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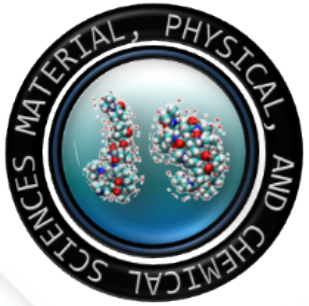

Crystal Plasticity Modeling of Microstructural Clones

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Sandia National Laboratories

March 5, 2024

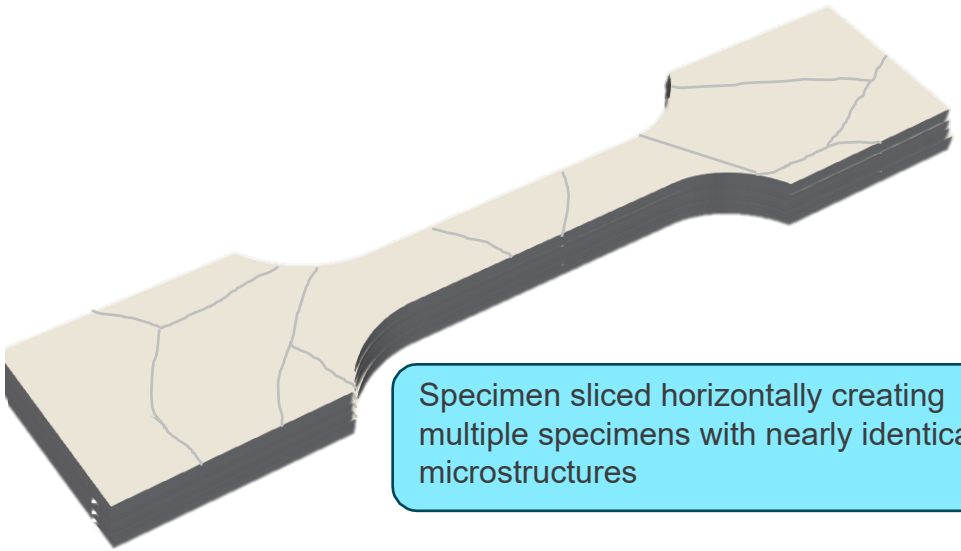
SAND2024-XXXXXX

Unclassified Unlimited Release

What are Microstructural Clones?

Multiple specimens in a set with nearly identical microstructures

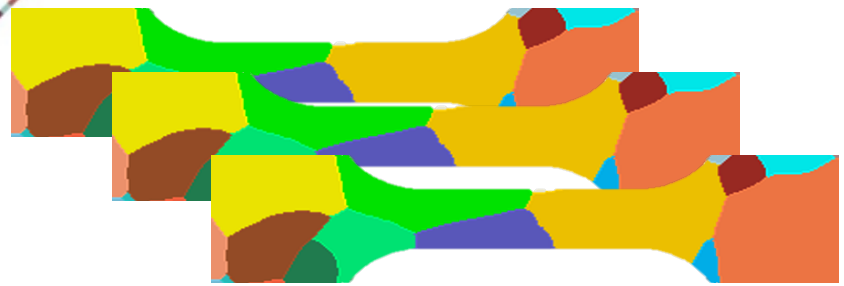
- 99.999% Nickel 0.25 in thick plate
- Heat treated to grow grains 10-20 mm in diameter
- Tensile specimens cut from locations with similar microstructure front and back

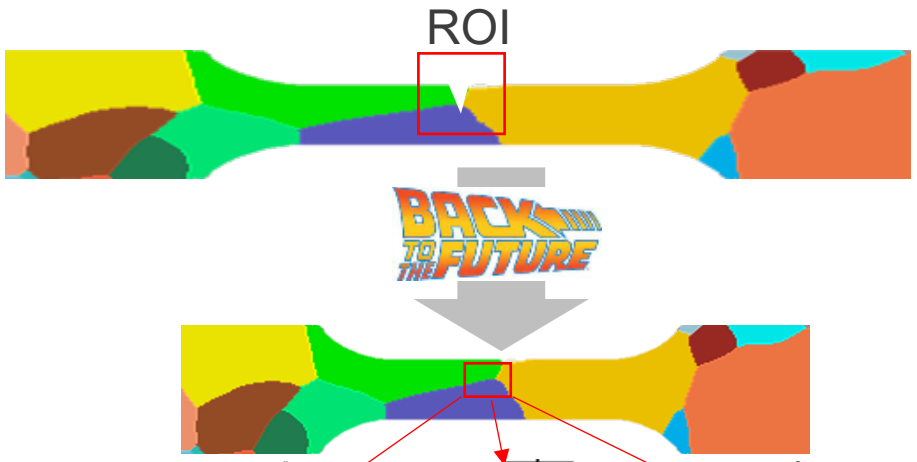


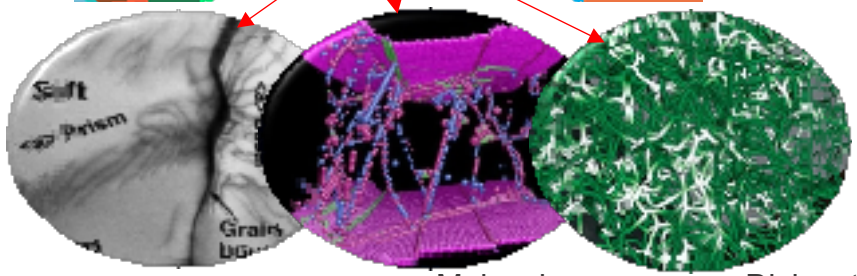
How to define microstructure clones? Some ideas:

1. **Same grain boundary locations within ~30 μm.**
2. **Same grain orientations within ~2°.**
3. **Same dislocation densities within a factor of 2.**

What can we do with Clones?



