MS&T22
Technical Meeting and Exhibition
MATERIALS SCIENCE & TECHNOLOGY

SAND2022-13885C

Investigating effects of particles and voids in plastic deformation of Al6061 using finite element simulations

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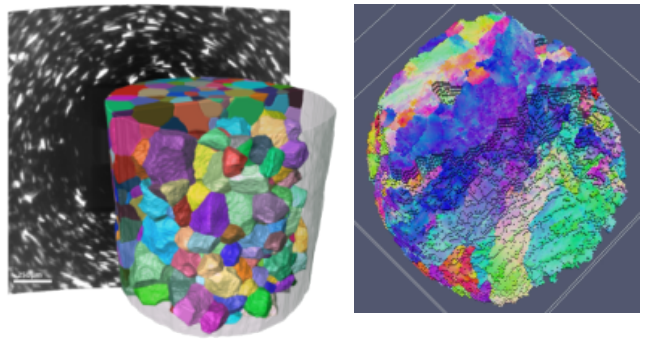
Objective

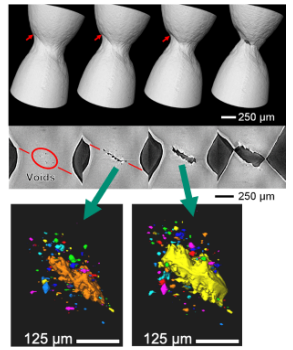
Goal: Predict failure based on the interaction of loading, microstructural features (e.g., crystal morphology, orientation), and defects such as pores, inclusions, and microcracks in structural alloys.

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

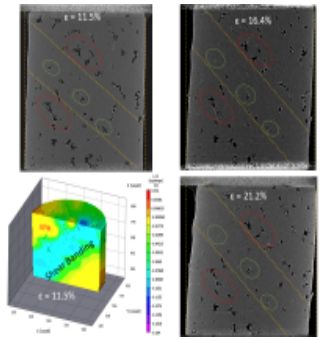


Diffraction Contrast Tomography (DCT)

3D Characterization



High Resolution µCT



Digital Volume Correlation (DVC)

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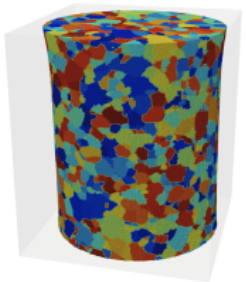
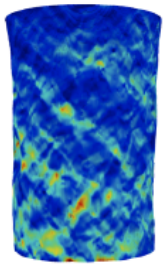
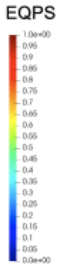
FAMU

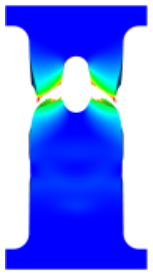
Finite element modeling

Deep Learning



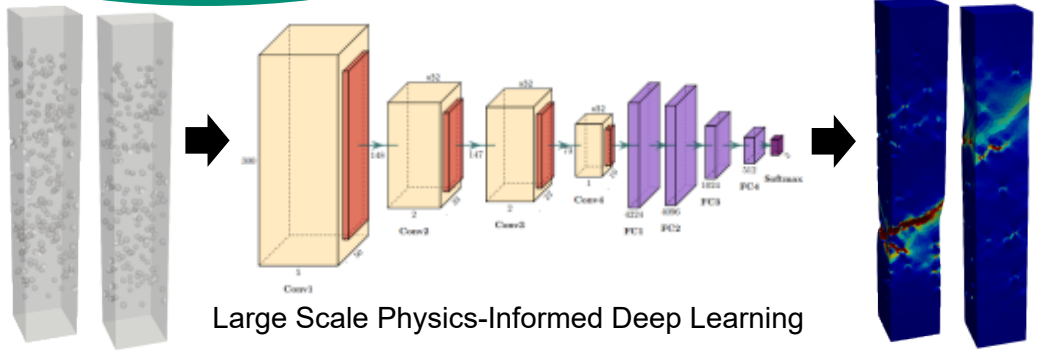






Crystal plasticity

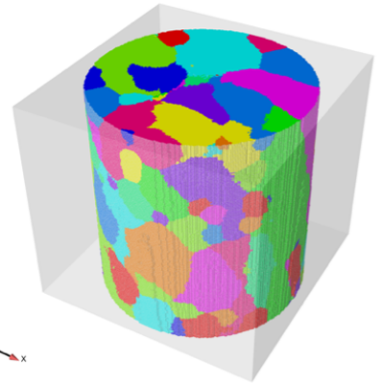
Continuum Plasticity and Damage Models



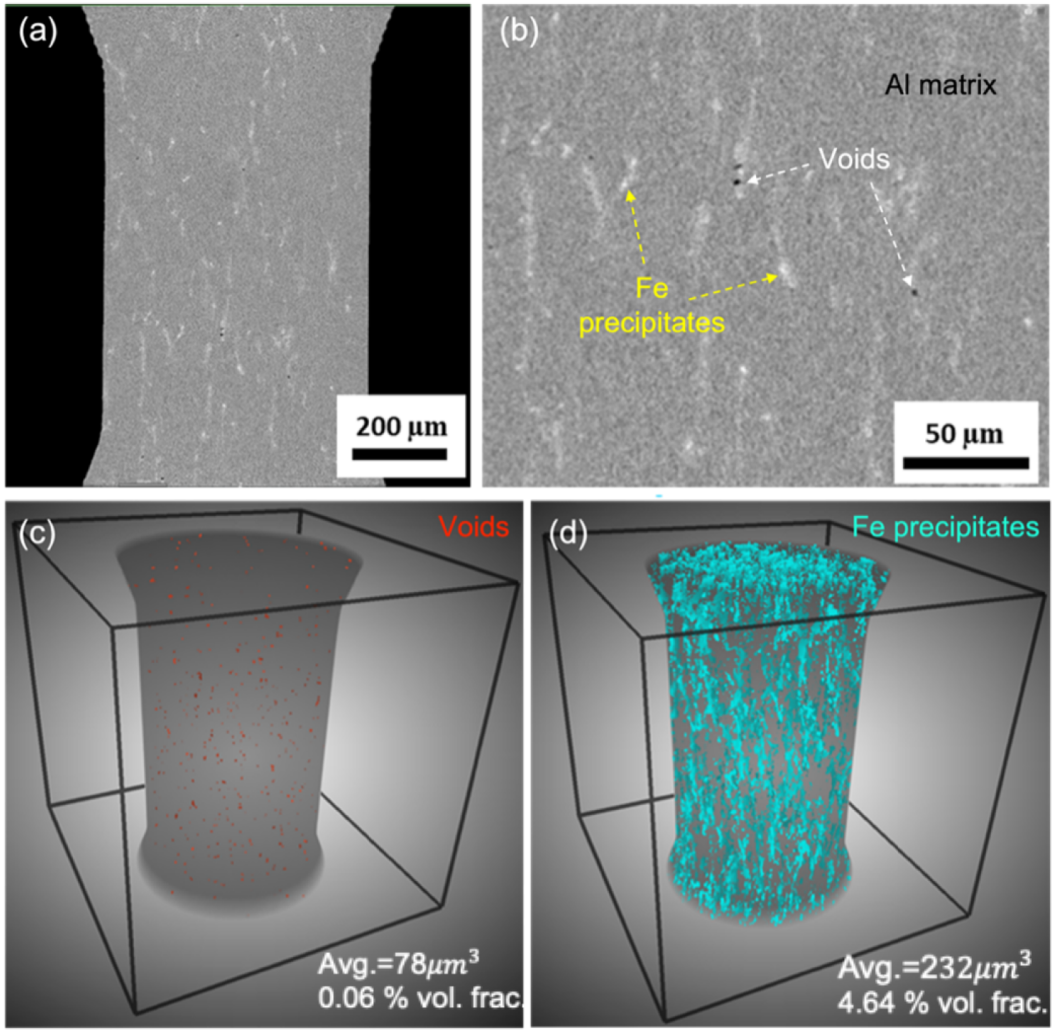
Large Scale Physics-Informed Deep Learning

Material characterization

Al6061-T6



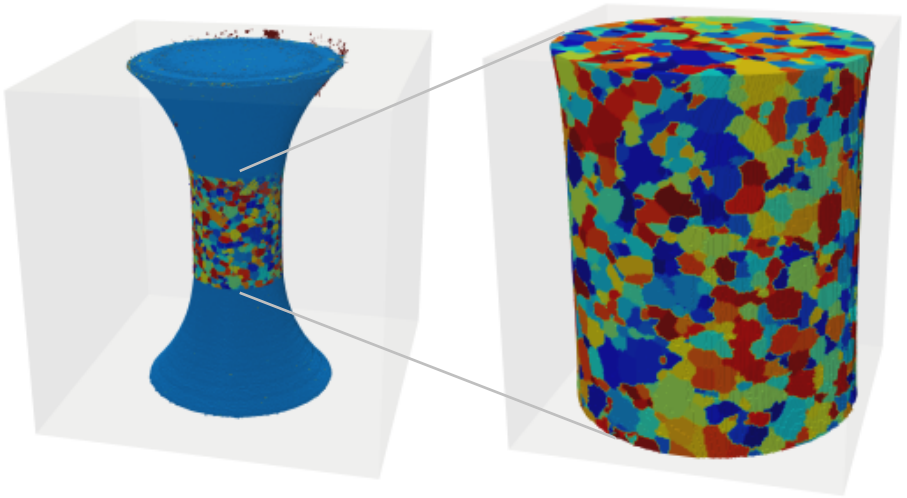
Grain morphology (DCT)

