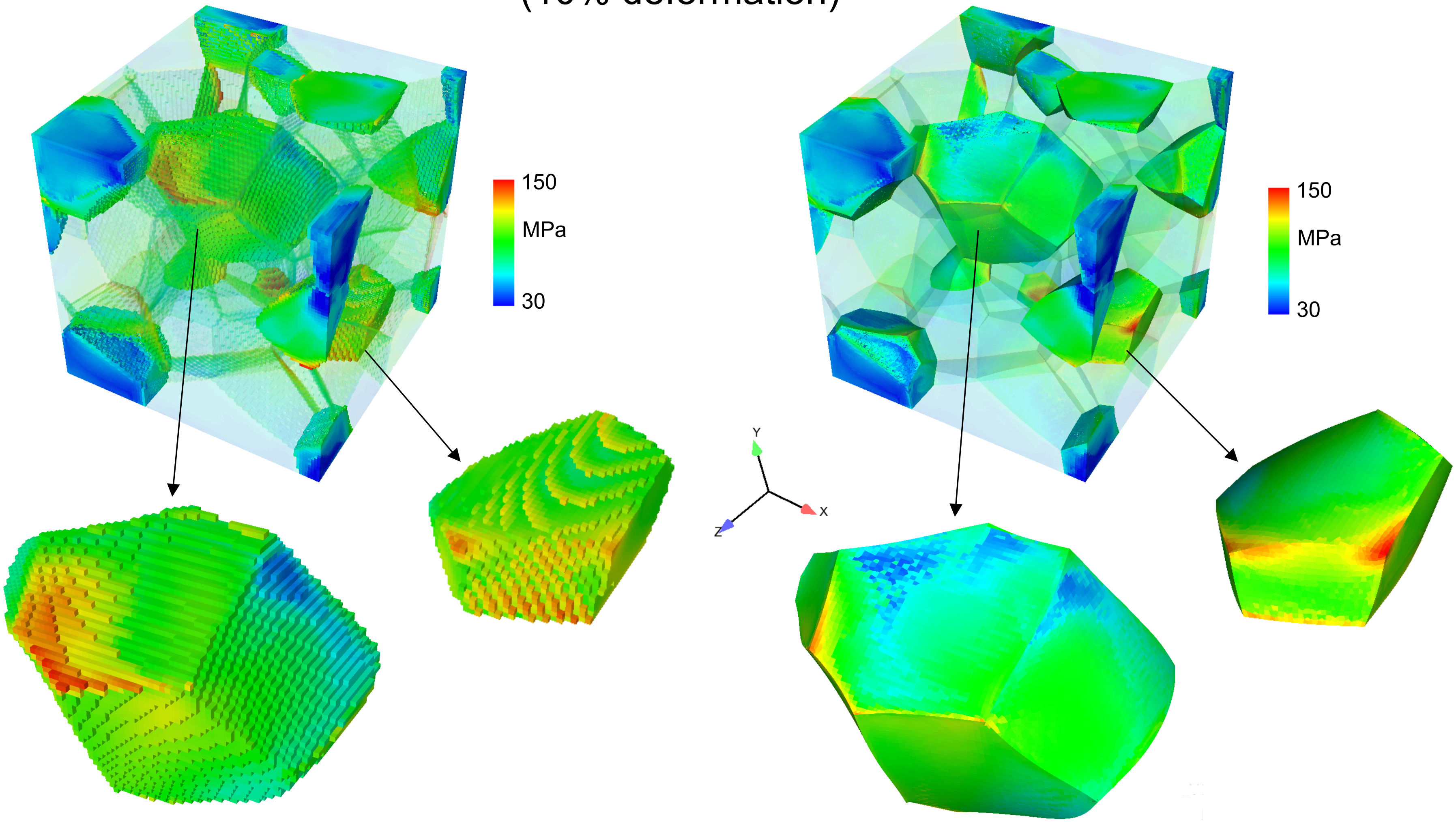
Conformal FE mesh



1,313,919 nodes
1,277,808 elements

Case 3: 3D microstructure

VonMises stress distributions
(10% deformation)