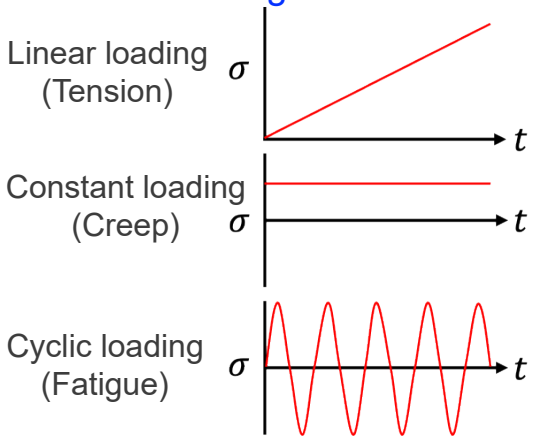




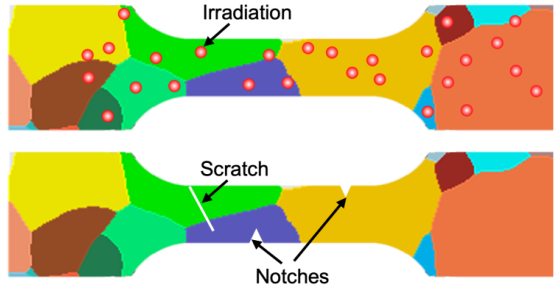
TEM | Molecular dynamics | Dislocation dynamics

- Will a unique microstructure always behave the same?
  - Stochasticity & Uncertainty quantification
- Perform multiple (destructive) experiments
  - Consistency of test setup

Different loading conditions

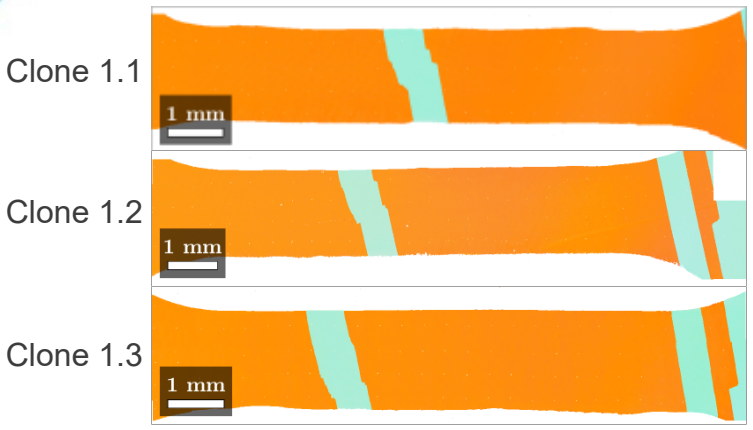


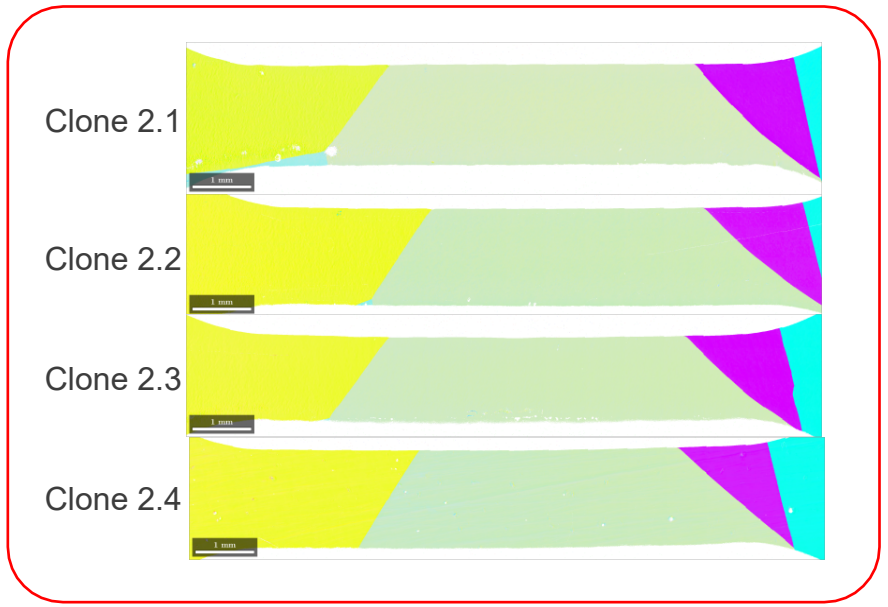
Microstructural/geometrical defects

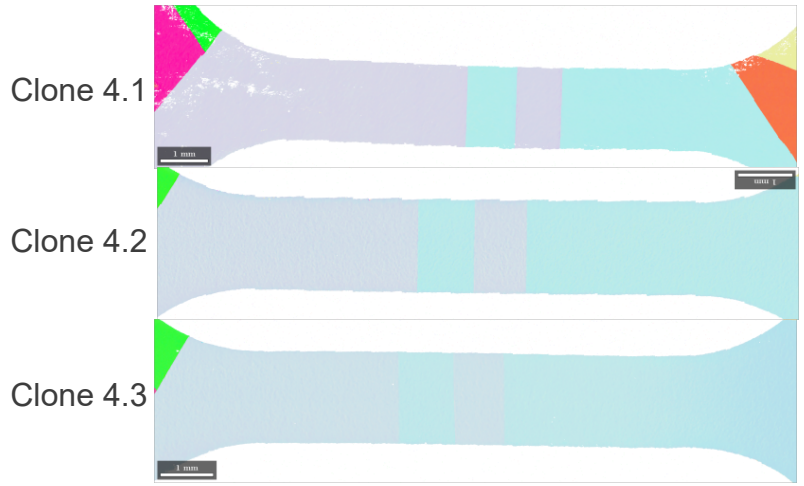


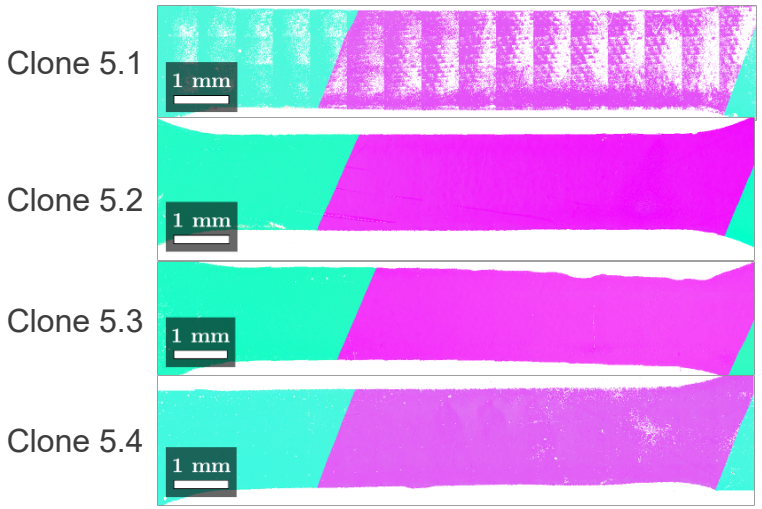
- How do you know where to look for high resolution exp./sim?
  - High resolution measurements often require you to know where to look ahead of time
  - Computational modeling can help predict location, but are not always correct
  - Identical microstructures can help “see the future” on where and how a specimen will deform

