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MMM10 The 10th International Conference on Multiscale Materials Modeling
Mechanics and Physics of Material Failure

Crystal plasticity and micro-CT characterization of voids in plastic deformation of Al6061

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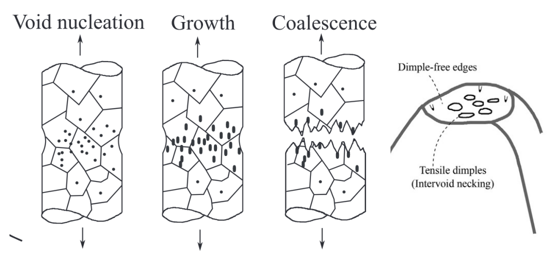
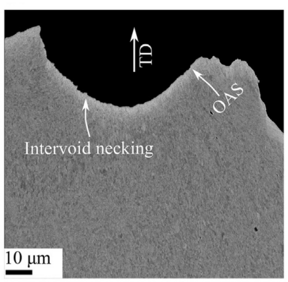
Introduction: Different failure mechanisms

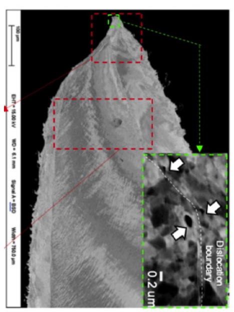
Intervoid necking



Void nucleation, growth and coalescence

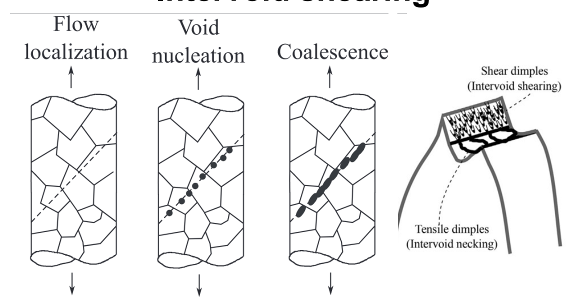


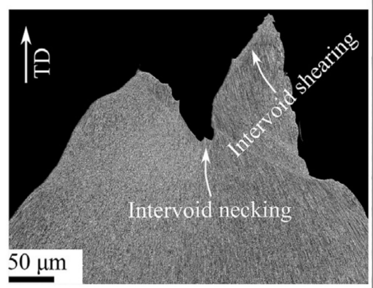
99.99% polycrystalline Cu



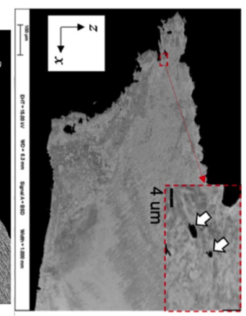
Ta [111] single crystal

Intervoid shearing



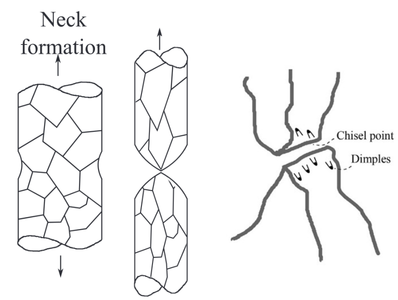


99.99% polycrystalline Ni

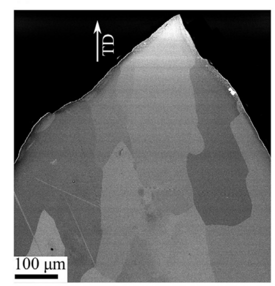


Ta [100] single crystal

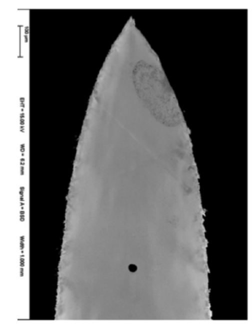
Necking to a point



Void-free rupture



99.999% polycrystalline Al



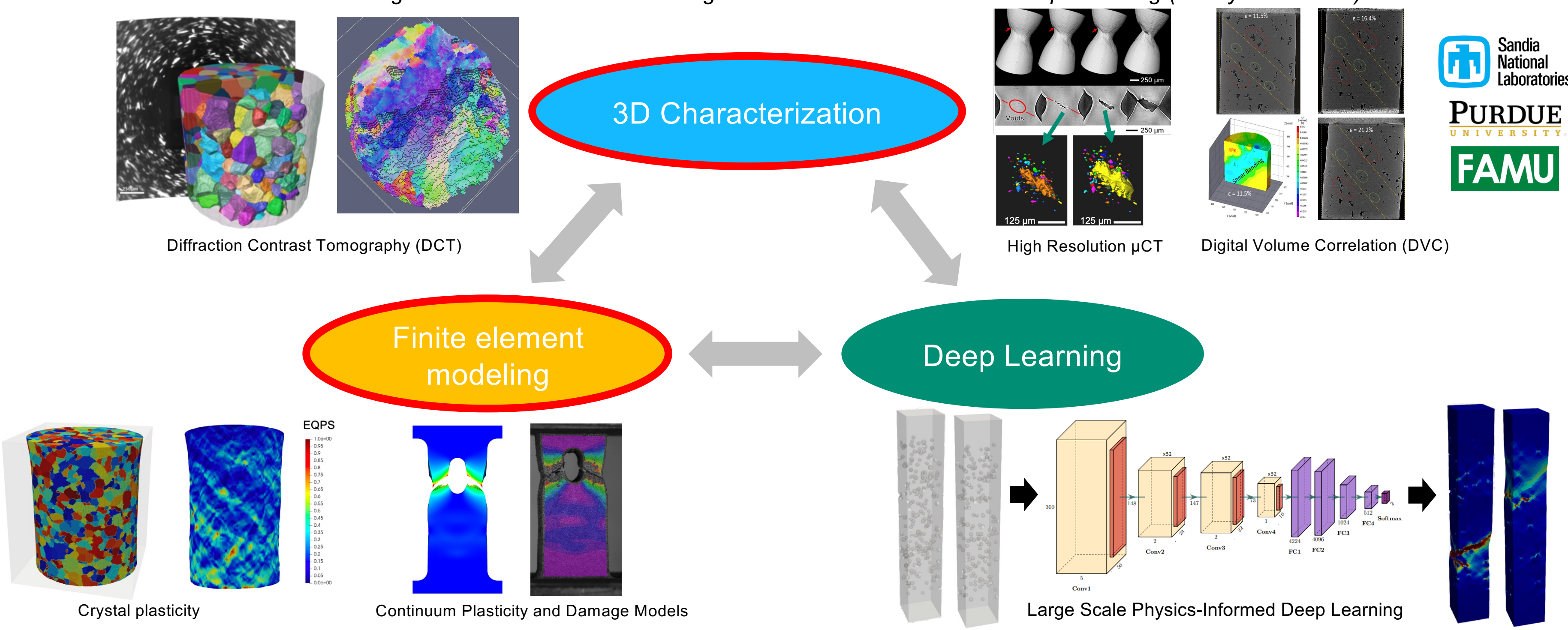
Ta [110] single crystal

Noell et al., Acta Mater. (2018) & Lim et al., Scripta Mater. (2021)

Objective

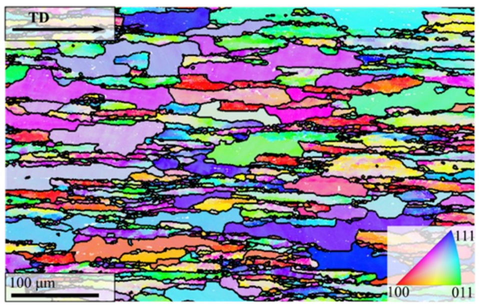
Goal: Predict failure based on the interaction of loading, microstructural features (e.g., crystal morphology, orientation), and defects such as pores, inclusions, and microcracks in structural alloys.

A New Paradigm for Failure Prediction Using 4-D Materials Science and Deep Learning (PI: Kyle Johnson)

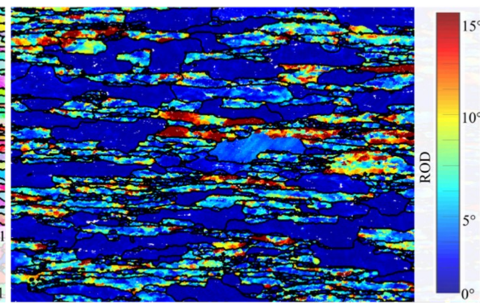


Material characterization: Al6061-T6

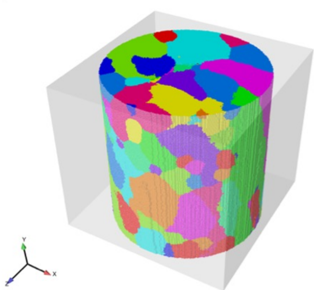
Al6061-T6 (rolled)



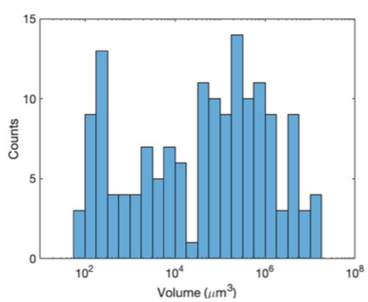
Inverse pole figure (IPF)



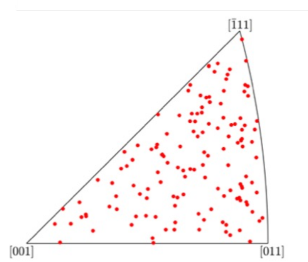
Reference orientation deviation (ROD)