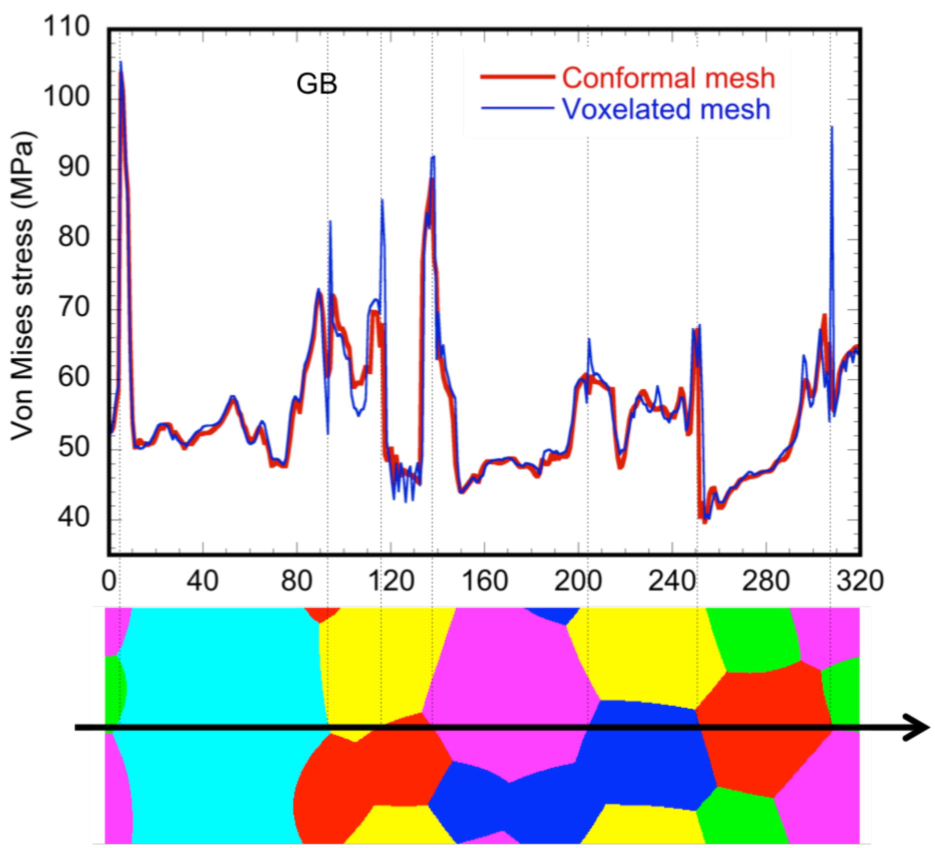


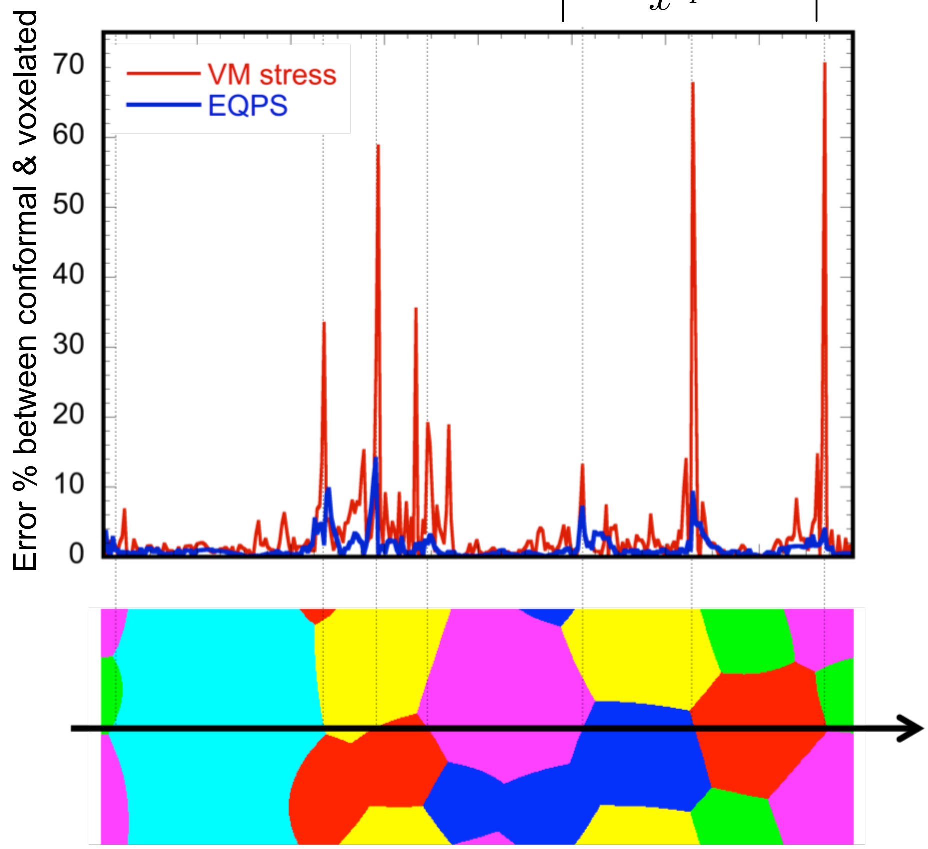
Voxelated mesh

Conformal mesh

Case 2: Columnar structure

$$\text{Error \%} = \left| \frac{x^{vox.} - x^{spl.}}{x^{spl.}} \right| \times 100$$





Large deviations near GB

Mesh more sensitive to stress