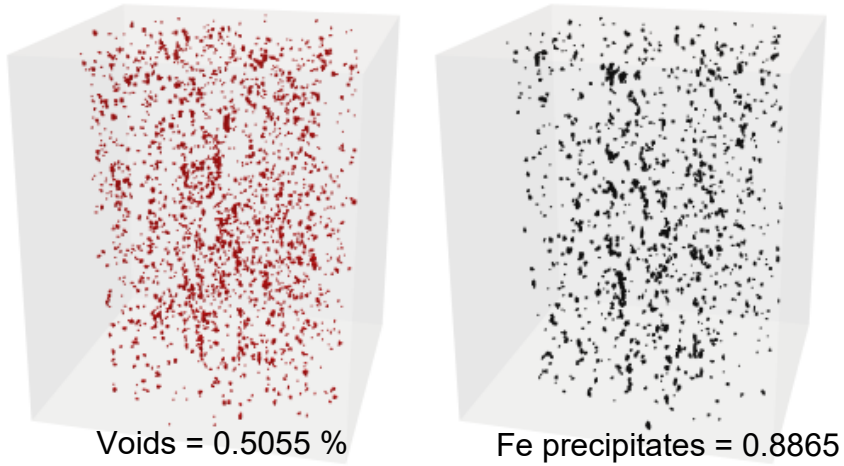


- 15M voxels (254×237×256)
- Diameter ~0.5mm, Height ~0.3 mm
- ~150 grains, 2.5 µm voxel size

XCT measurements

Al2219



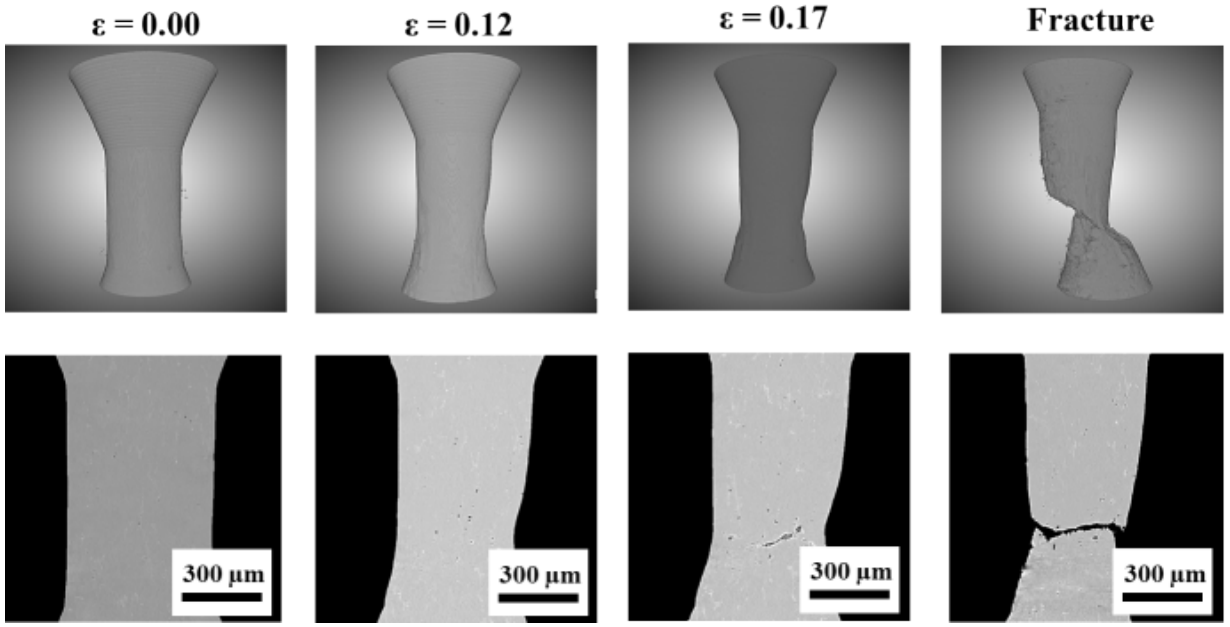


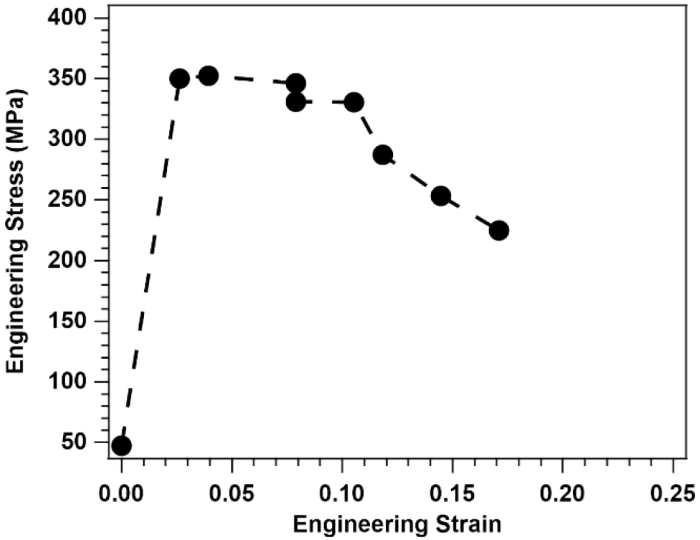
Voids = 0.5055 %

Fe precipitates = 0.8865 %

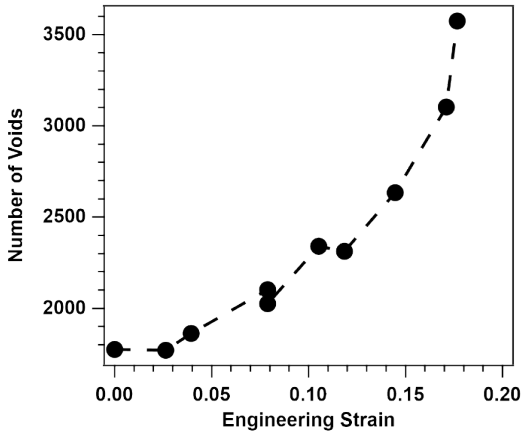
- ~310M voxels (674x672x686) /~10M voxels (209x206x245)
- Diameter ~1mm, Height ~1.2mm
- ~3700 grains, 5um voxel size

In-situ XCT measurements – Al6061

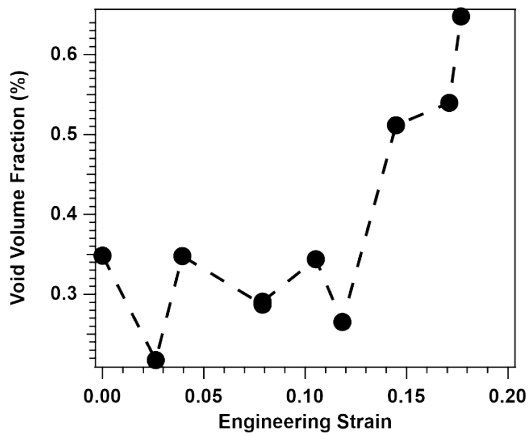




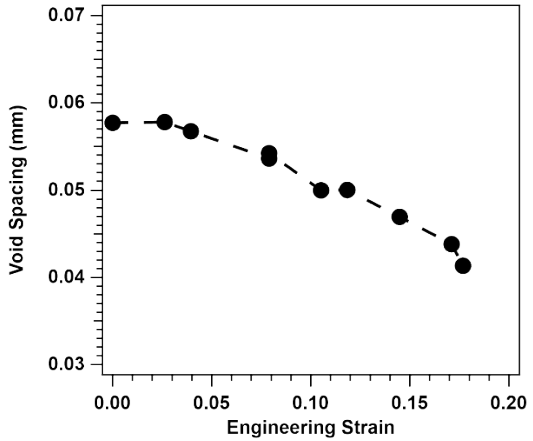
In situ stress-strain results. Markers indicate CT scan points