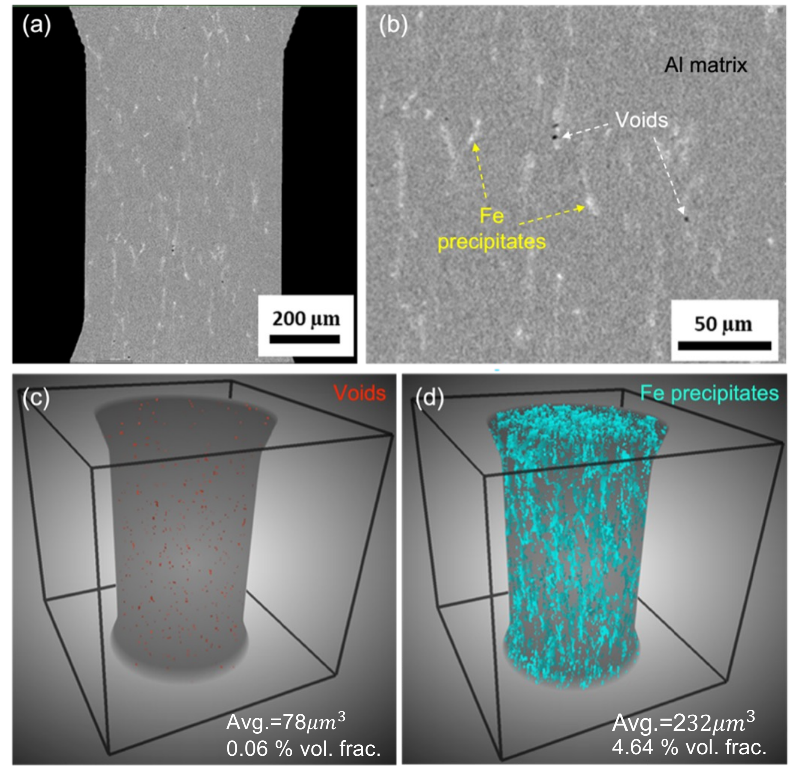
Grain morphology (DCT)



Volume distribution

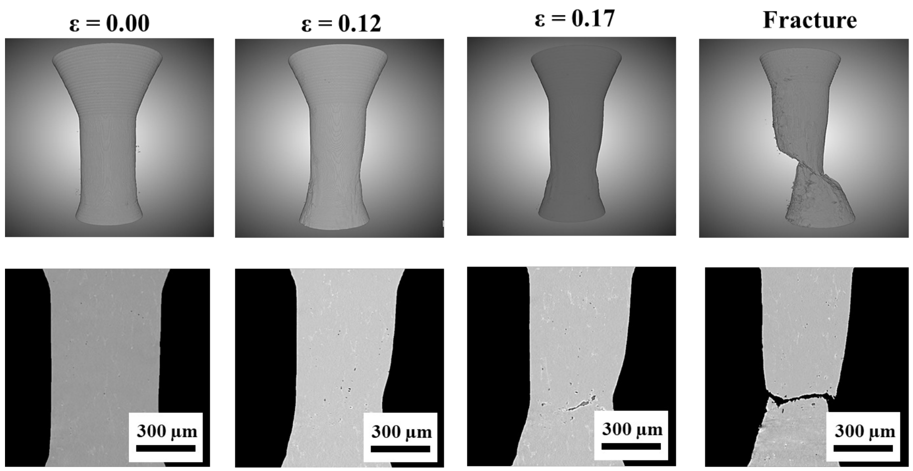


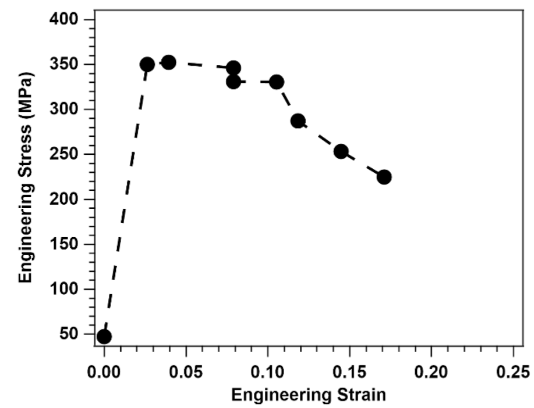
IPF (tensile direction)



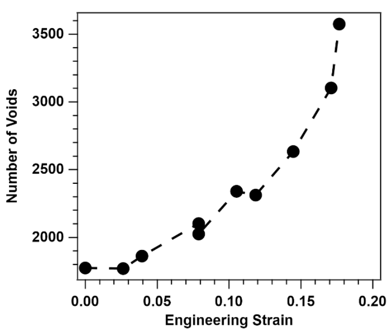
XCT measurements

In-situ XCT measurements

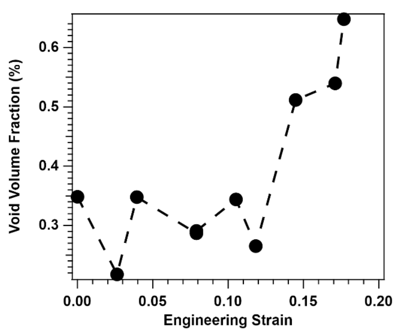




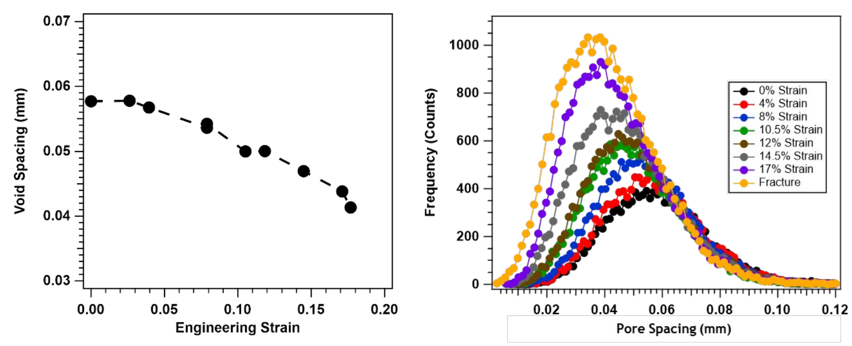
In situ stress-strain results. Markers indicate CT scan points



Void Nucleation



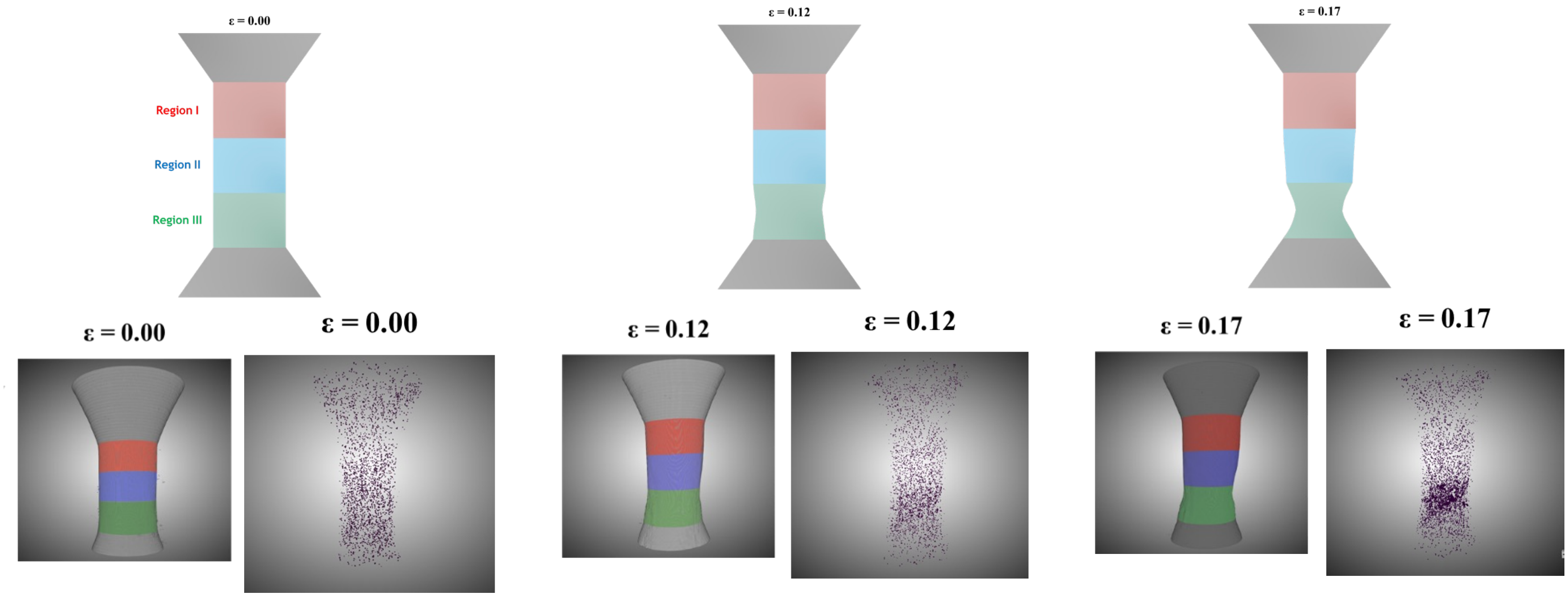
Void Nucleation + Growth



Void Coalescence

Seede et al. Scripta Mater. (submitted)

In-situ XCT measurements: Particles

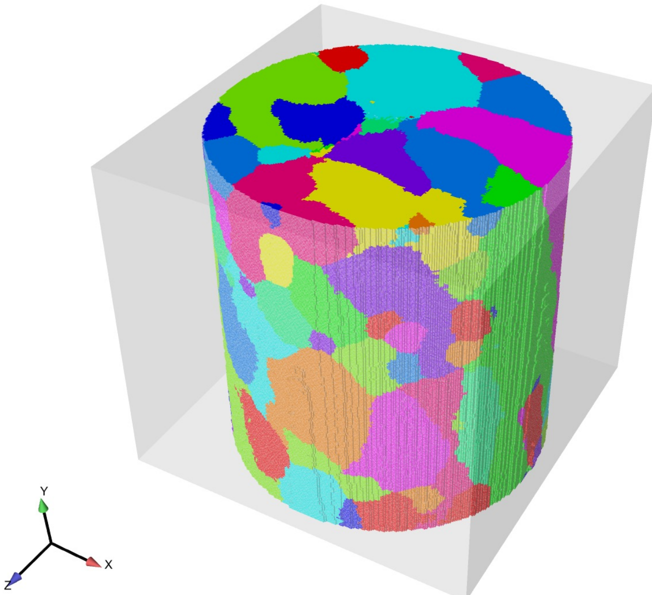


Location	Region I	Region II	Region III
Total Particle Volume (mm^3)	0.00218	0.00188	0.00215
Average Particle Spacing (mm)	0.03536	0.03530	0.03274