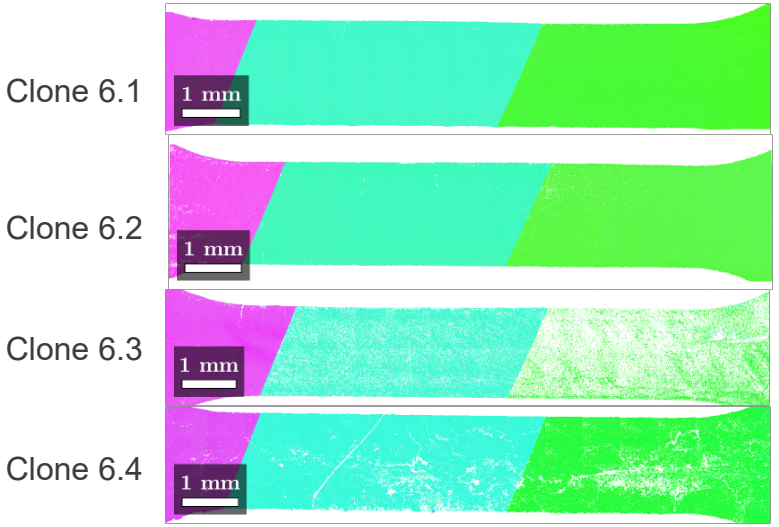
Family of Ni Clones

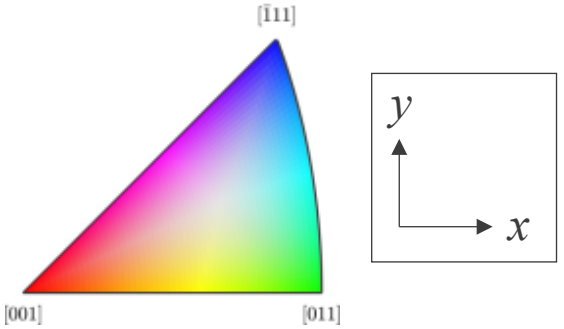










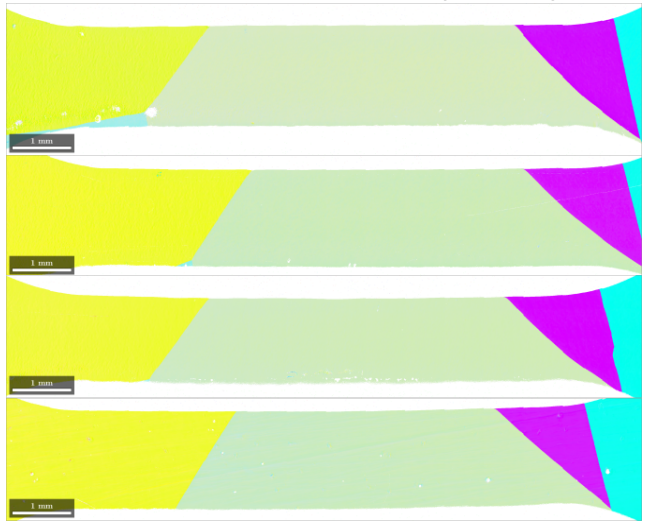


+ many more single & multi-crystal clone families

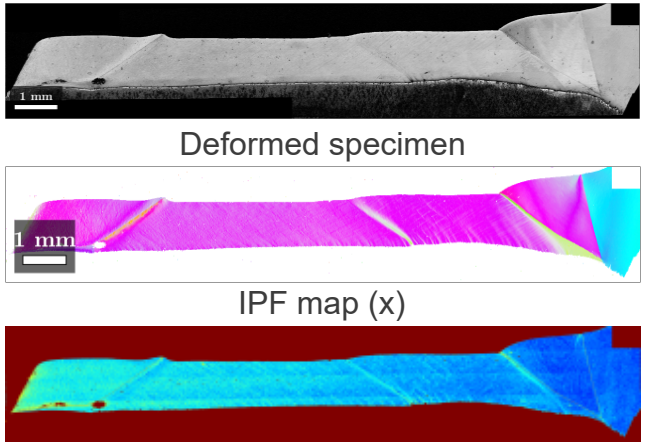
Kaitlynn Fitzgerald et al., ”Microstructure Clones”, 5:40PM

Clone 2.x - Experiments

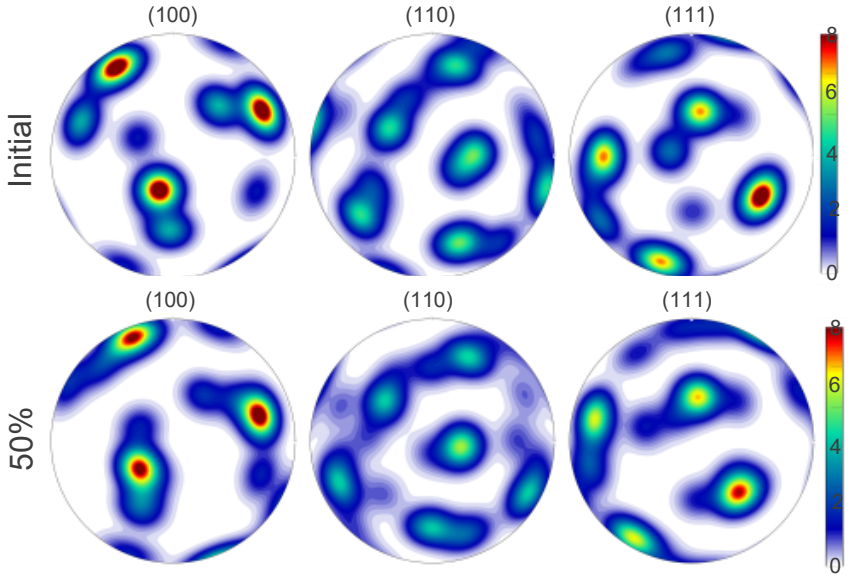
Initial microstructures (EBSD)