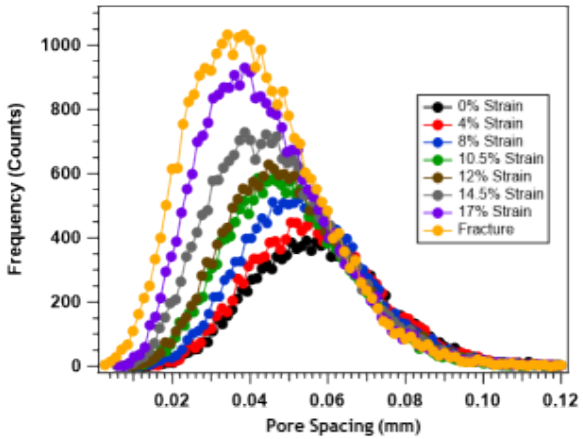


Void Nucleation



Void Nucleation + Growth

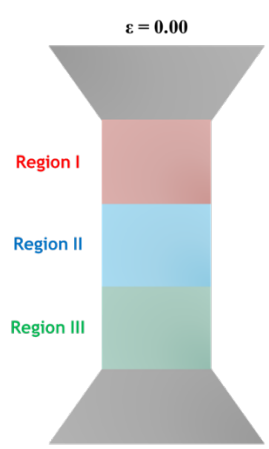


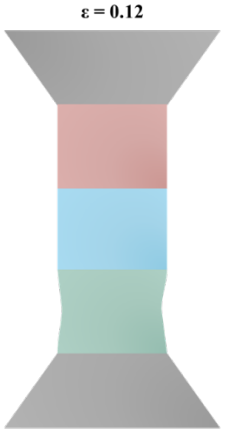


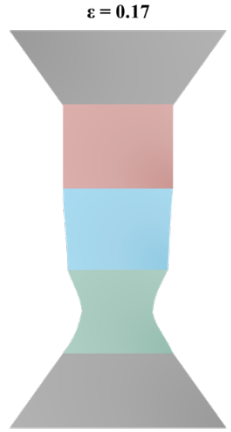
Void Coalescence

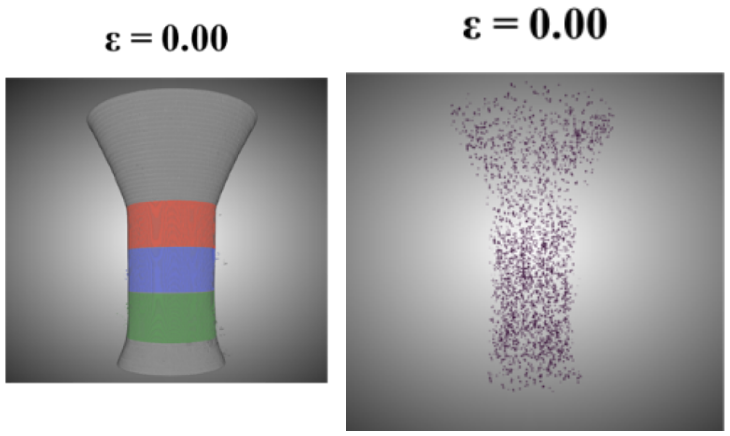
Seede et al. Scripta Mater. (submitted)

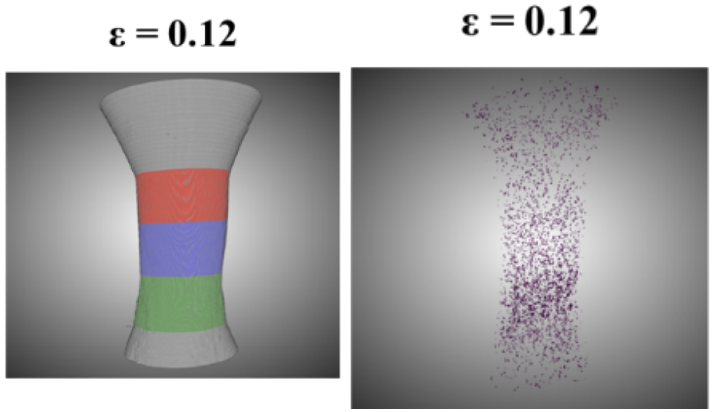
In-situ XCT measurements: Particles

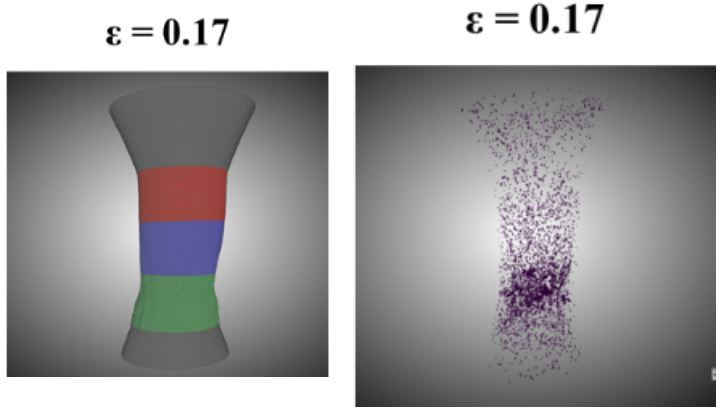










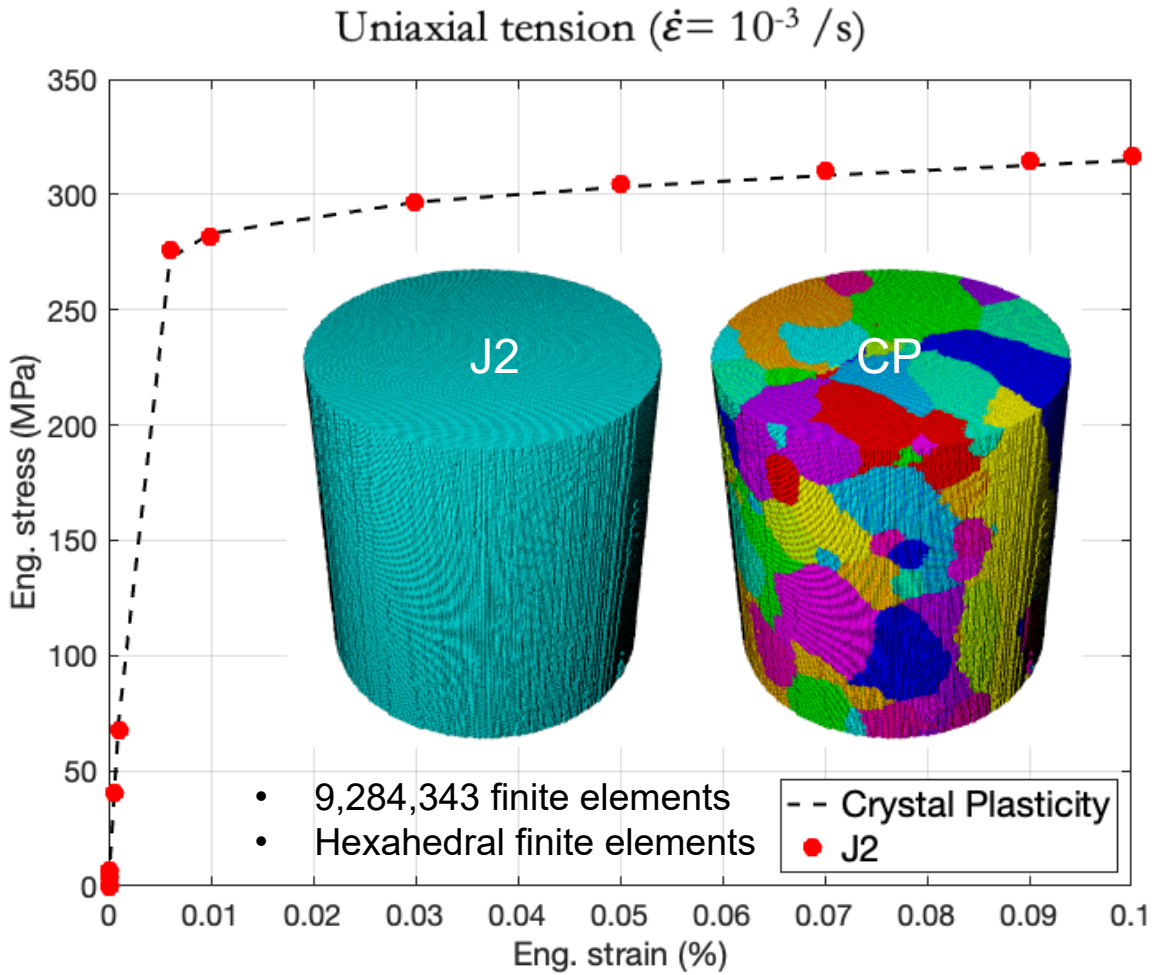


Location	Region I	Region II	Region III
Total Particle Volume (mm^3)	0.00218	0.00188	0.00215
Average Particle Spacing (mm)	0.03536	0.03530	0.03274

Region III contains high particle volume and low particle spacing

Seede et al. Scripta Mater. (submitted)