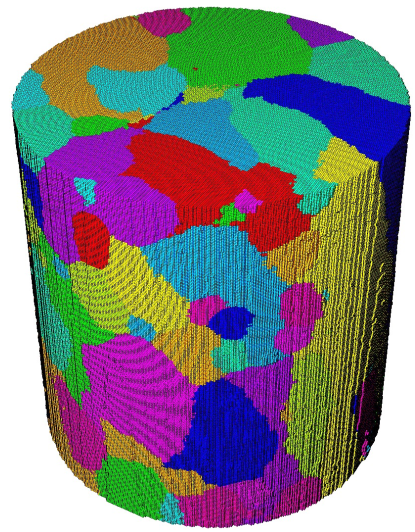
Region III contains high particle volume and low particle spacing

CT data to computational microstructure/FE mesh

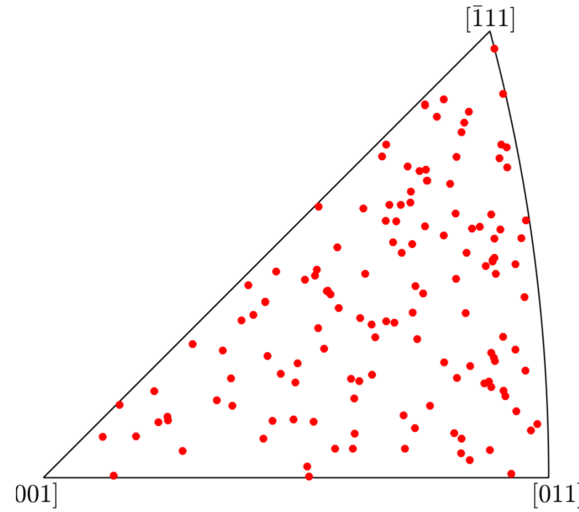
DCT data



FE mesh



Initial crystal orientations
(IPF along the TD)



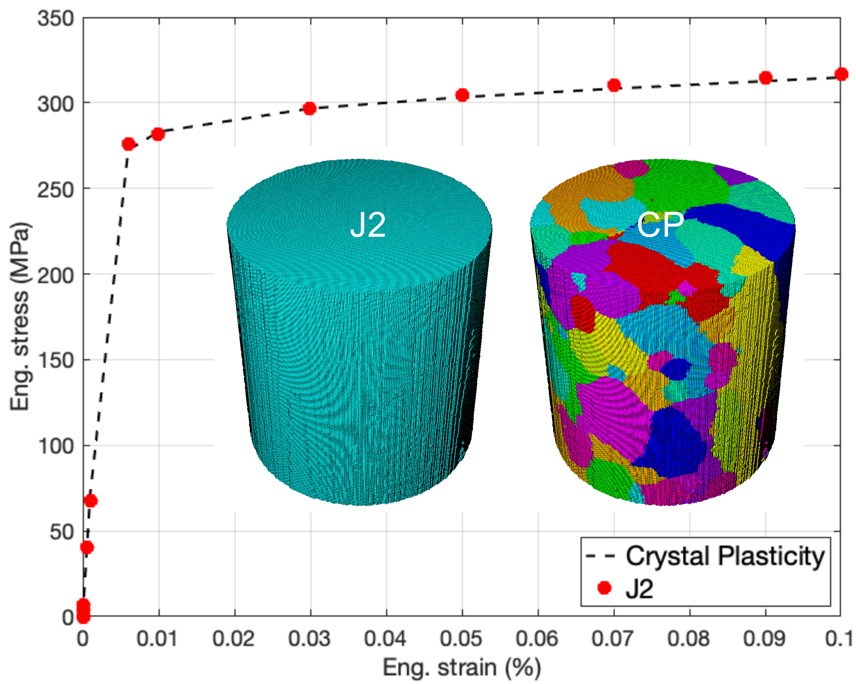
- 15,410,688 data points (254×237×256)
- Diameter 565 μm, Height 295 μm
- ~156 grains, 2.5 μm voxel size
- Removed all grains < 10 voxels

- 9,284,343 finite elements
- Hexahedral finite elements

- No significant texture

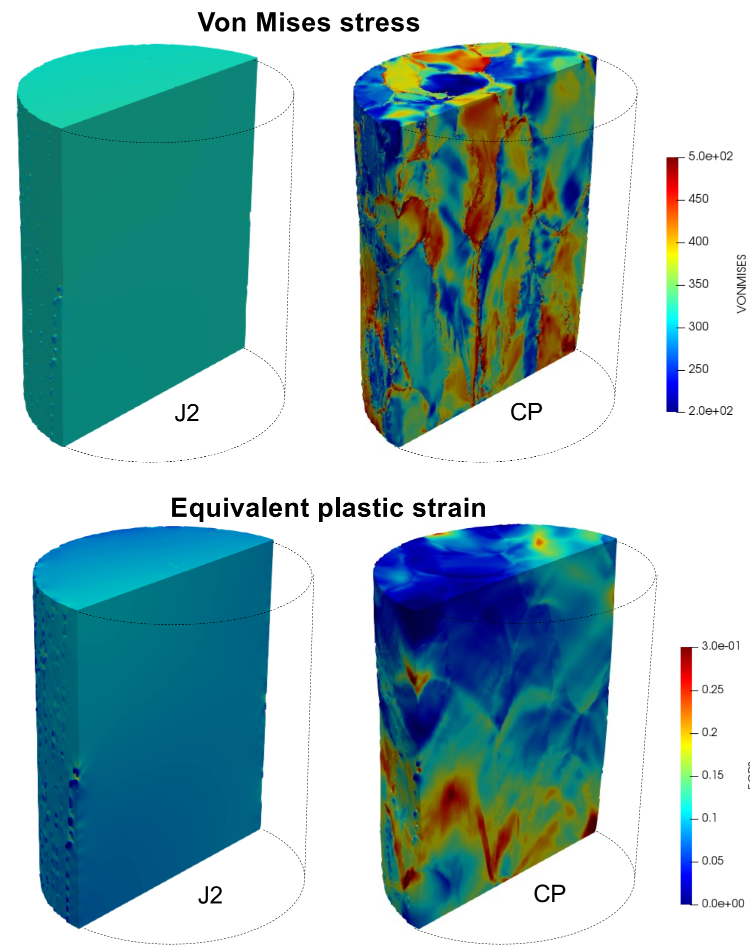
Finite element simulations

Uniaxial tension ($\dot{\varepsilon}$= 10^{-3} /s)

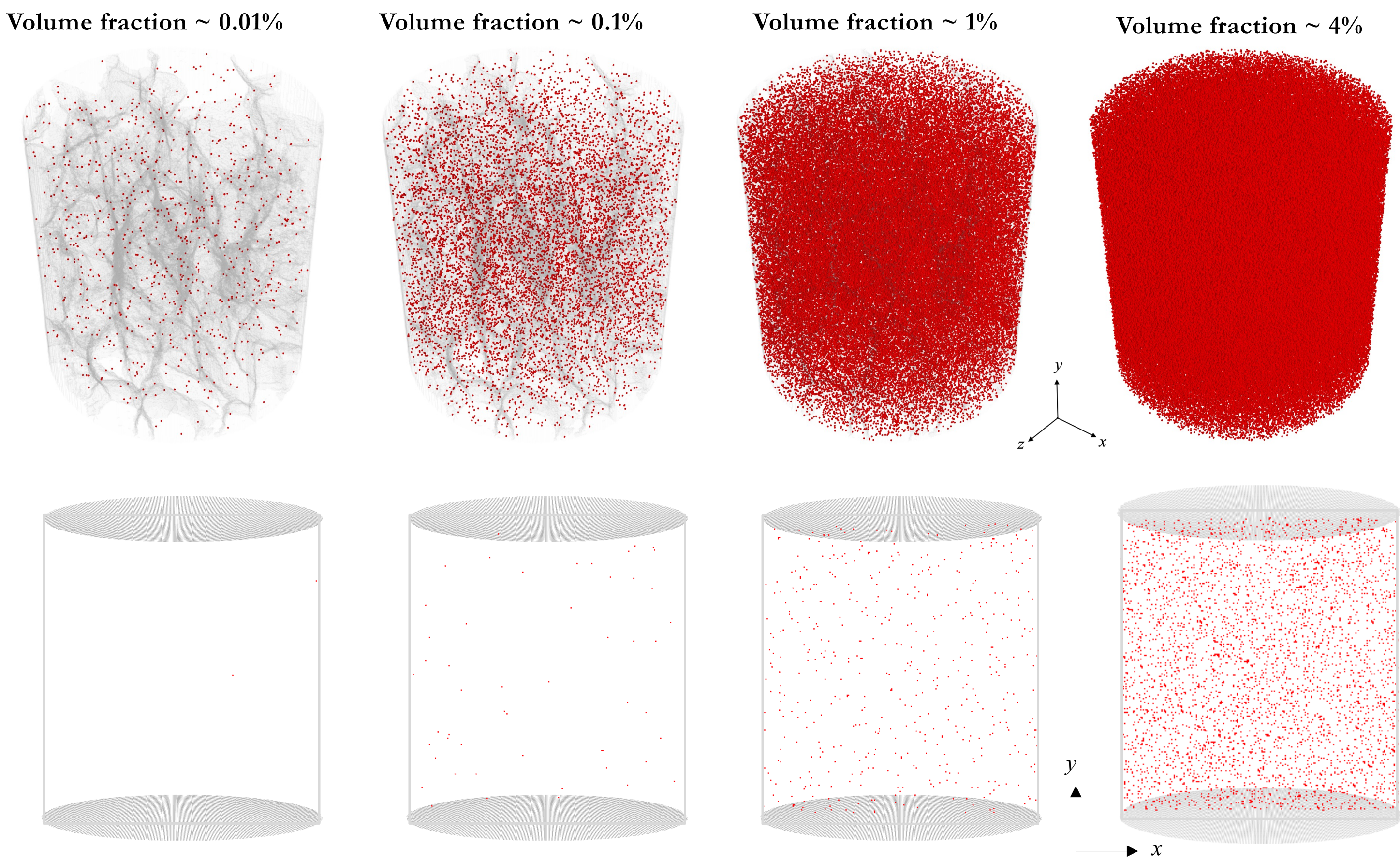


$$g^{\alpha} = g_0 + A\mu b\sqrt{\sum_{\beta=1}^{12} H^{\alpha\beta}\rho^{\beta}} \qquad d\rho^{\alpha} = \left(\kappa_1\sqrt{\sum_{\beta=1}^{12}\rho^{\beta}} - \kappa_2\rho^{\alpha}\right)|d\gamma|$$