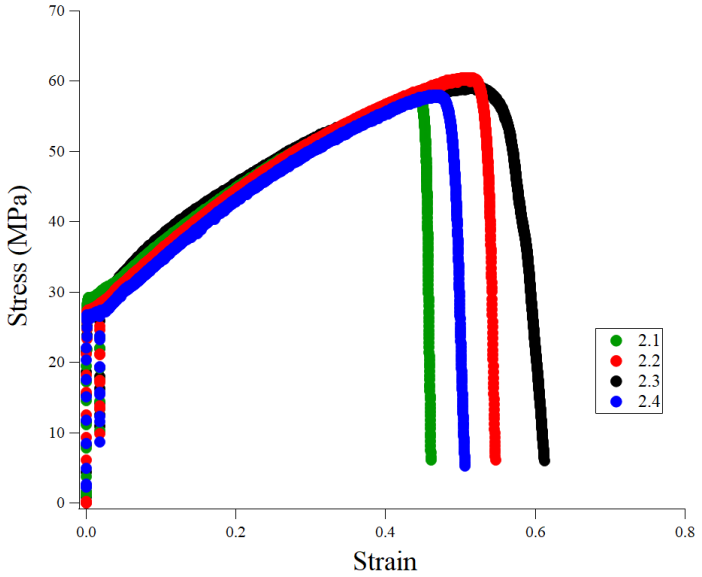
Deformed microstructures (EBSD, Clone 2.1)



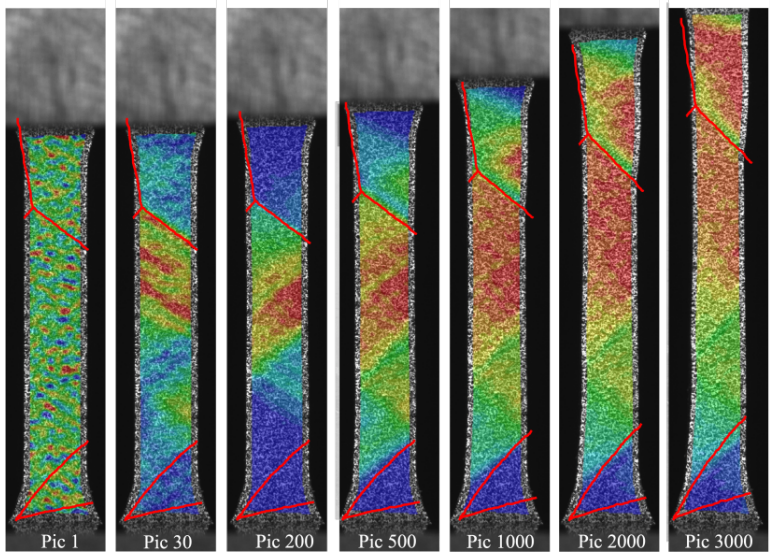
Texture (EBSD, Clone 2.1)



Uniaxial tension tests



In-situ surface strain fields (DIC, Clone 2.1)



Failed specimens (optical)

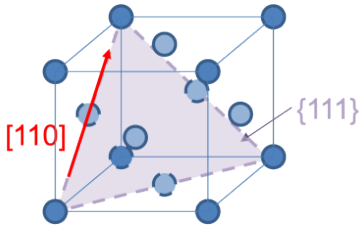
Crystal Plasticity FE simulations

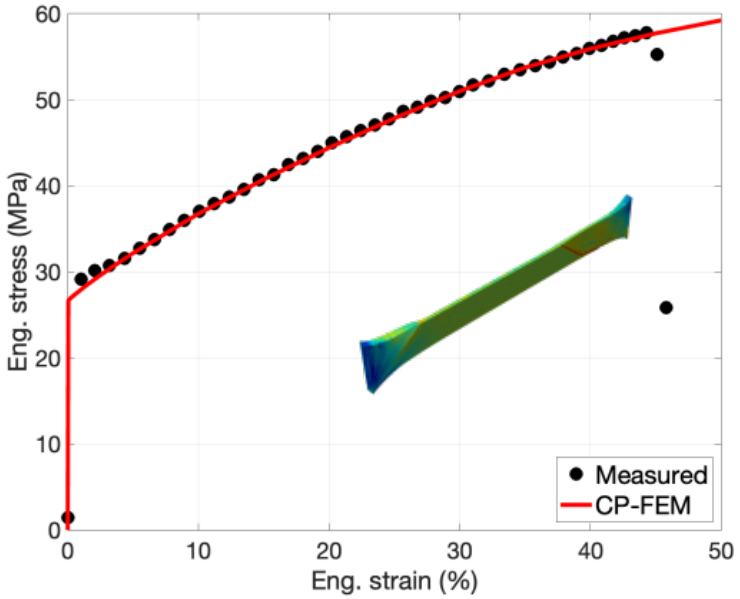
- *Slip rate:* $\dot{\gamma}^{\alpha} = \dot{\gamma}^{0}\left(\frac{\tau^{\alpha}}{g^{\alpha}}\right)^{1/m}$
- *Slip resistance:* $g^{\alpha} = g_0 + A\mu b\sqrt{\sum_{\beta=1}^{12} H^{\alpha\beta}\rho^{\beta}}$
- *Dislocation evolution:*

$$d\rho^{\alpha} = \left(\kappa_1\sqrt{\sum_{\beta=1}^{12}\rho^{\beta}} - \kappa_2\rho^{\alpha}\right)|d\gamma|$$

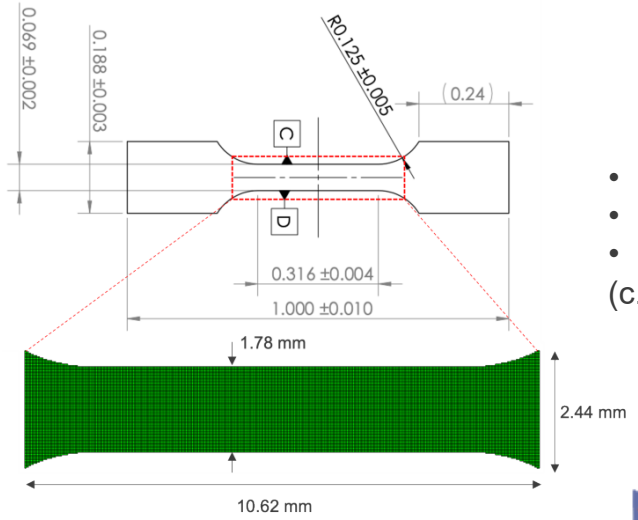
- *Hardening matrix:* $H^{\alpha\beta} = \mathbf{n}^{\alpha}\cdot\xi^{\beta}$
- *12 {111}<110> slip systems for FCC*