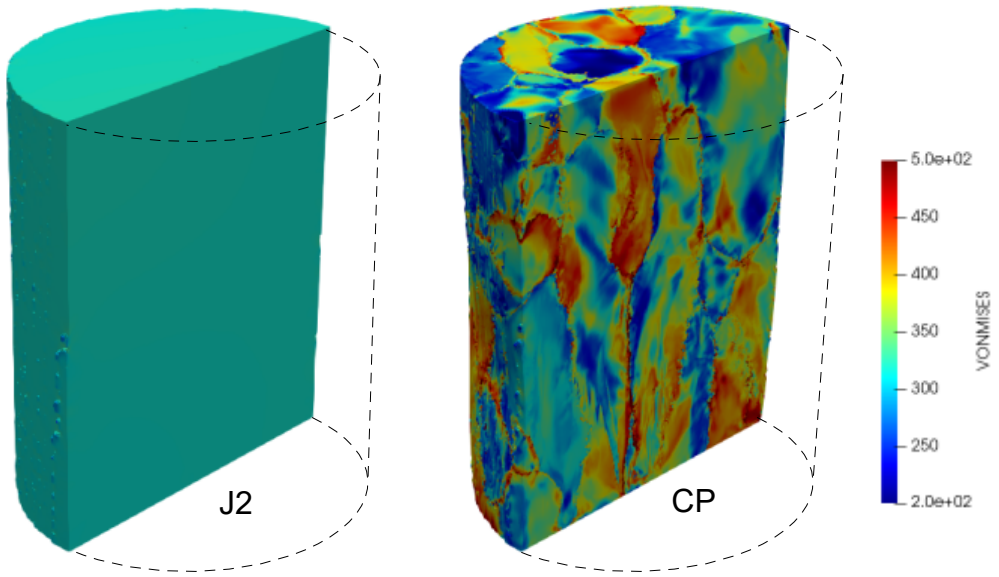
Finite element simulations



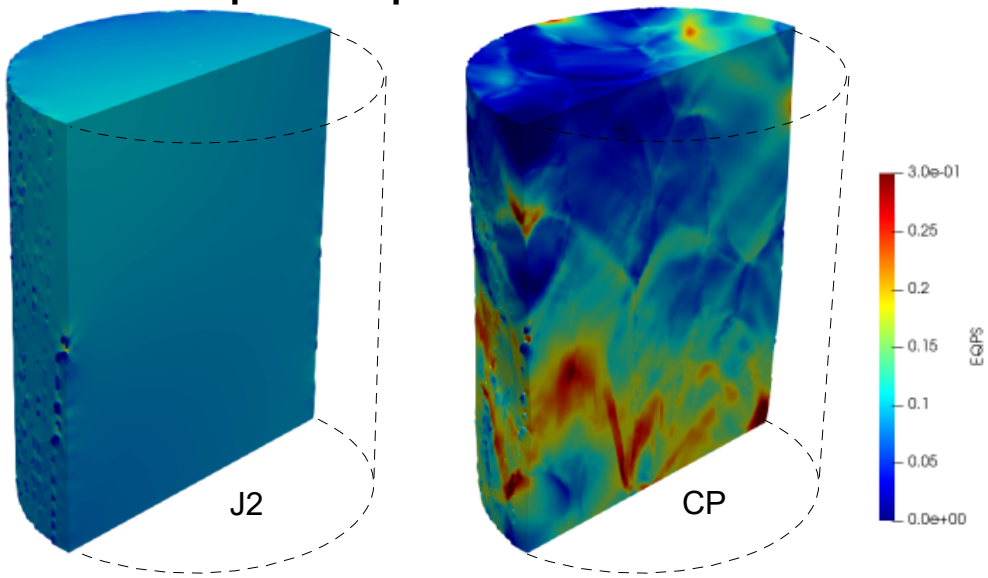
Crystal plasticity: $g^{\alpha} = g_0 + A\mu b\sqrt{\sum_{\beta=1}^{12} H^{\alpha\beta}\rho^{\beta}}$ $\quad d\rho^{\alpha} = \left(\kappa_1\sqrt{\sum_{\beta=1}^{12}\rho^{\beta}} - \kappa_2\rho^{\alpha}\right)|d\gamma|$

J2 plasticity: $\sigma = \sigma_0 + A\epsilon^n$

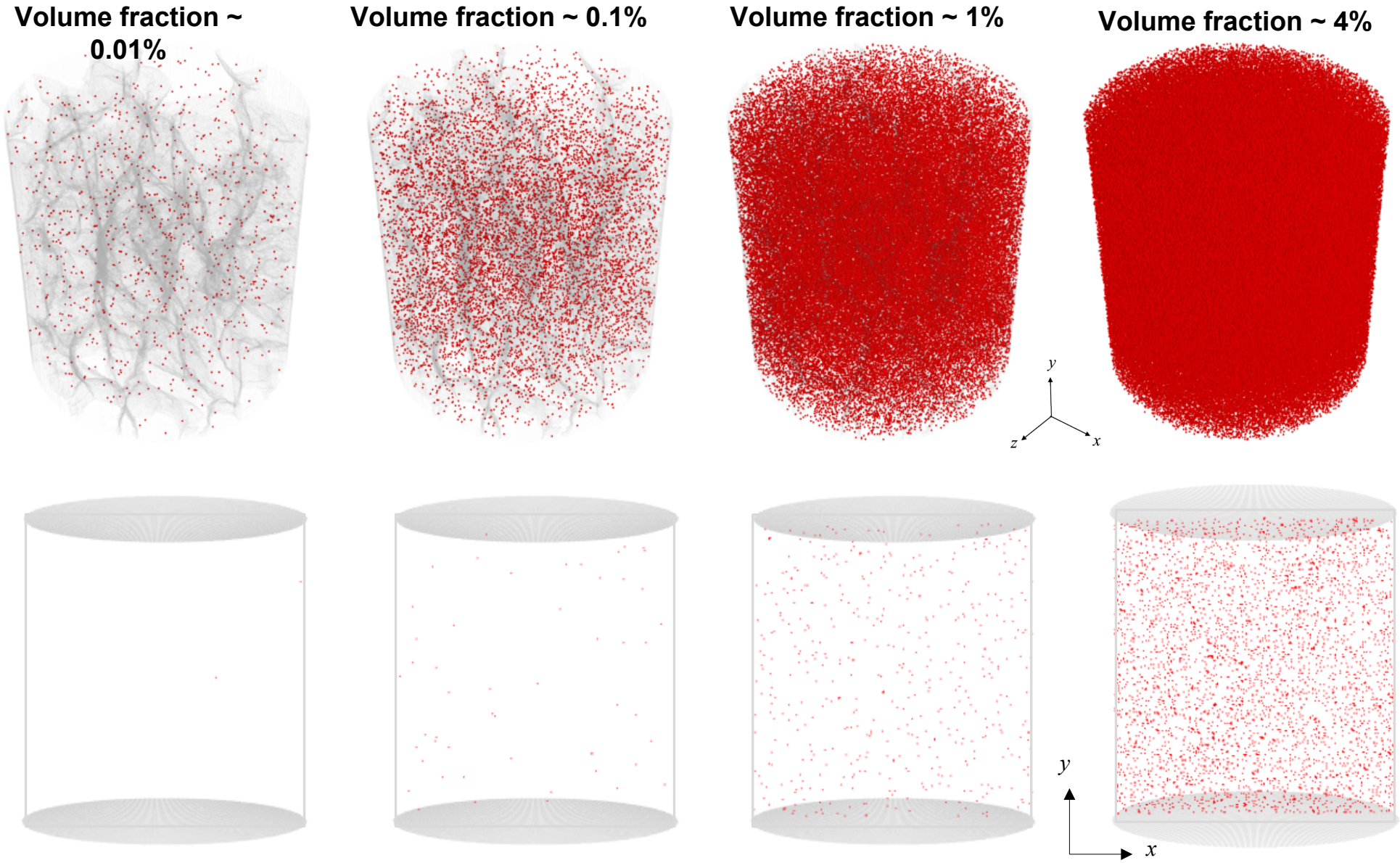
Von Mises stress



Equivalent plastic strain



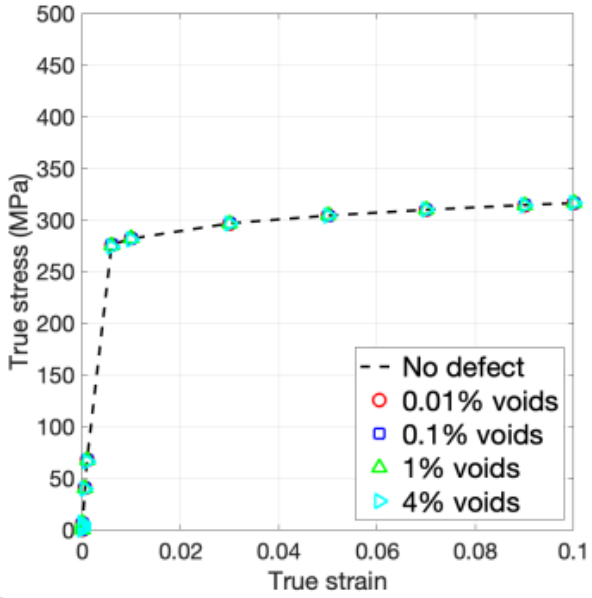
Incorporating volumetric defects in FE mesh

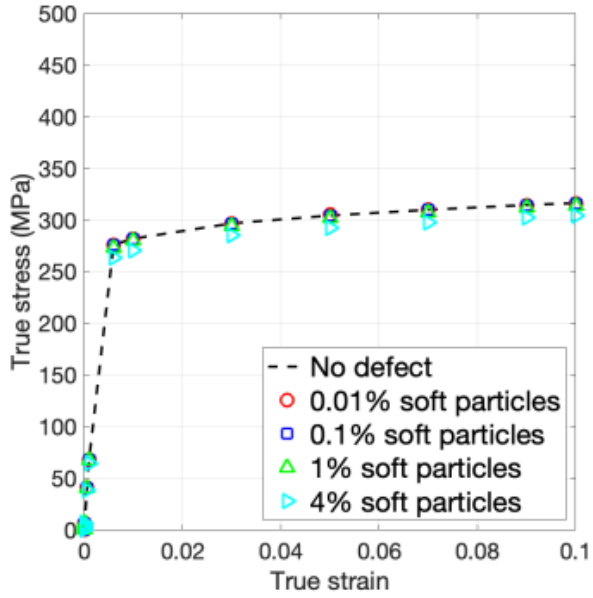


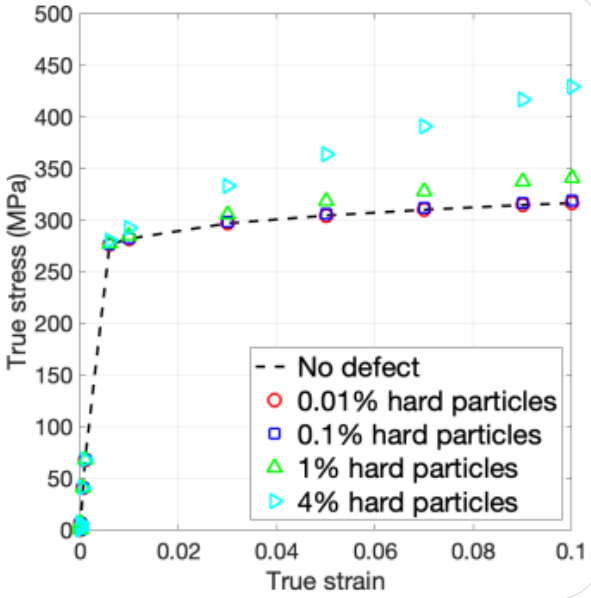
- Single element defects (2.5 μm), randomly distributed (vol. frac. 0.001 - 4%)
- "Defect elements" are converted to hard particles, soft particles and voids.
- Hard particles: 100× yield strength of Al matrix
- Soft particles: 1/100× yield strength of Al matrix
- Voids: defect elements removed from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