$$\sigma = \sigma_0 + A\epsilon^n$$



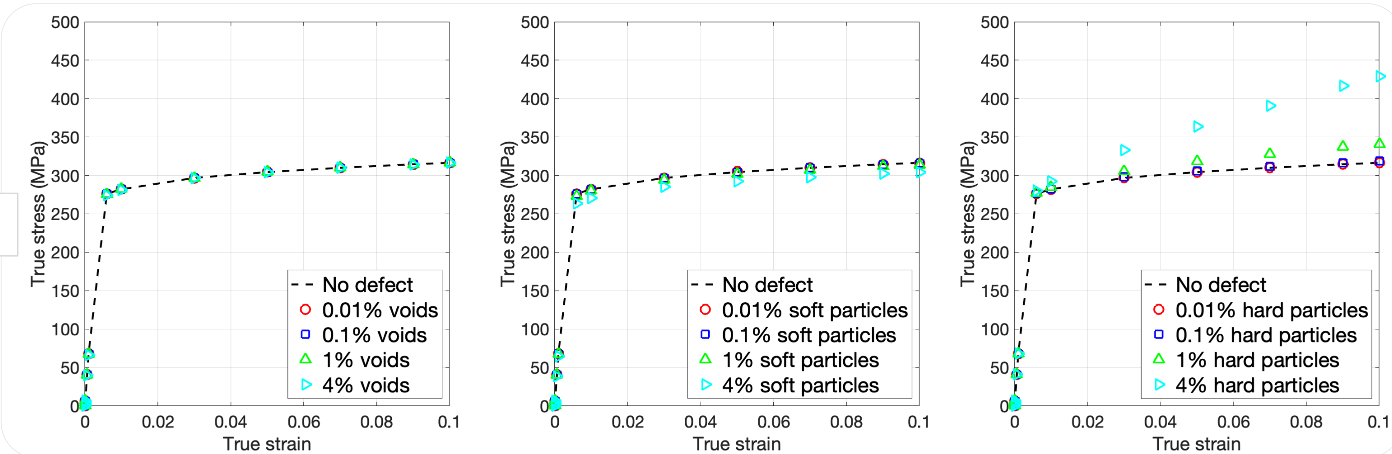
Incorporating volumetric defects in FE mesh



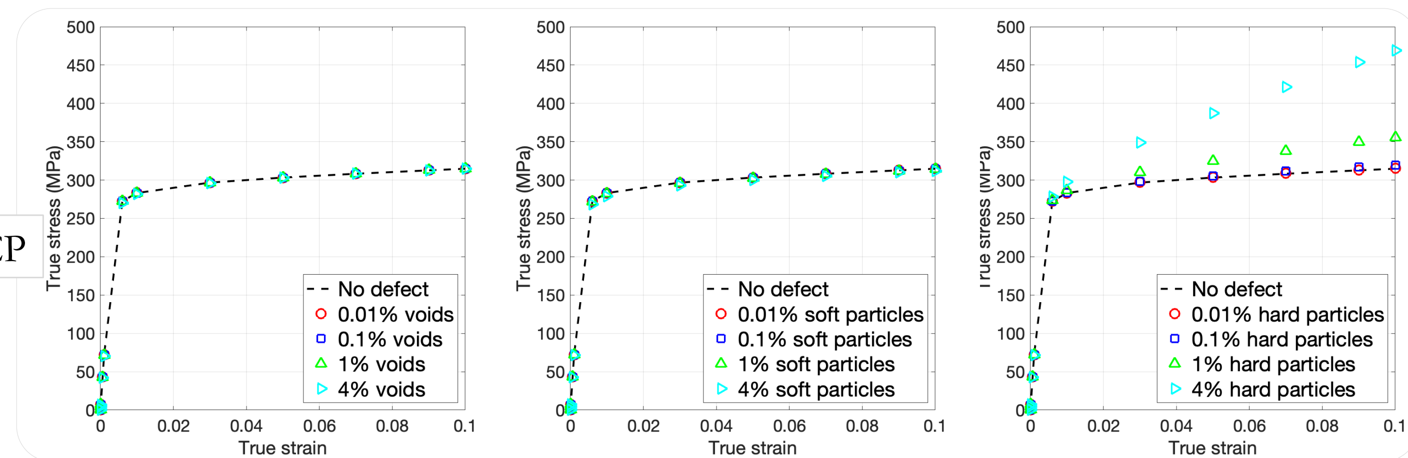
- Single element defects (2.5 μm), randomly distributed (vol. frac. 0.001 - 4%)
- “Defect elements” are converted to hard particles, soft particles and voids.
- Hard particles: 100× yield strength of Al matrix
- Soft particles: 1/100× yield strength of Al matrix
- Voids: defect elements removed from the mesh