Face Centered Cubic structure





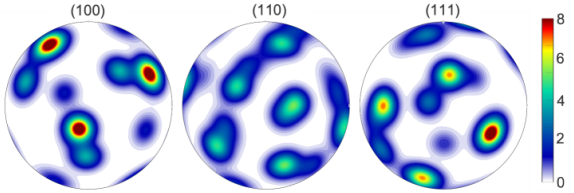
Property	Value
C_{11}	108.2 GPa
C_{12}	61.3 GPa
C_{44}	28.5 GPa
μ	25.7 GPa
$\dot{\gamma}_0$	10^{-5} s^{-1}
m	0.012
A	0.4
b	2.86×10^{-10} m
ρ_0	2.6×10^{13} m^{-2}



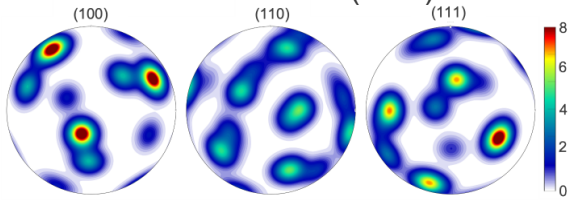
- FE mesh with 8-node hexahedron element
- Total of ~ 620k FE elements
- FE size~25um

(c.f. EBSD size ~4um, DIC size ~50um)

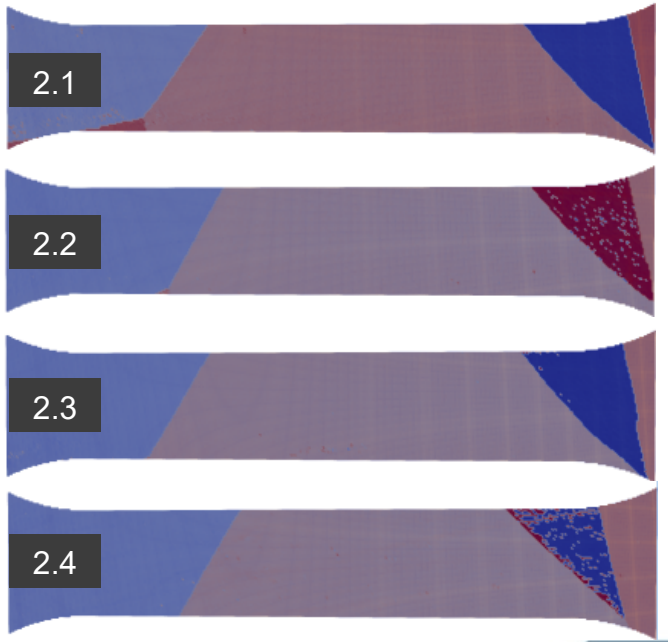
Initial texture (EBSD)



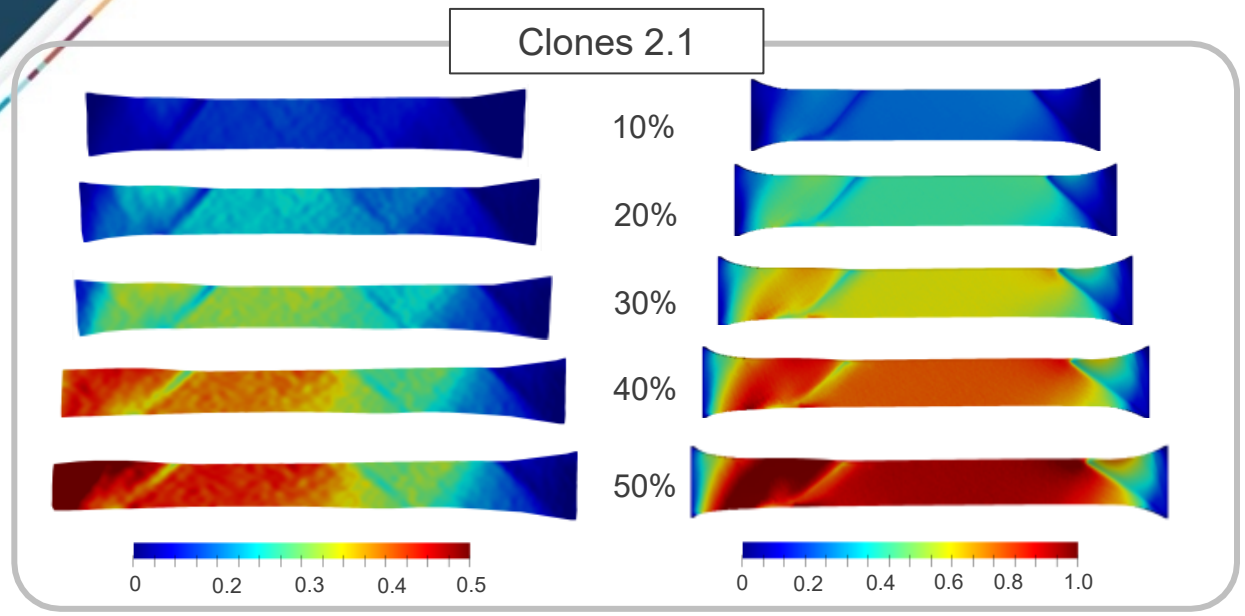
Initial texture (Sim.)