Macroscopic stress-strain response

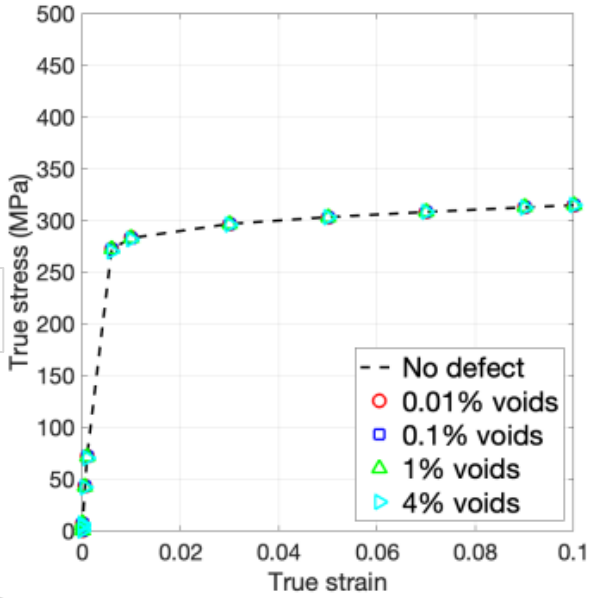
J2

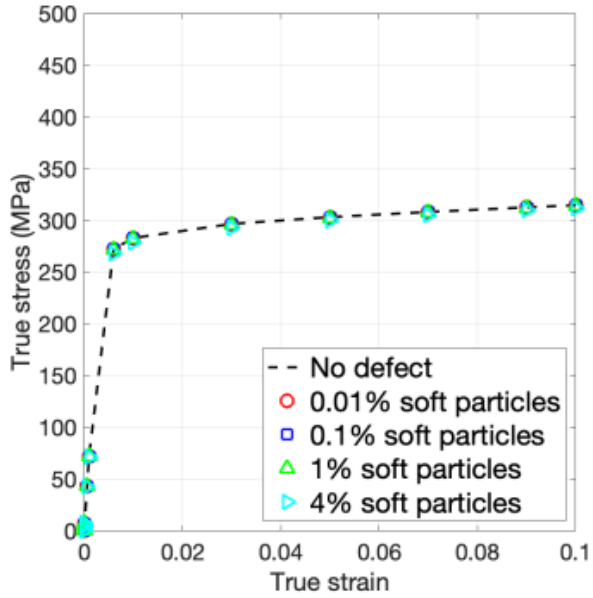


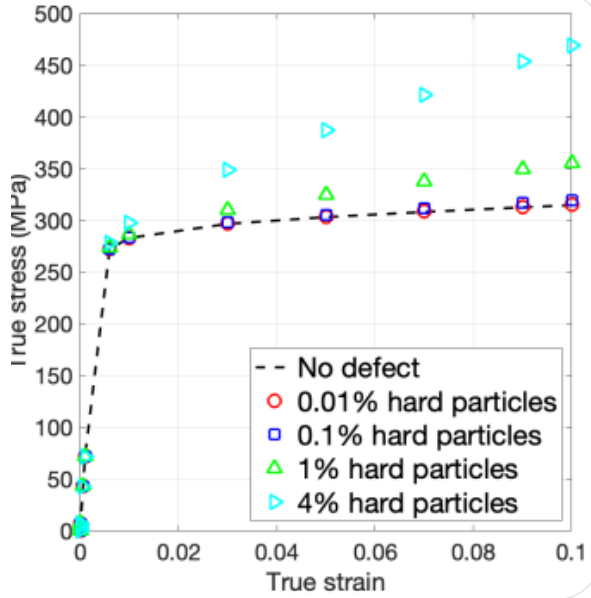




CP

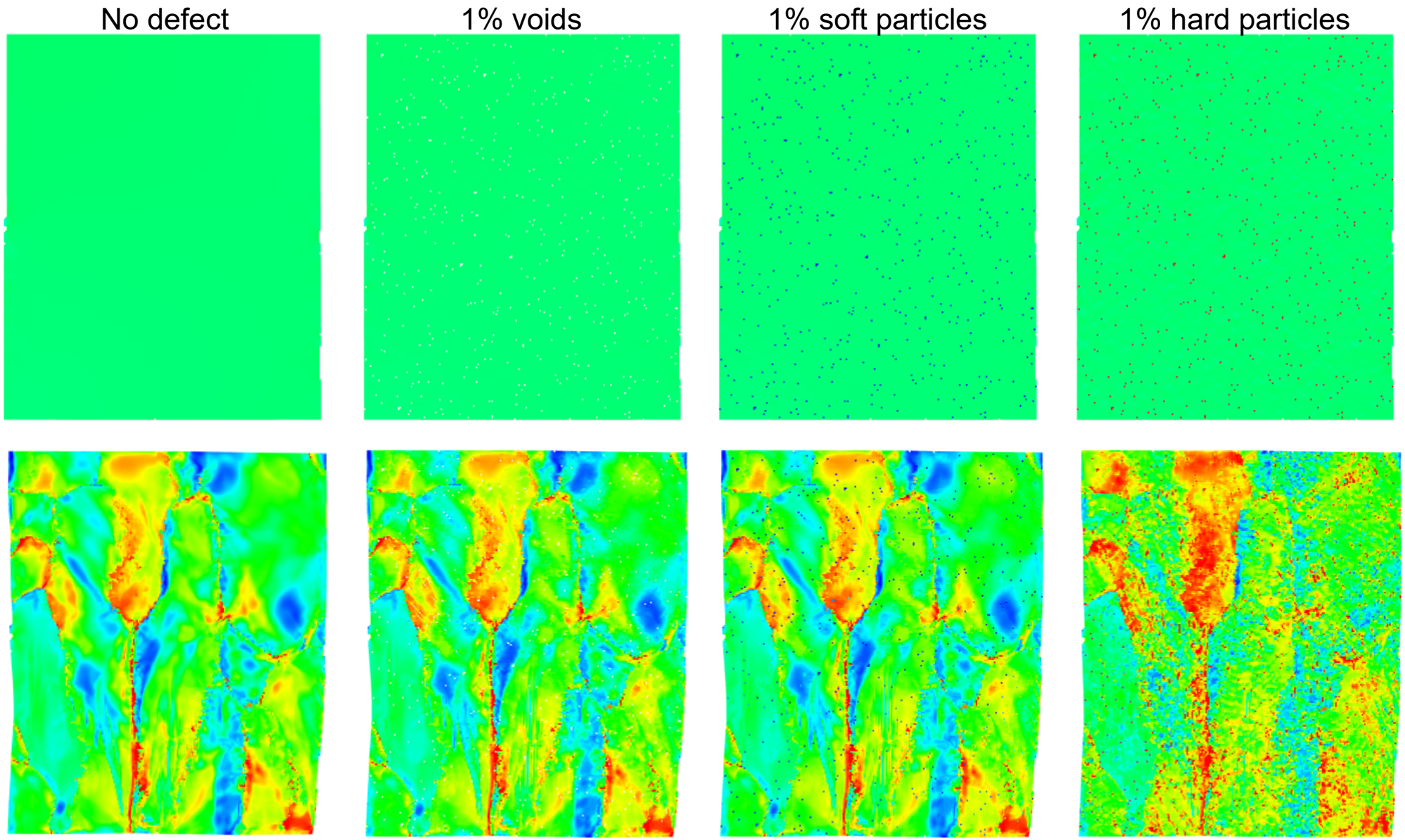




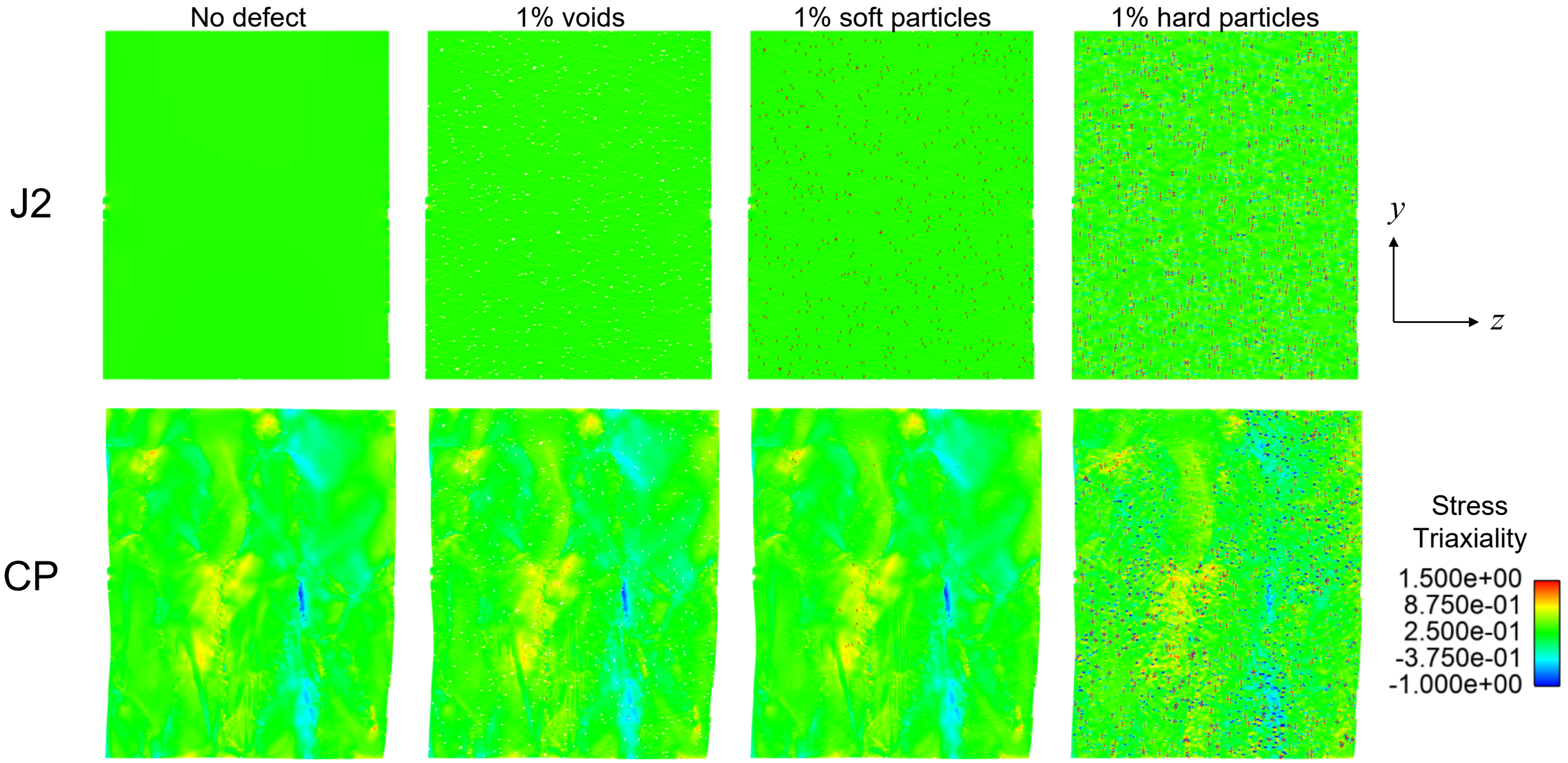


- Voids and soft particles have negligible effects
- Hard particles increase the strength