Macroscopic stress-strain response

J2

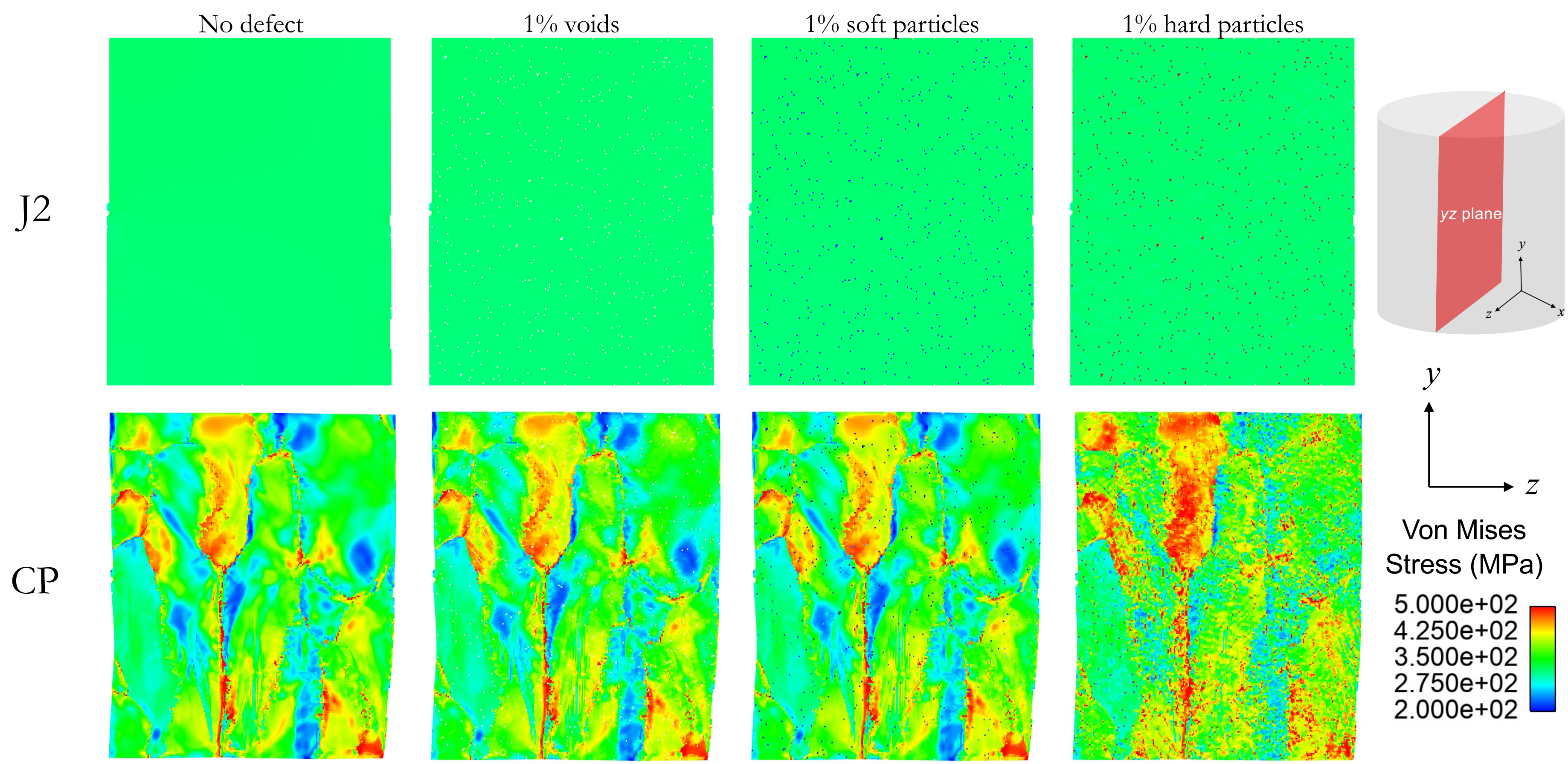


CP

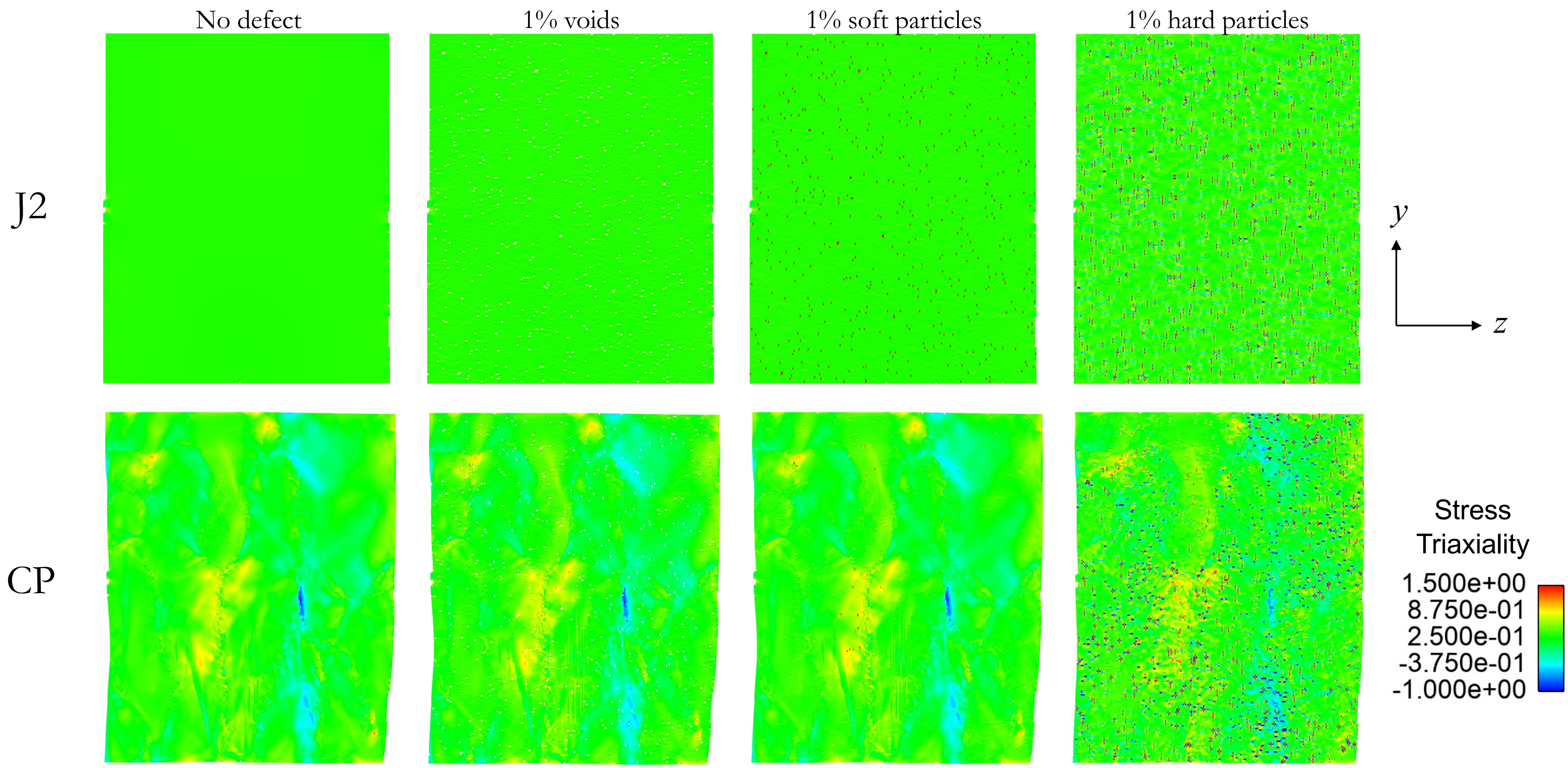


- Voids and soft particles have negligible effects
- Hard particles increase the strength
- CP is more sensitive to hard particles (see figures in the next slides) – hard particles increased stress fields in neighboring elements in CP.

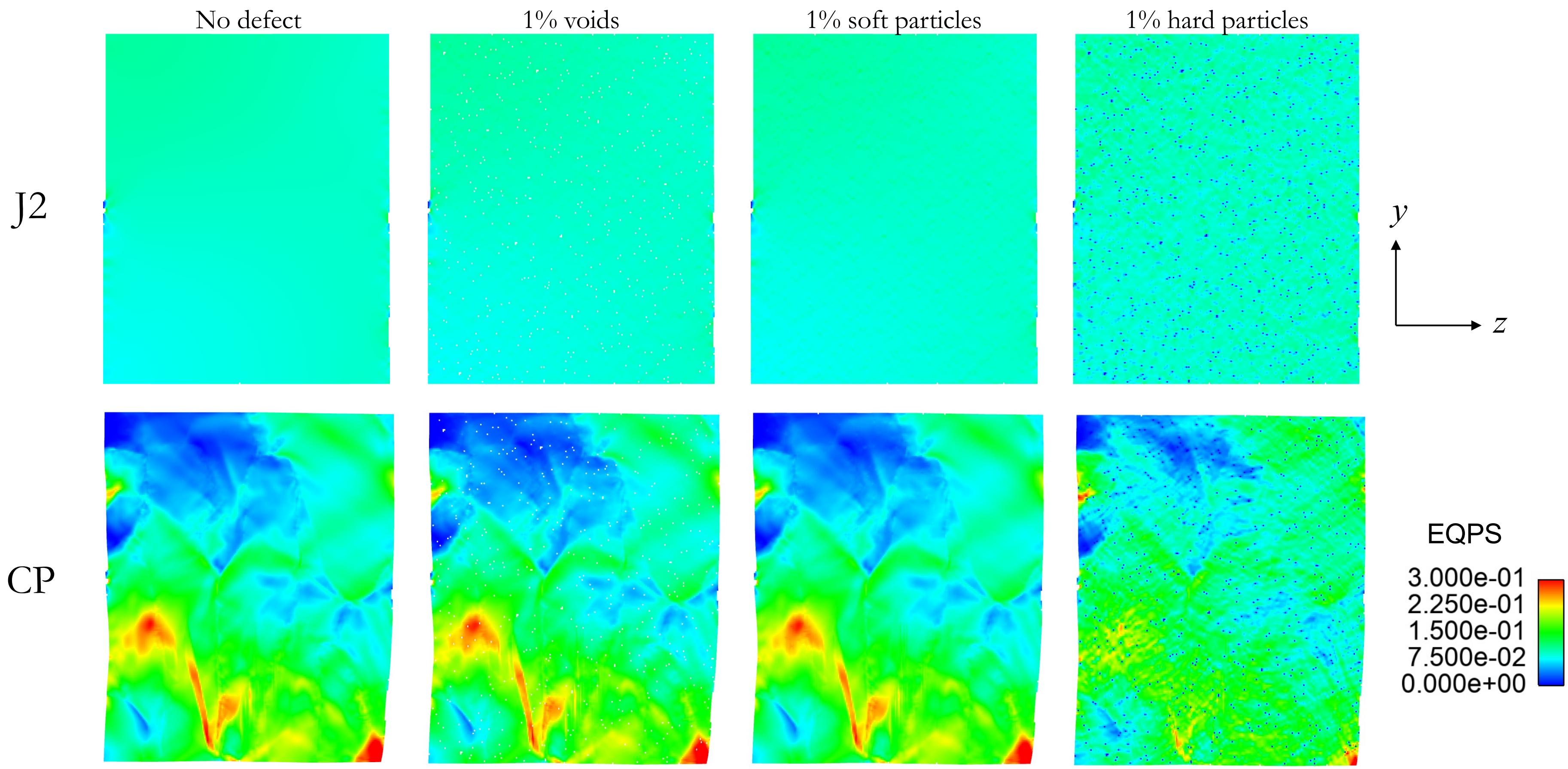
Von Mises stress after 10% deformation



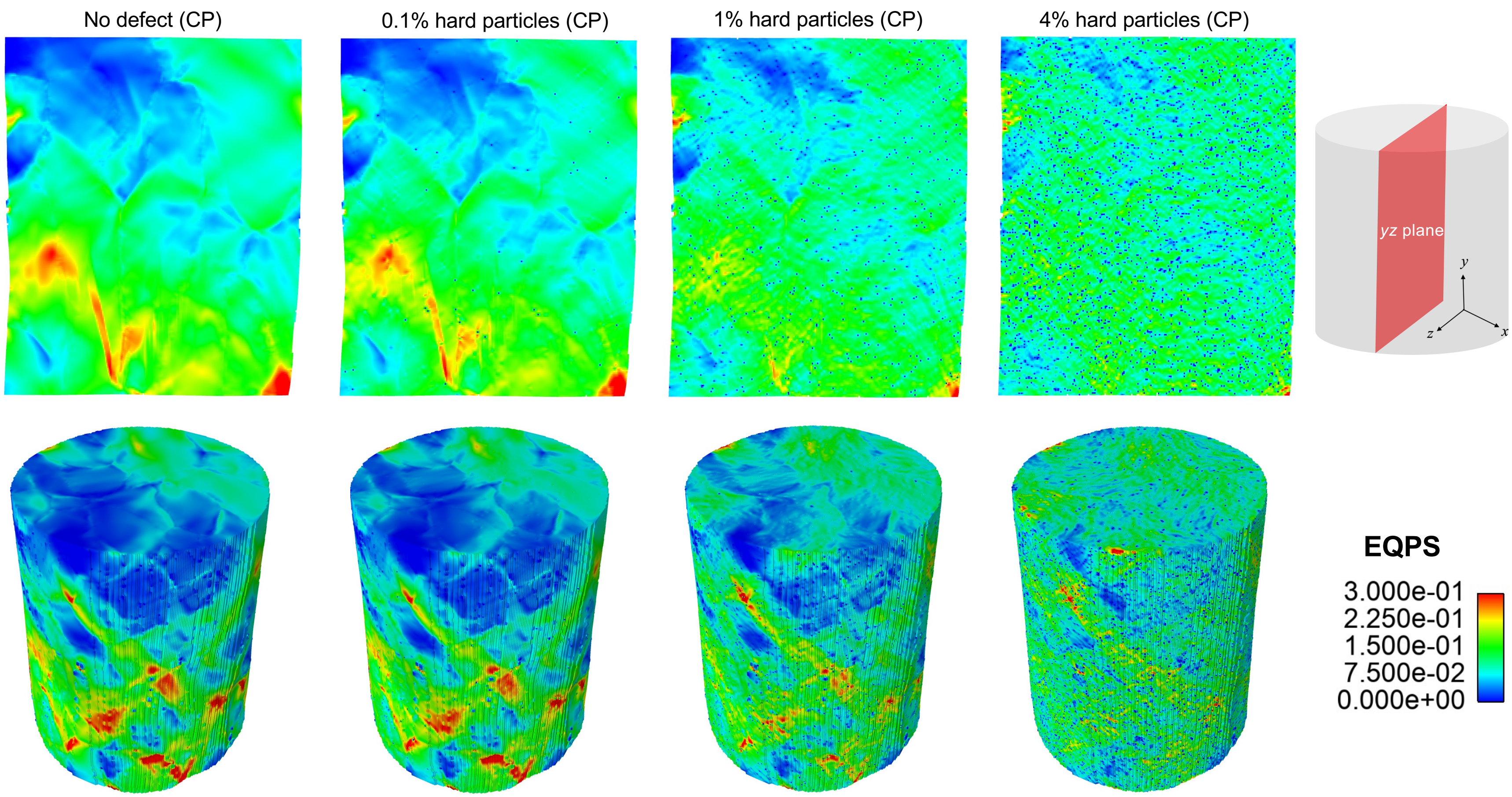
Stress triaxiality after 10% deformation