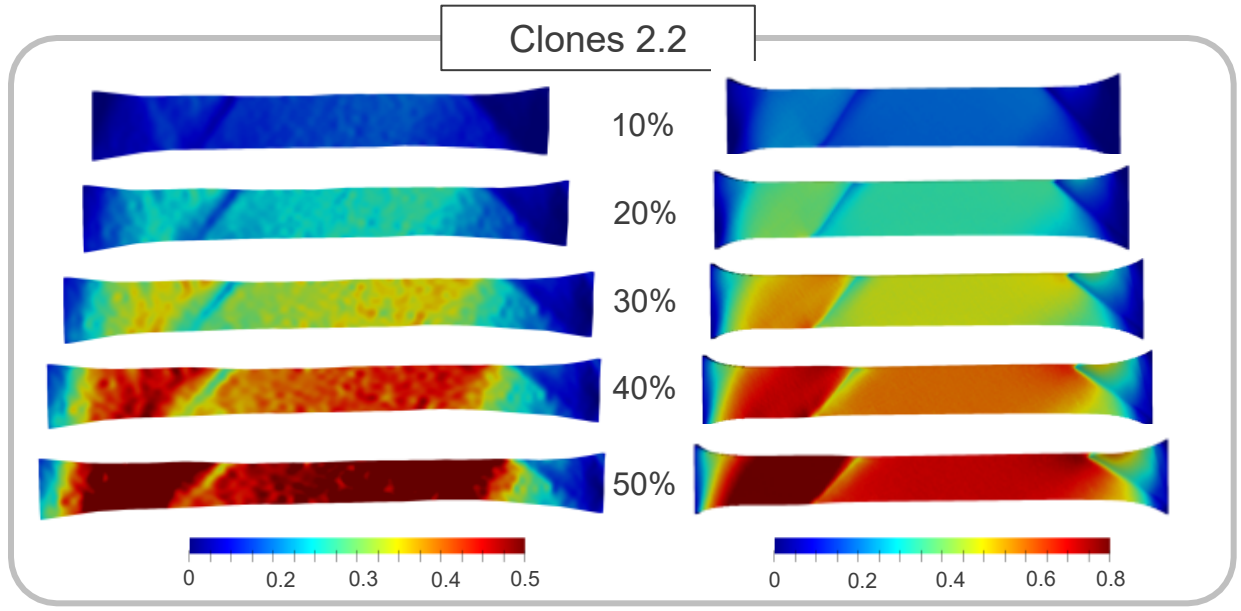


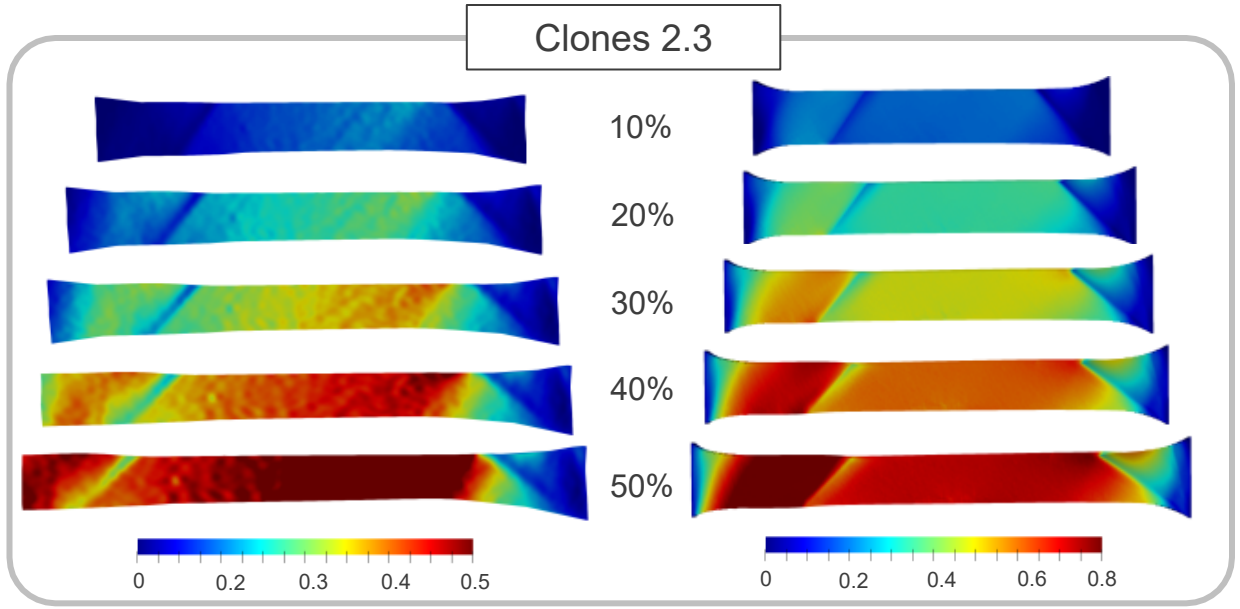
FE meshes

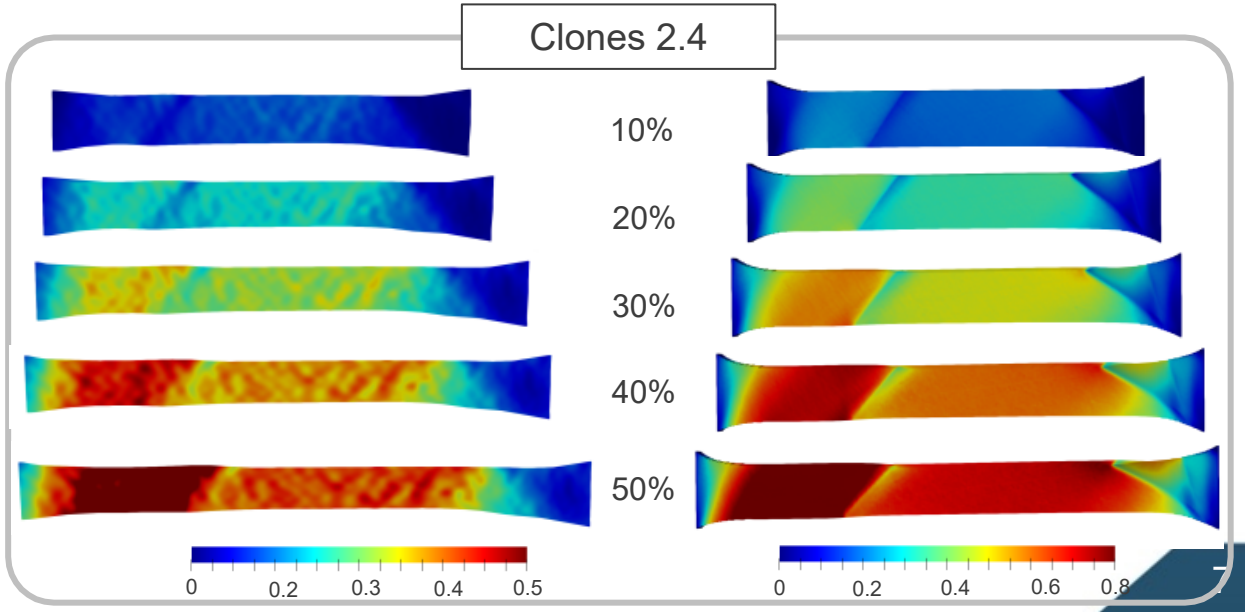


Surface strain field comparisons





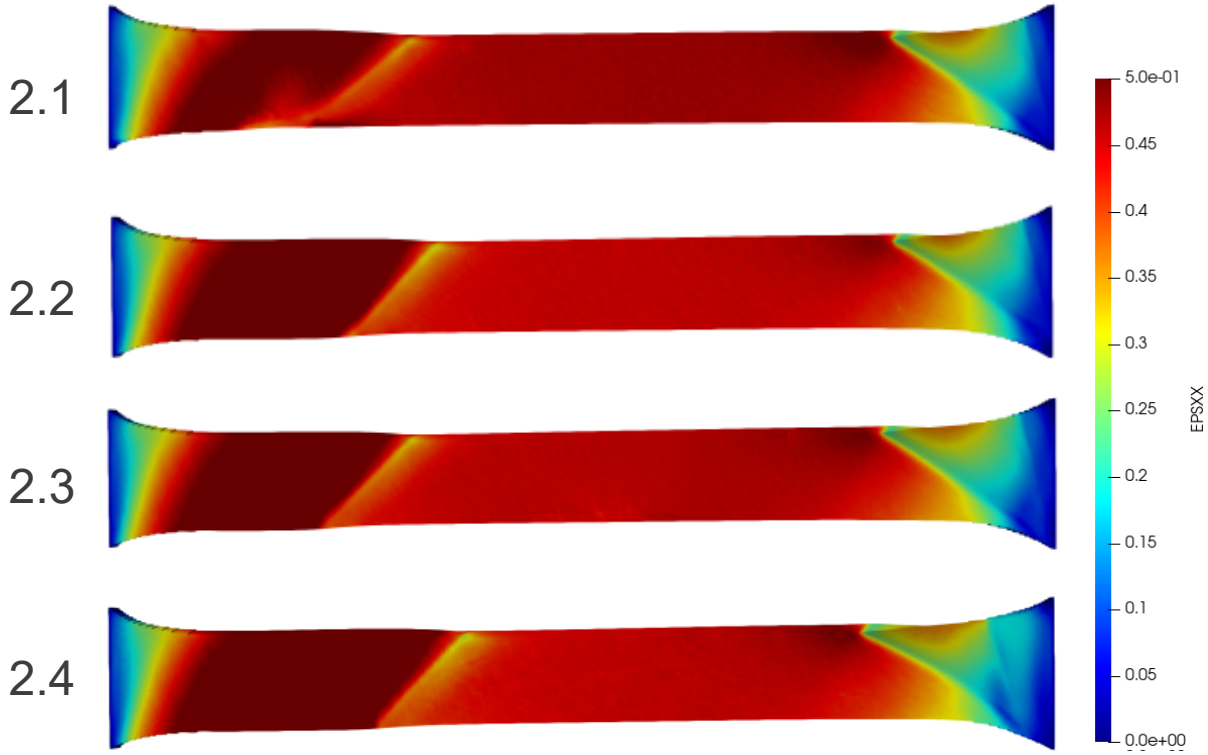




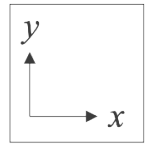
Failure locations and CP predictions

Optical

CP simulations (50% deformation)



- Surface strain predictions from CP simulations are very similar between Clones2.1 – 2.4.
- Current CP models do not incorporate damage.
- Different failure locations seem to be caused by difference in thicknesses.

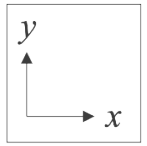