- CP is more sensitive to hard particles (see figures in the next slides) – hard particles increased stress fields in neighboring elements in CP.

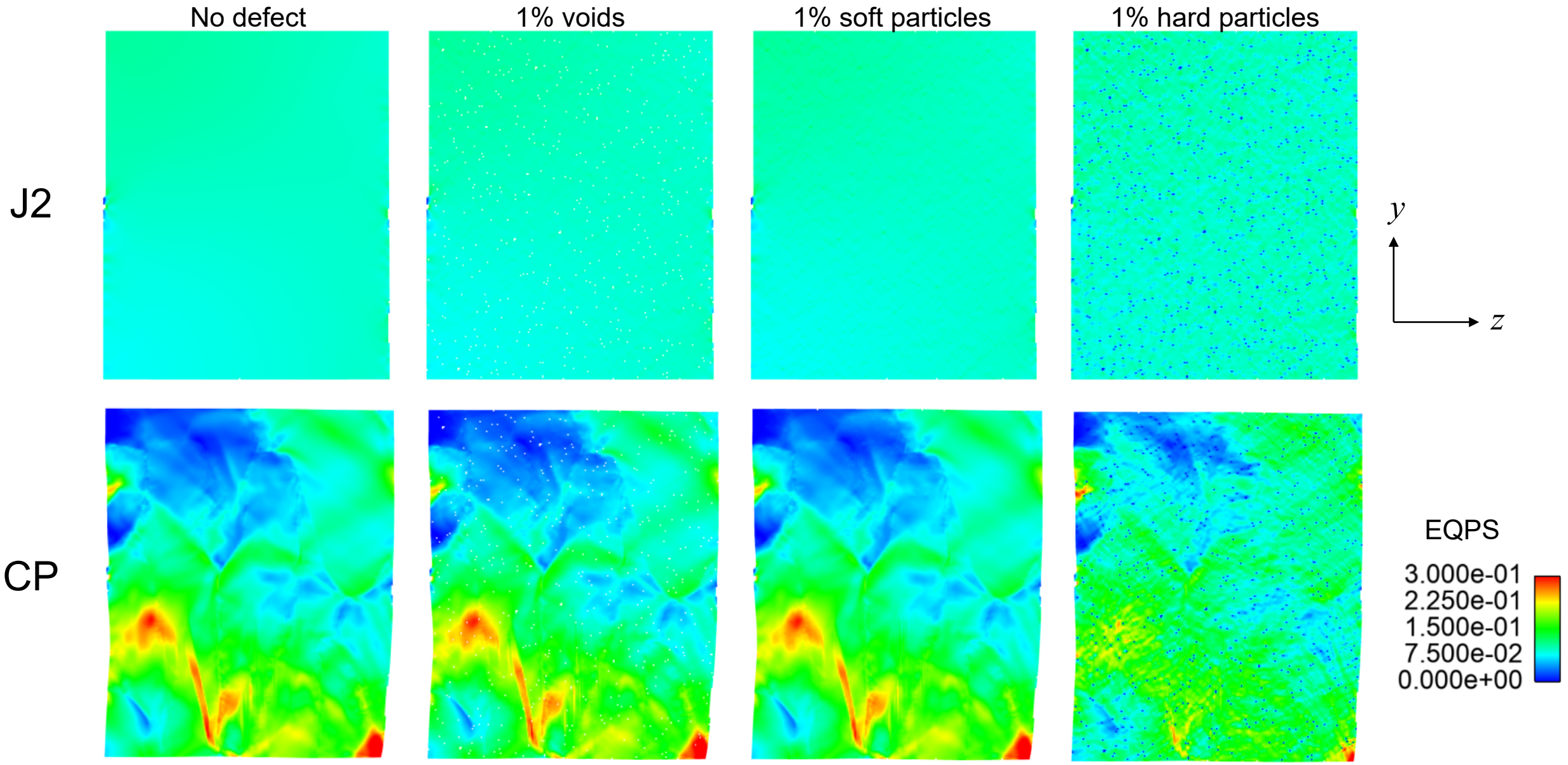
Von Mises stress after 10% deformation



Stress triaxiality after 10% deformation



EQPS after 10% deformation



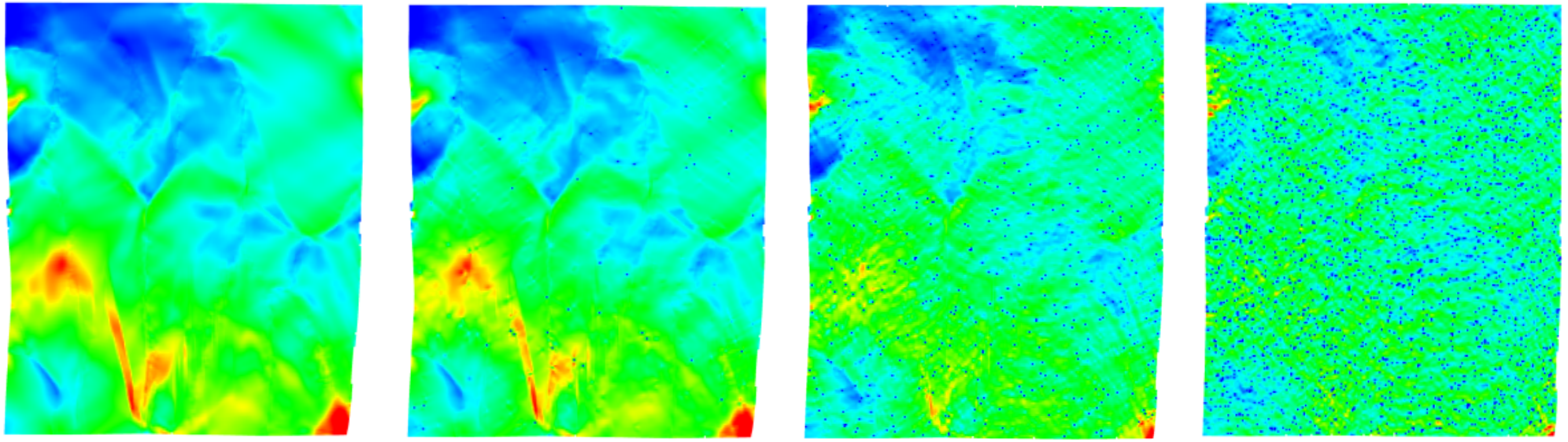
EQPS after 10% deformation: Effects of hard particles

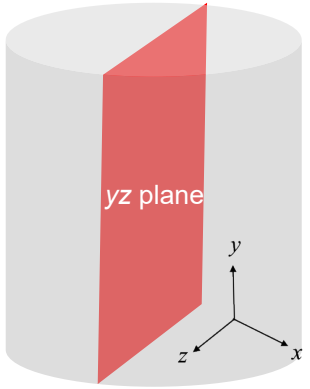
No defect (CP)