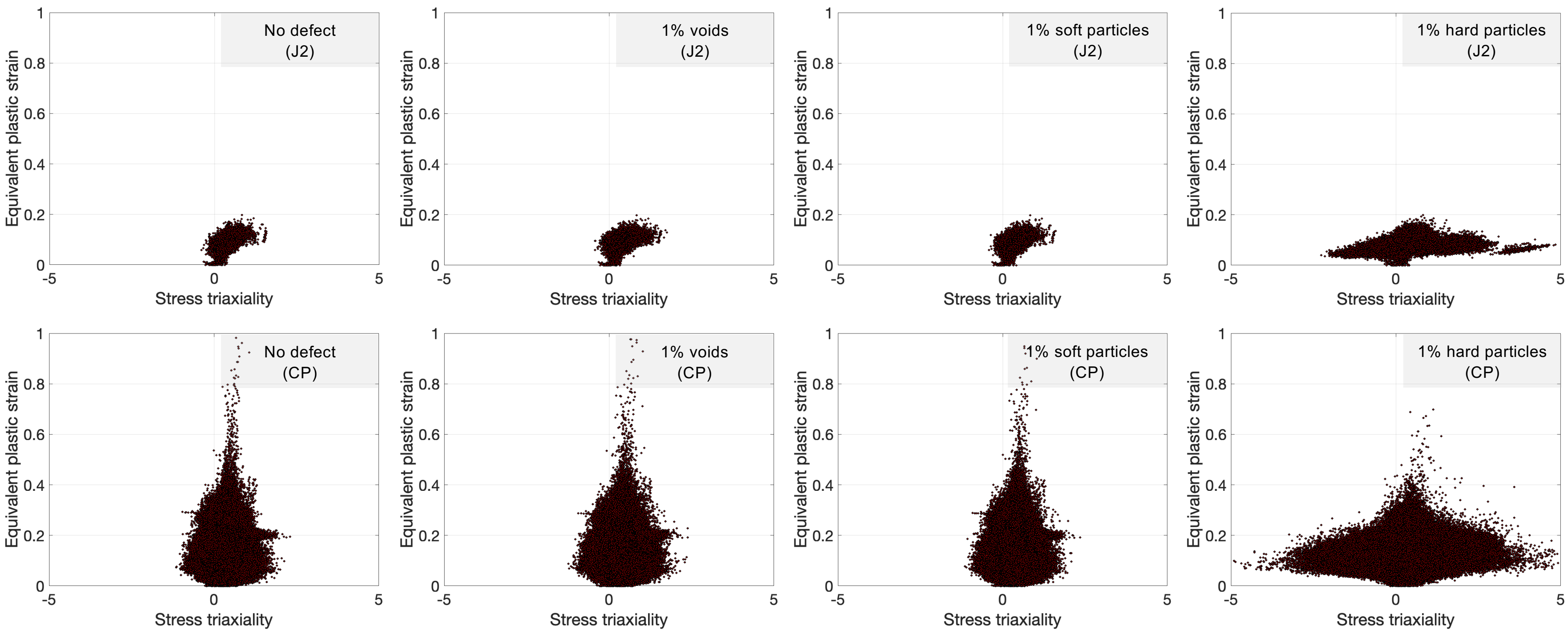
EQPS after 10% deformation



EQPS after 10% deformation: Effects of hard particles



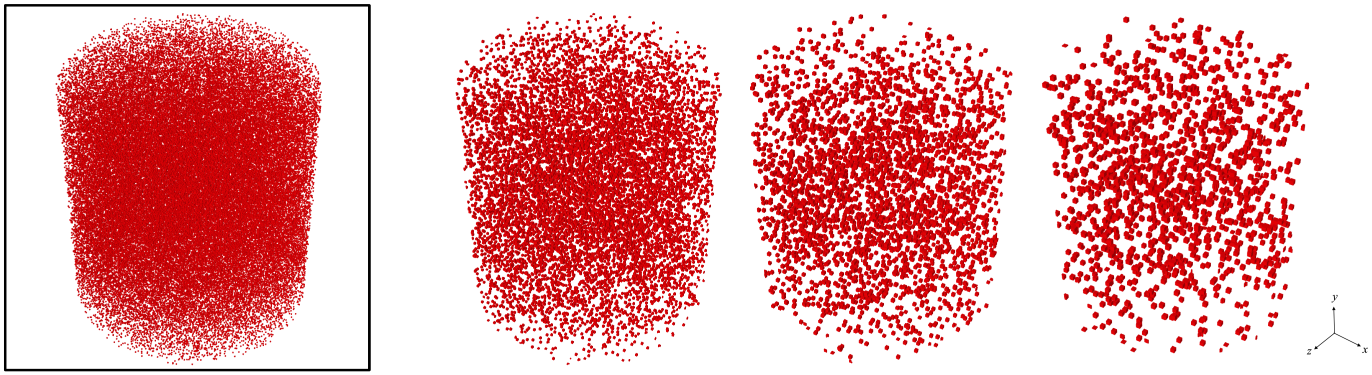
EQPS vs. stress triaxiality: All elements



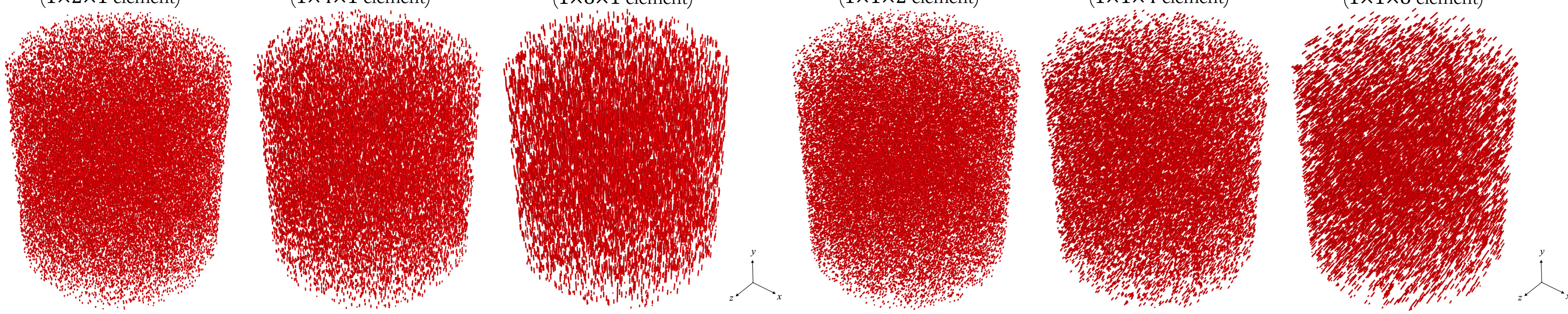
- Larger EQPS and stress triaxiality scatters in CP compared to J2 simulation.
- Voids and soft particles have small effects on local strain and stress triaxiality.
- Hard particles significantly increase scatter in stress triaxiality.

Effects of defect sizes/shapes (Volume fraction ~1%)

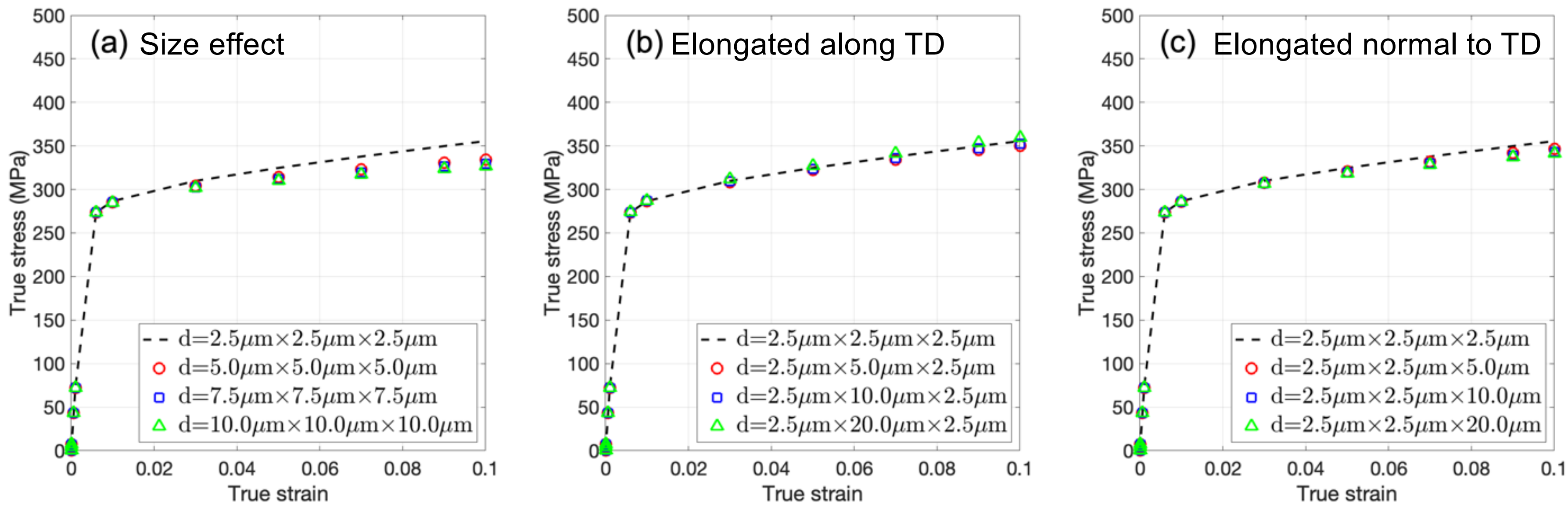
$(2.5\mu m\times 2.5\mu m\times 2.5\mu m)$ (1×1×1 element)
$(5.0\mu m\times 5.0\mu m\times 5.0\mu m)$ (2×2×2 element)
$(7.5\mu m\times 7.5\mu m\times 7.5\mu m)$ (3×3×3 element)
$(10.0\mu m\times 10.0\mu m\times 10.0\mu m)$ (4×4×4 element)