Kaitlynn Fitzgerald et al., ”Microstructure Clones”, 5:40PM

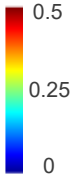
Front vs. back surfaces: CP predictions at 50% strain

DIC side (front)

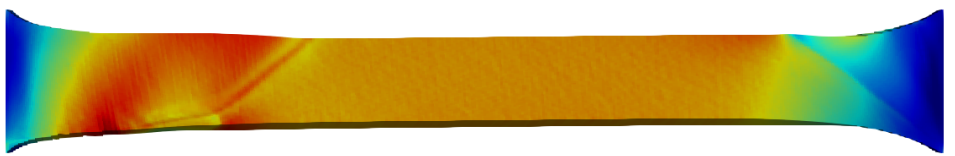
EBSD/Optical side (back)

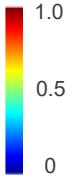


ϵ_{xx}

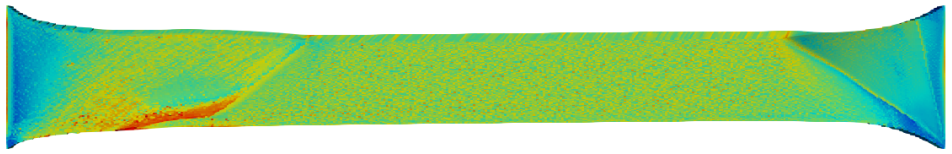


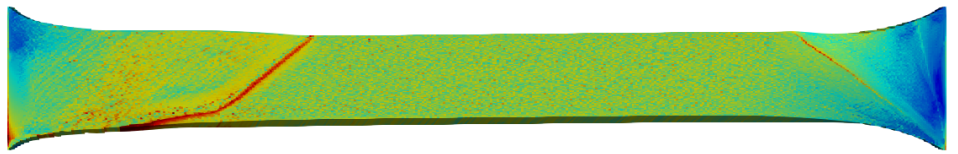
EQPS

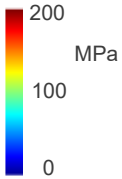




Damage stress







Damage stress: $\sigma^* = \sigma_{mises}\left[\frac{2}{3}(1+\nu)+3(1-2\nu)\eta^2\right]^{\frac{1}{2}}\Big|_{\eta\geq-\frac{1}{3}}$