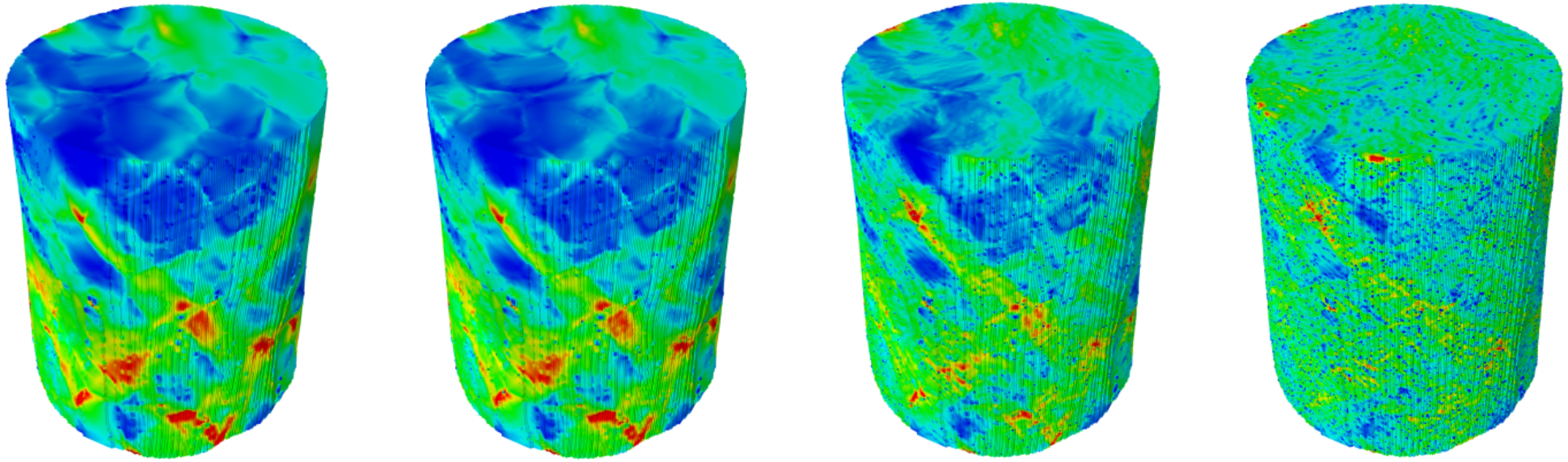
0.1% hard particles (CP)

1% hard particles (CP)

4% hard particles (CP)



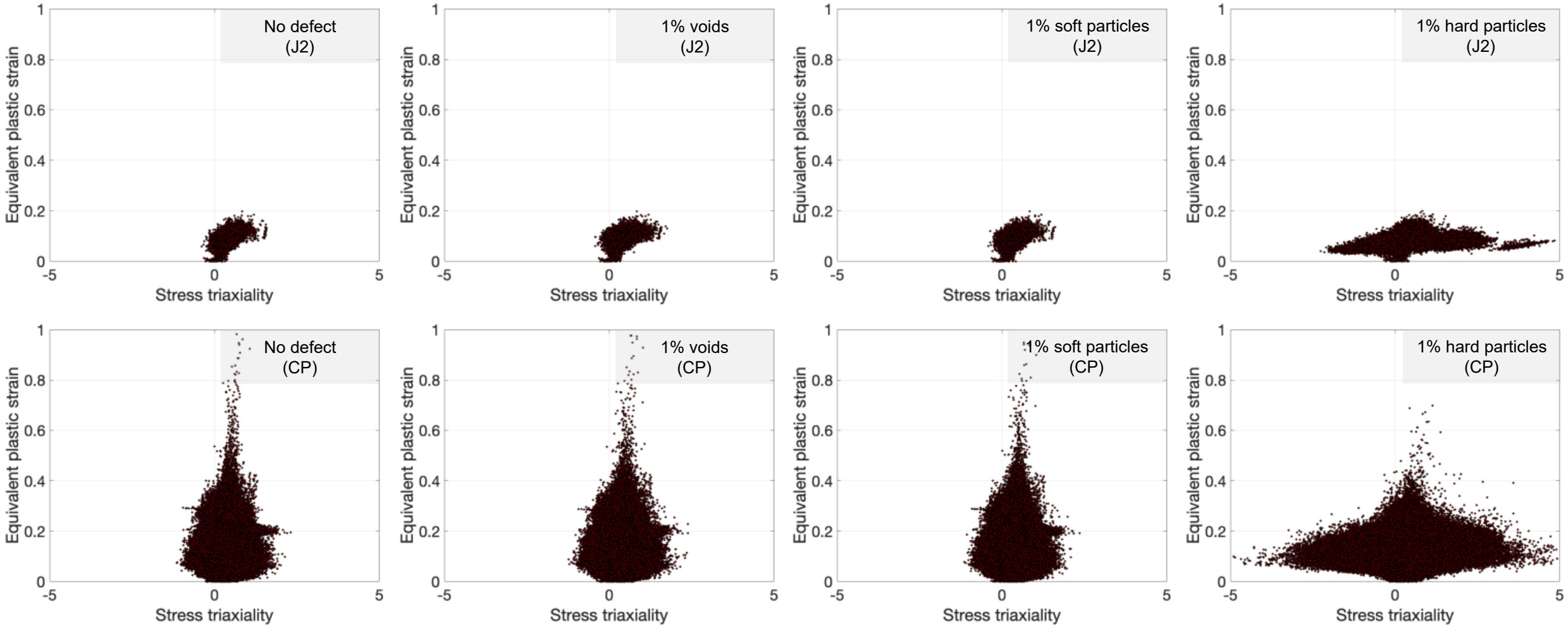




EQPS

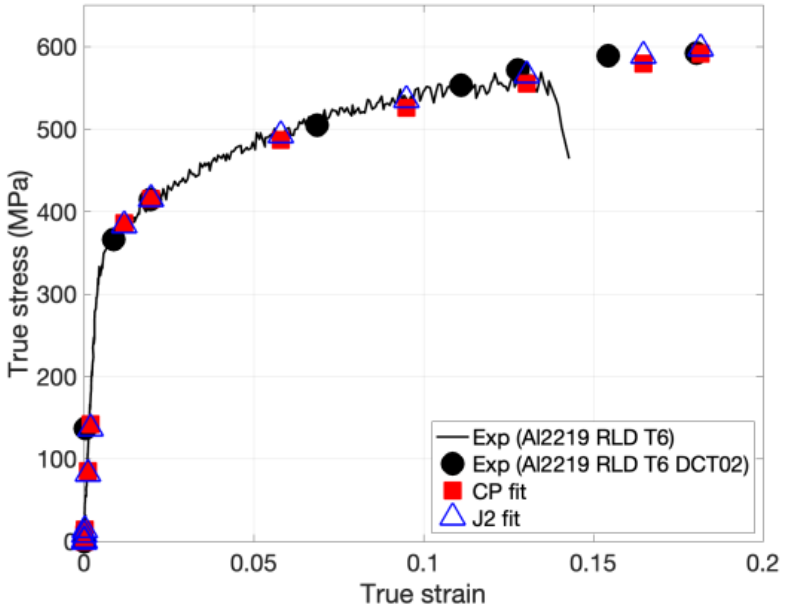
3.000e-01
2.250e-01
1.500e-01
7.500e-02
0.000e+00

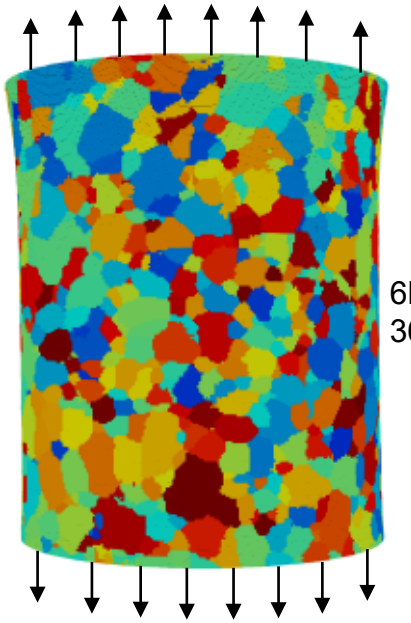
EQPS vs. stress triaxiality: All elements



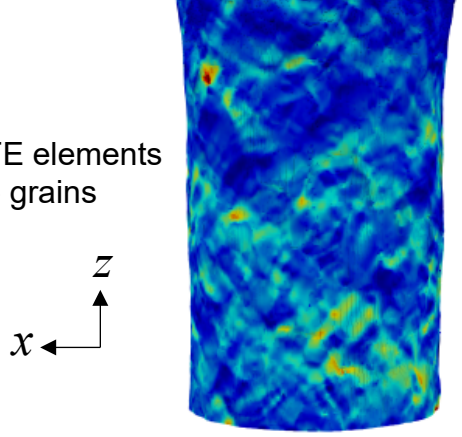
- Larger EQPS and stress triaxiality scatters in CP compared to J2 simulation.
- Voids and soft particles have small effects on local strain and stress triaxiality.
- Hard particles significantly increase scatter in stress triaxiality.