$(2.5\mu m\times 5.0\mu m\times 2.5\mu m)$ (1×2×1 element)
$(2.5\mu m\times 10.0\mu m\times 2.5\mu m)$ (1×4×1 element)
$(2.5\mu m\times 20.0\mu m\times 2.5\mu m)$ (1×8×1 element)
$(2.5\mu m\times 2.5\mu m\times 5.0\mu m)$ (1×1×2 element)
$(2.5\mu m\times 2.5\mu m\times 10.0\mu m)$ (1×1×4 element)
$(2.5\mu m\times 2.5\mu m\times 20.0\mu m)$ (1×1×8 element)

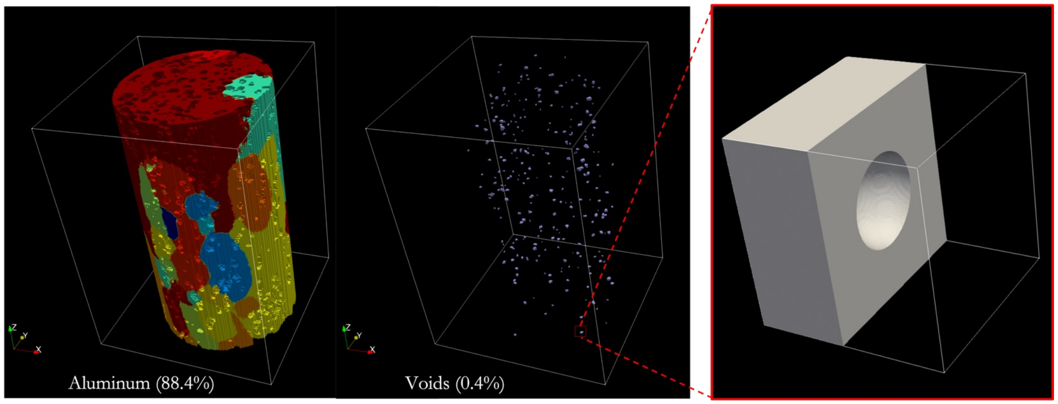


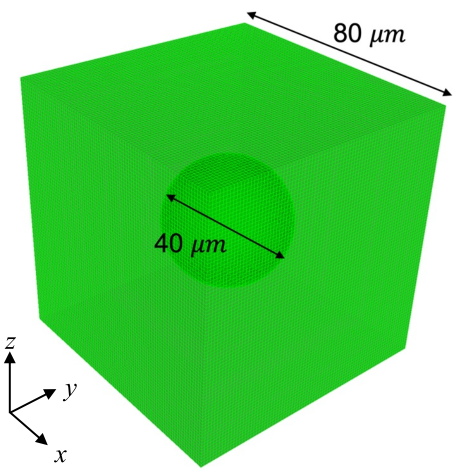
Stress-strain response

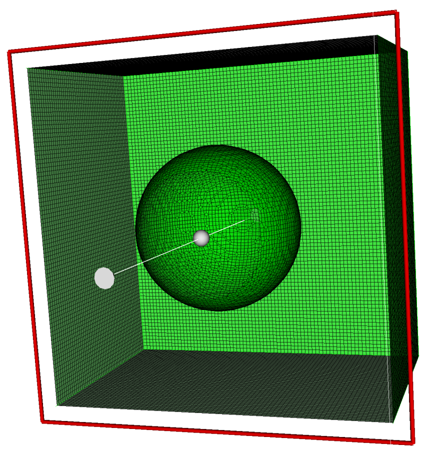


- Larger particles reduce the strength (shorter mean free path)
- Shape had less effect. Long particles along the TD increased the strength.
- Long particles normal to the TD decreased the strength.
- Limitation: The current CP model does not consider motion and dislocations and their interactions with particles.

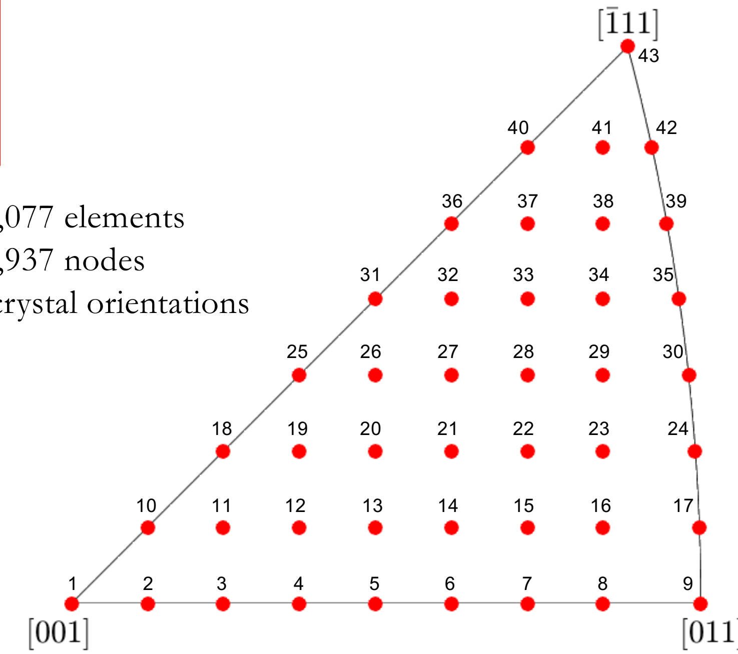
Effects of voids and particles in polycrystalline deformation