Local fields at 19% tension

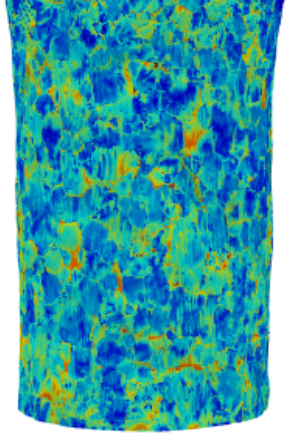




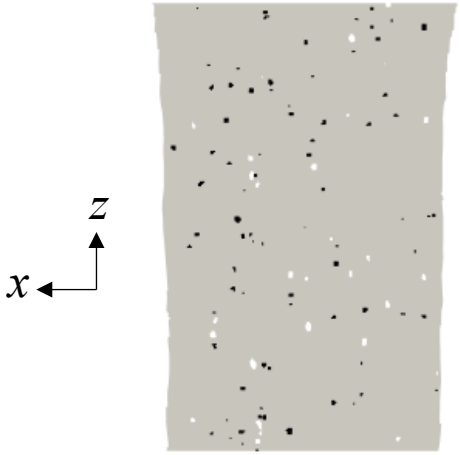
6M FE elements
3695 grains



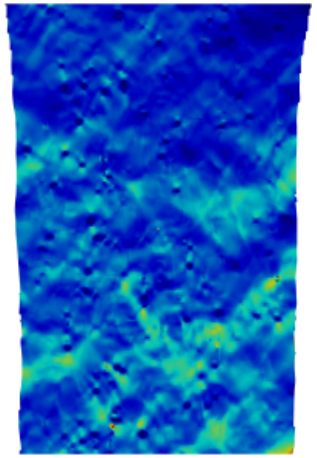
EQPS



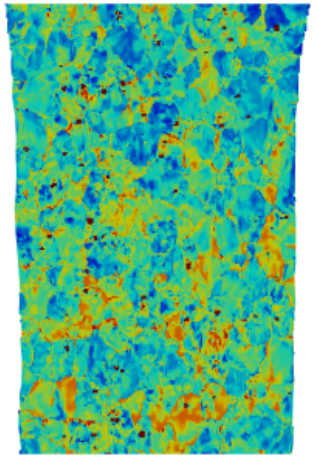
VM stress



Al
Fe precipitate
Void

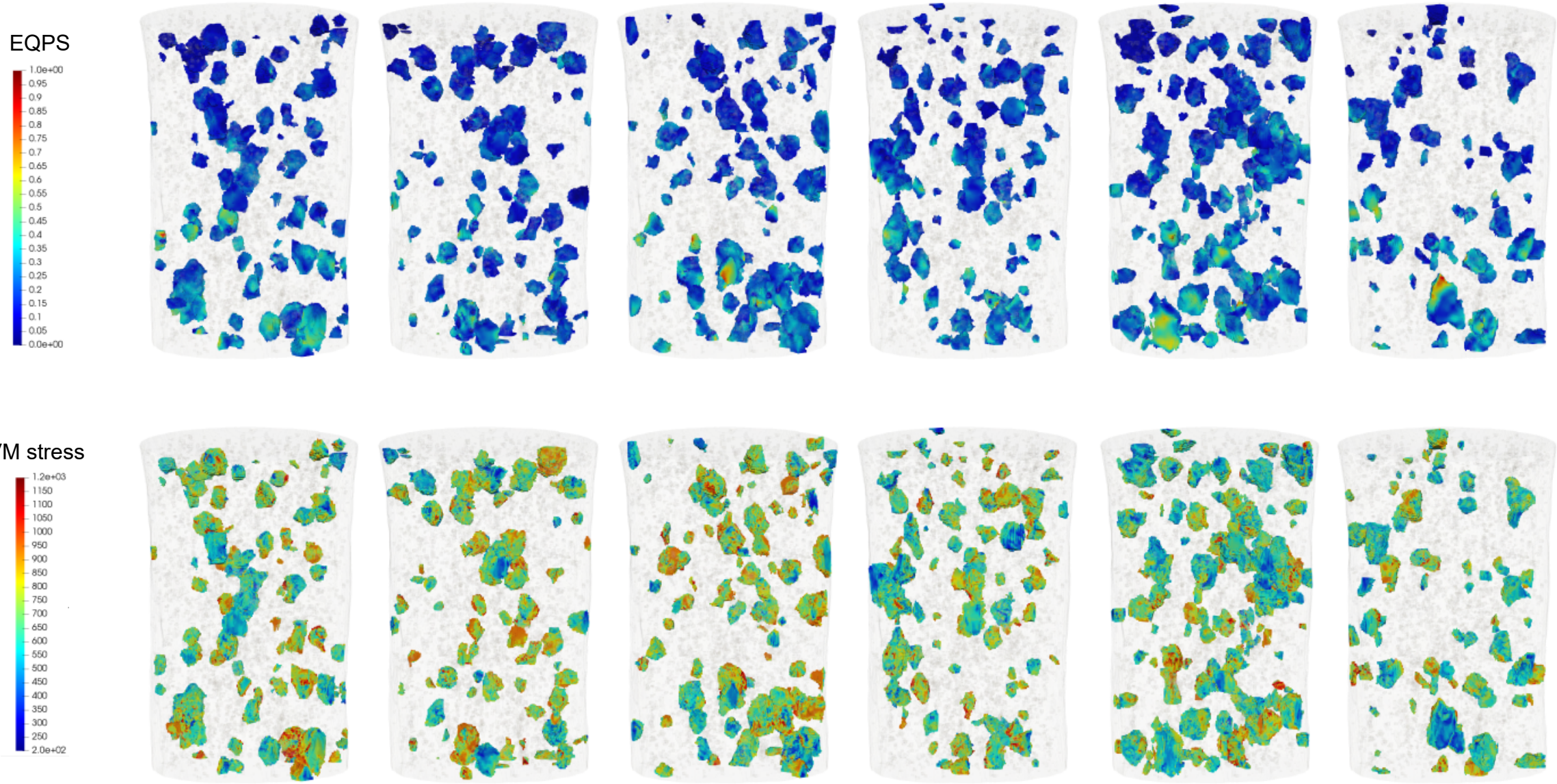


EQPS

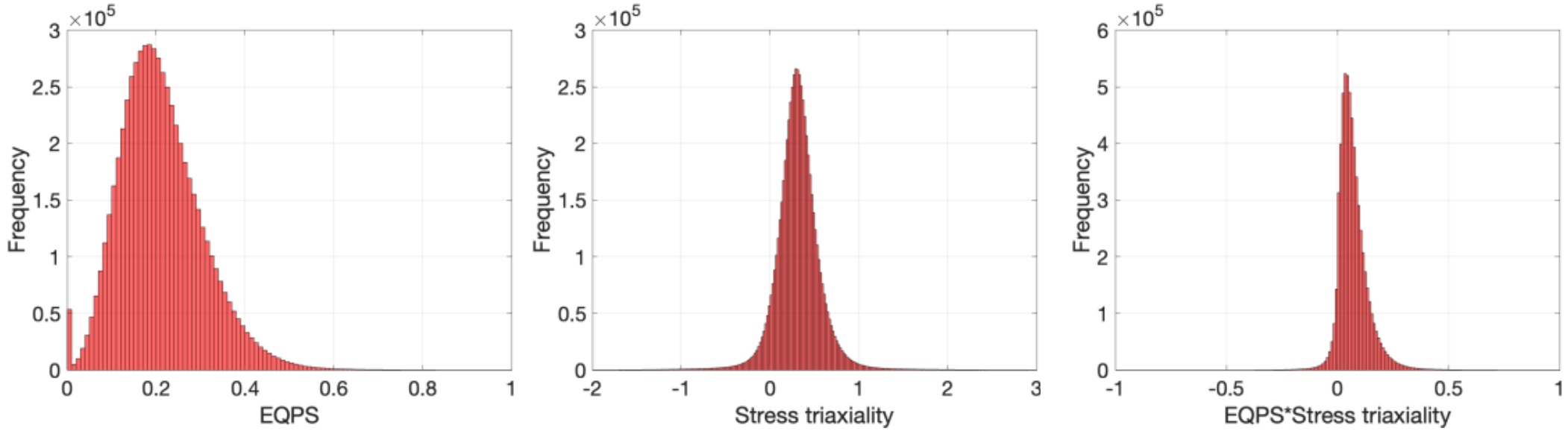


VM stress

Al2219 CP simulations: Local fields at 19% tension per grain



Distributions of local fields



Where do we see the hotspot?

- ✓ Surface vs. interior?
- ✓ Near the neck region?
- ✓ Big or small grains?
- ✓ Near voids?
- ✓ Near particles?
- ✓ Near grain boundaries?
- ✓ Near triple junctions?
- ✓ High or low max. Schmid factors?

Summary: Local fields from CP simulations at 19% deformation

	EQPS	stress triaxiality	stress triaxiality * EQPS
All domain	**0.211±0.093**	**0.314 ±0.283**	**0.070±0.070**
Center (within 25μm)	0.212±0.082	0.310±0.287	0.069±0.071
Surface (within 25μm)	0.095±0.046	0.283±0.184	0.028±0.025
Neck (within 25μm)	0.267±0.114	0.292±0.297	0.085±0.100
Big grains (10 biggest)	0.212±0.088	0.318±0.266	0.071±0.068
Small grains (10 smallest)	0.171±0.076	0.302±0.164	0.051±0.044
Near voids (next to voids)	0.226±0.114	0.322±0.315	0.082±0.108
Near particles (next to particles)	0.112±0.082	0.280±0.831	0.047±0.150
Near GB (next to GB)	0.208±0.089	0.310±0.267	0.068±0.068
Near TJ (next to TJ)	0.206±0.087	0.305±0.264	0.066±0.067
High Schmid factors (>0.499)	0.236±0.085	0.348±0.335	0.084±0.082
Low Schmid factors (<0.330)	0.141±0.071	0.268±0.166	0.039±0.034

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.
  - **Microstructural features influence both macroscopic behavior and local fields.**

- **Investigated factors that may influence the local fields**
  - Elements near voids and the neck region had **increased** EQPS and stress triaxiality.

THANK YOU !

Advanced Simulation & Computing (ASC)

Materials Margins Assurance

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