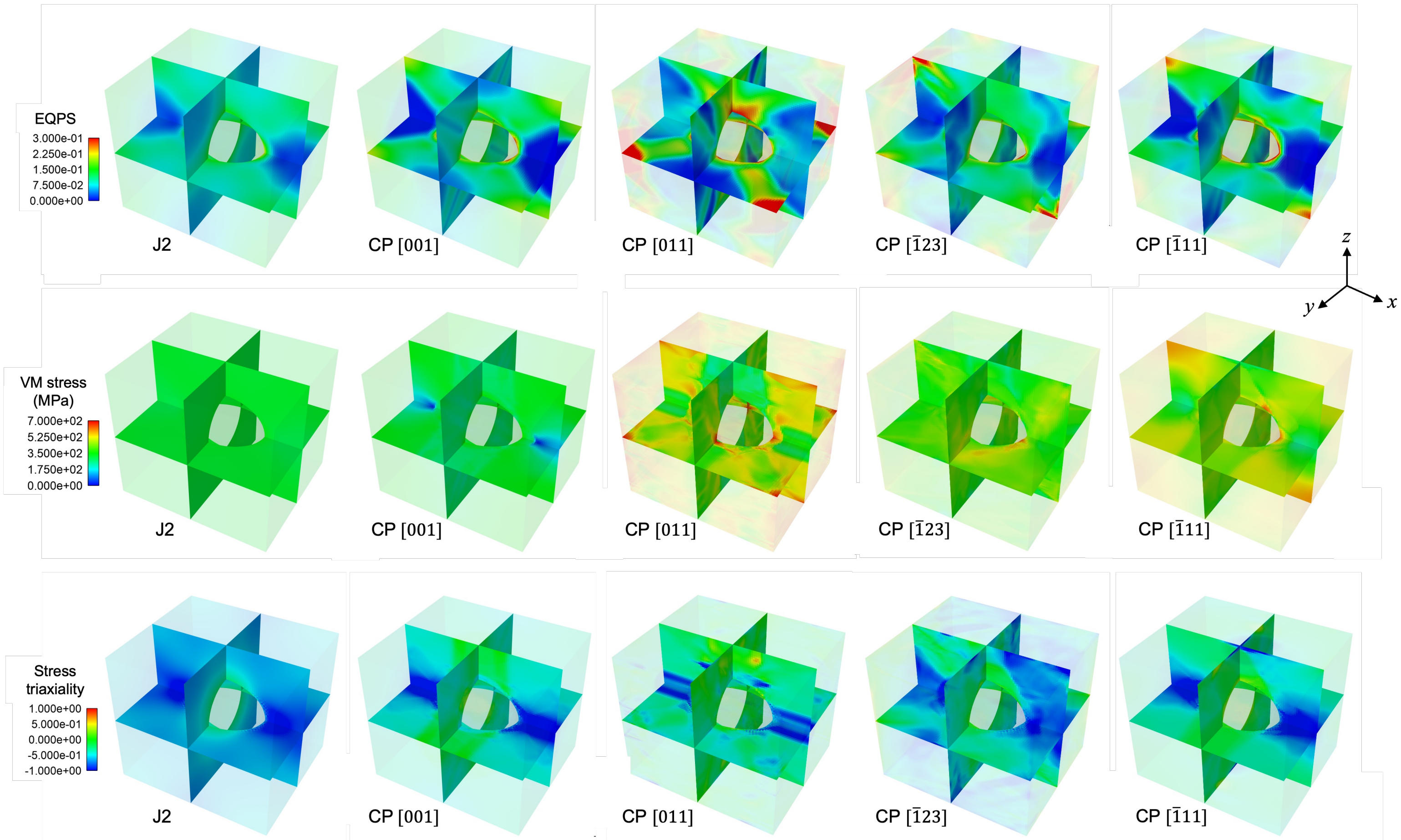




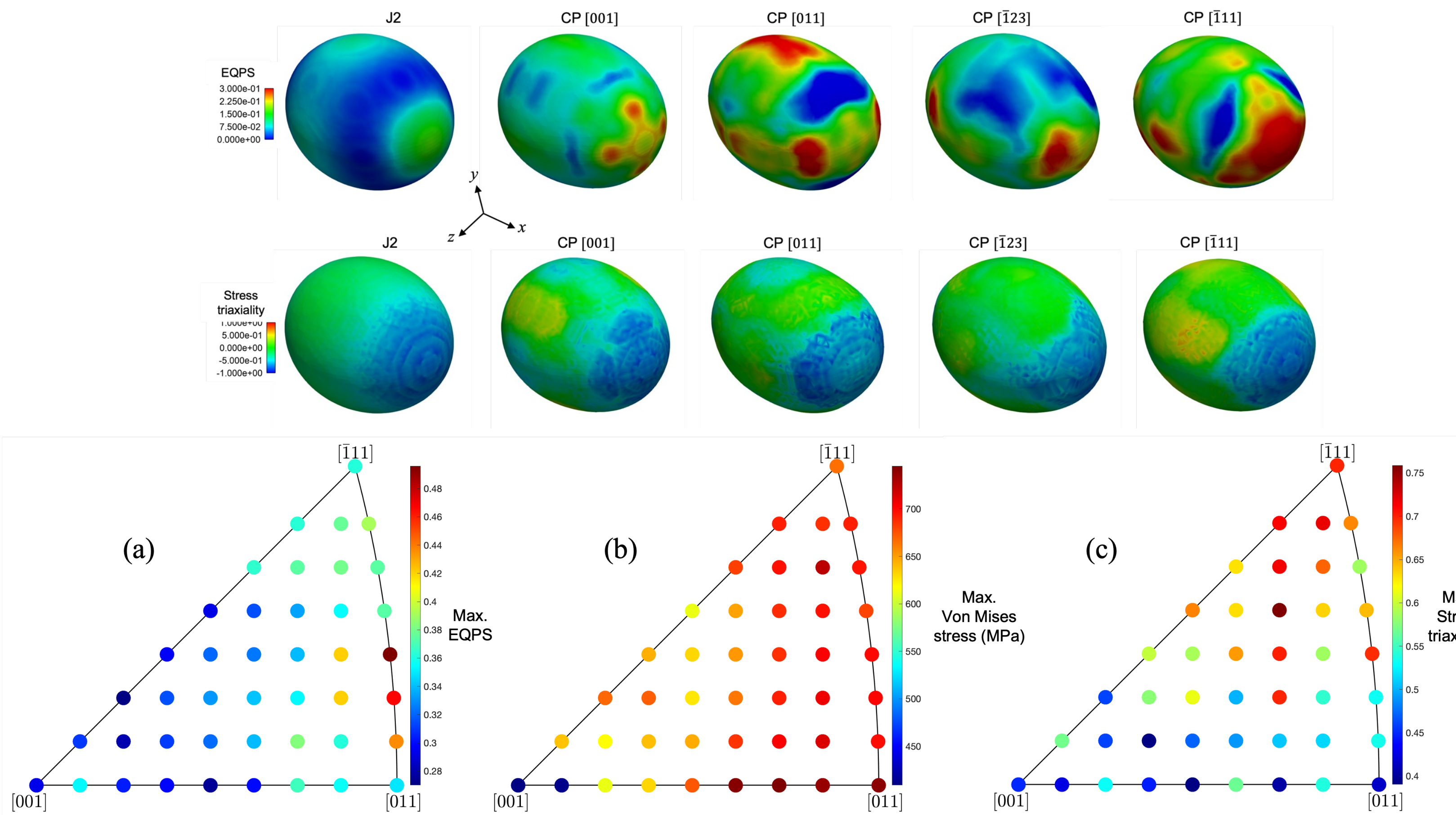
496,077 elements
518,937 nodes
43 crystal orientations



Local fields at 10% deformation

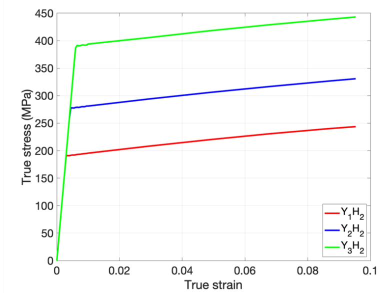


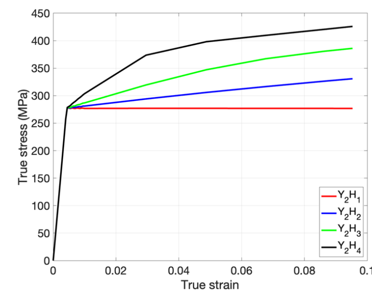
Local fields at 10% deformation (void surface)



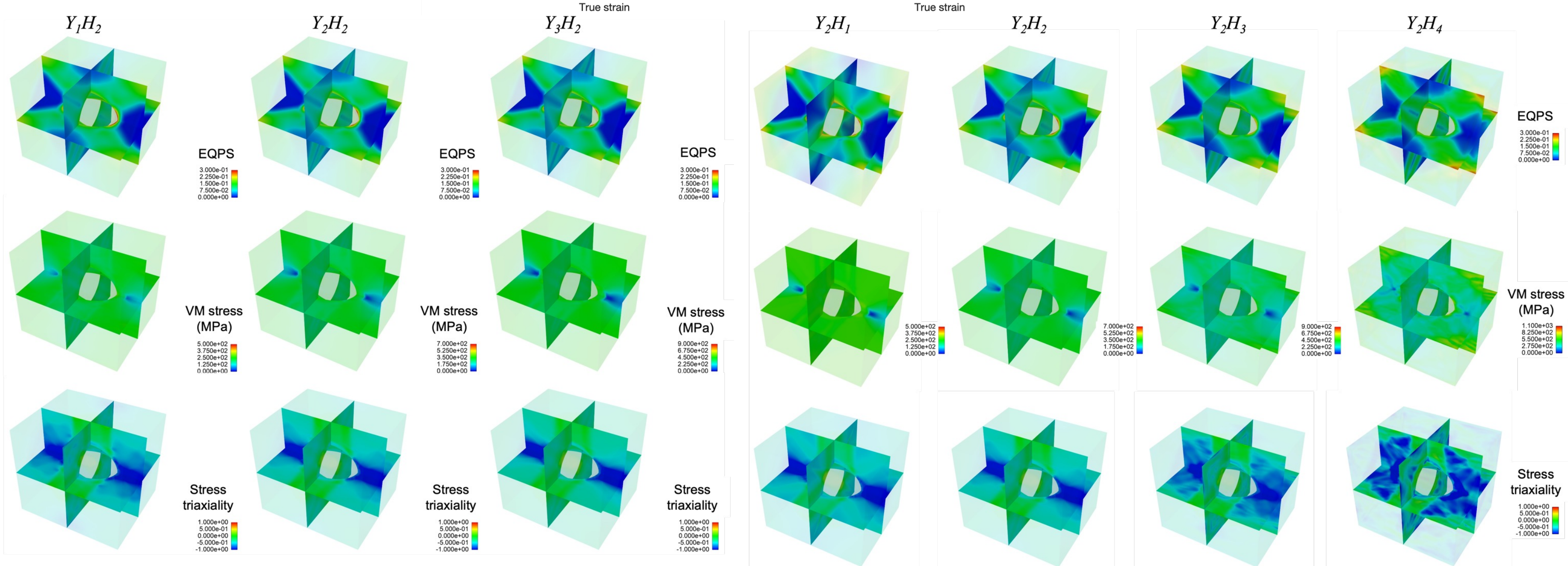
Effects of flow stress

Yield stress: $Y_1 < Y_2 < Y_3$





Hardening: $H_1 < H_2 < H_3 < H_4$



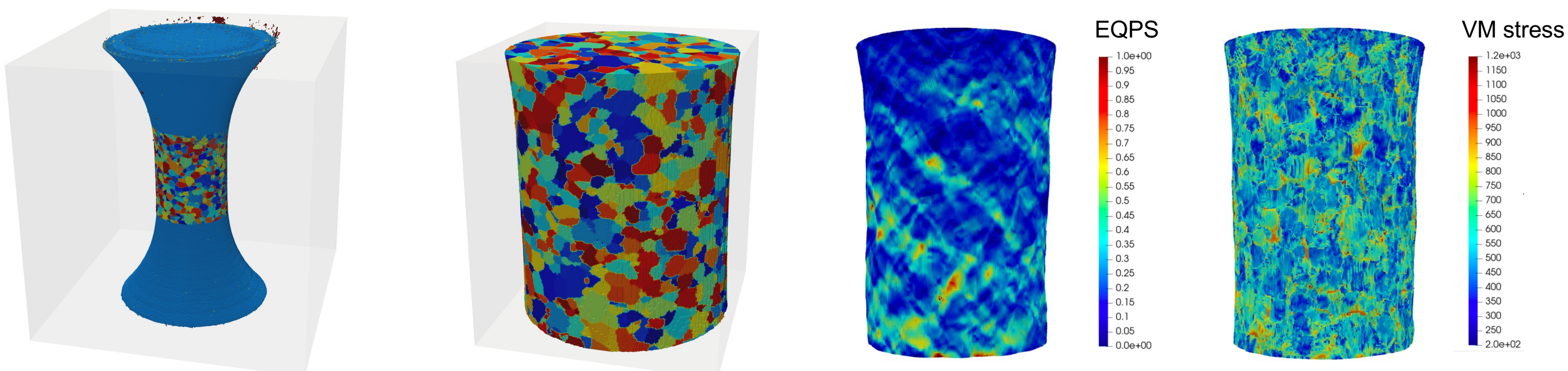
Summary

- ❖ **Performed 3D in-situ characterization of voids and particles using DCT/XCT.**

- ❖ **Developed a framework that reproduces 3D computational microstructures from experimental DCT/XCT data with grain orientations, phases, and defects**.

- ❖ **Microstructural features influence both macroscopic behavior and local fields.**
  - Inclusions of voids and soft particles had small effect in widely used CP and J2 models.
  - Hard particles significantly altered both macroscopic and local responses.
  - Inclusions of hard particles increased the strength and reduced strain heterogeneity and localization.
  - The shape and size of hard particles had moderate effect on deformation of polycrystalline.

- ❖ **Local crystal orientation near the void significantly influences local stress/strain fields.**



THANK YOU !

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Advanced Simulation & Computing (ASC)

Materials Margins Assurance

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