σ_{mises}: Von Mises stress

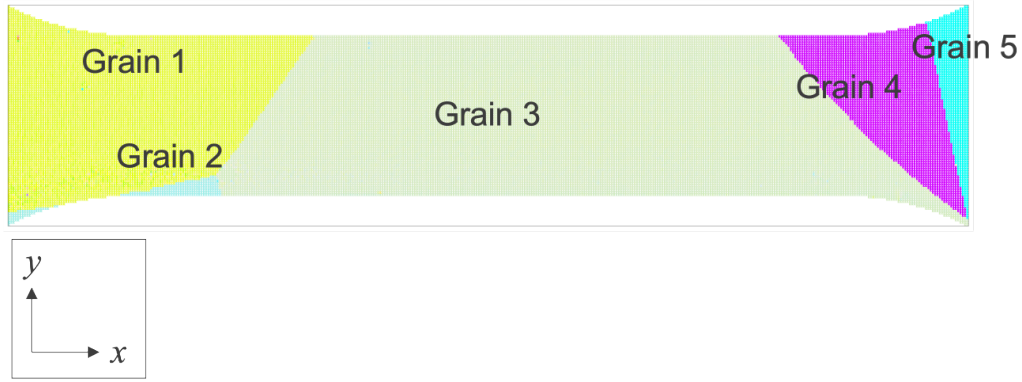
ν: Poisson's ra

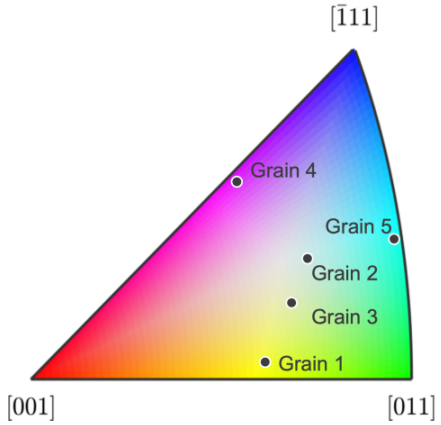
η: Stress triax

J. Lemaitre, Nuc. Eng. Des. (1984)

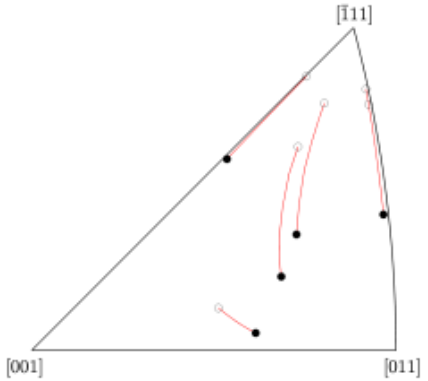
P.O. Bouchard et al., Int. J. Mater. Form. (2011)

Crystal rotation / texture evolution

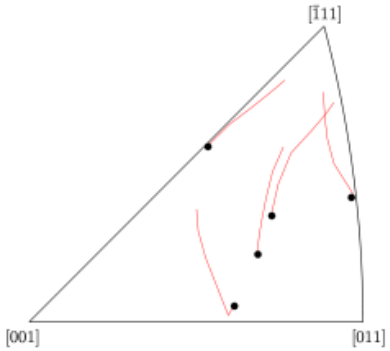




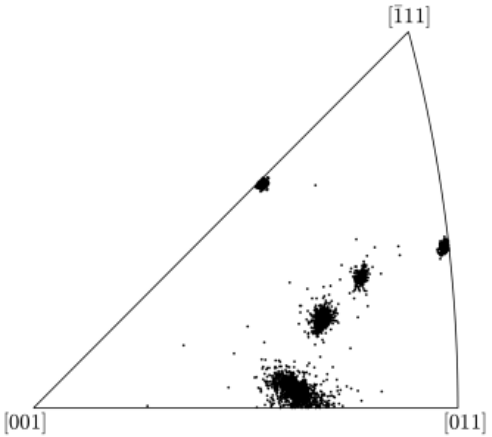
Isochoric deformation



Uniaxial deformation



CP predictions of crystallographic texture



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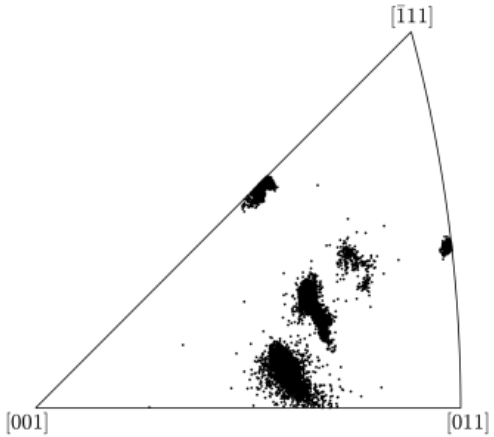
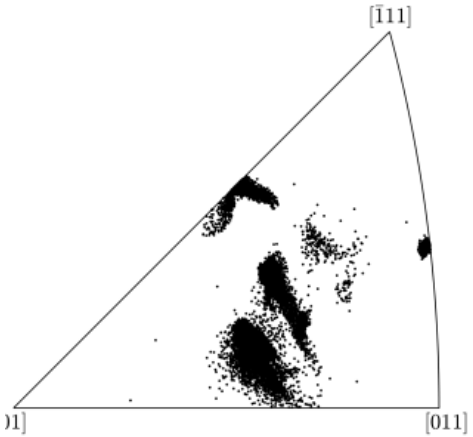
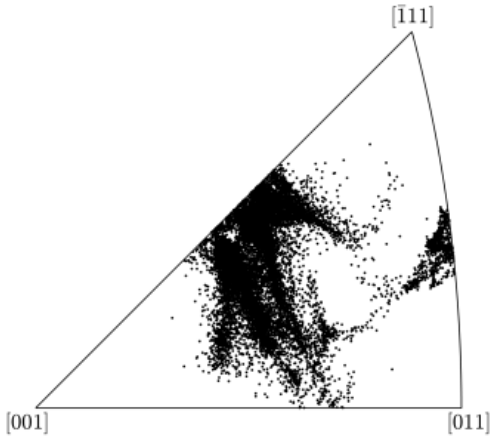


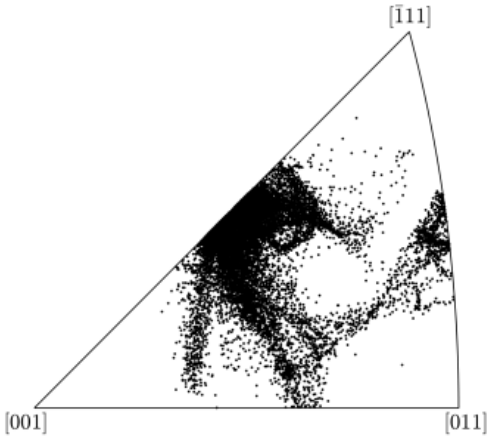
5%



10%



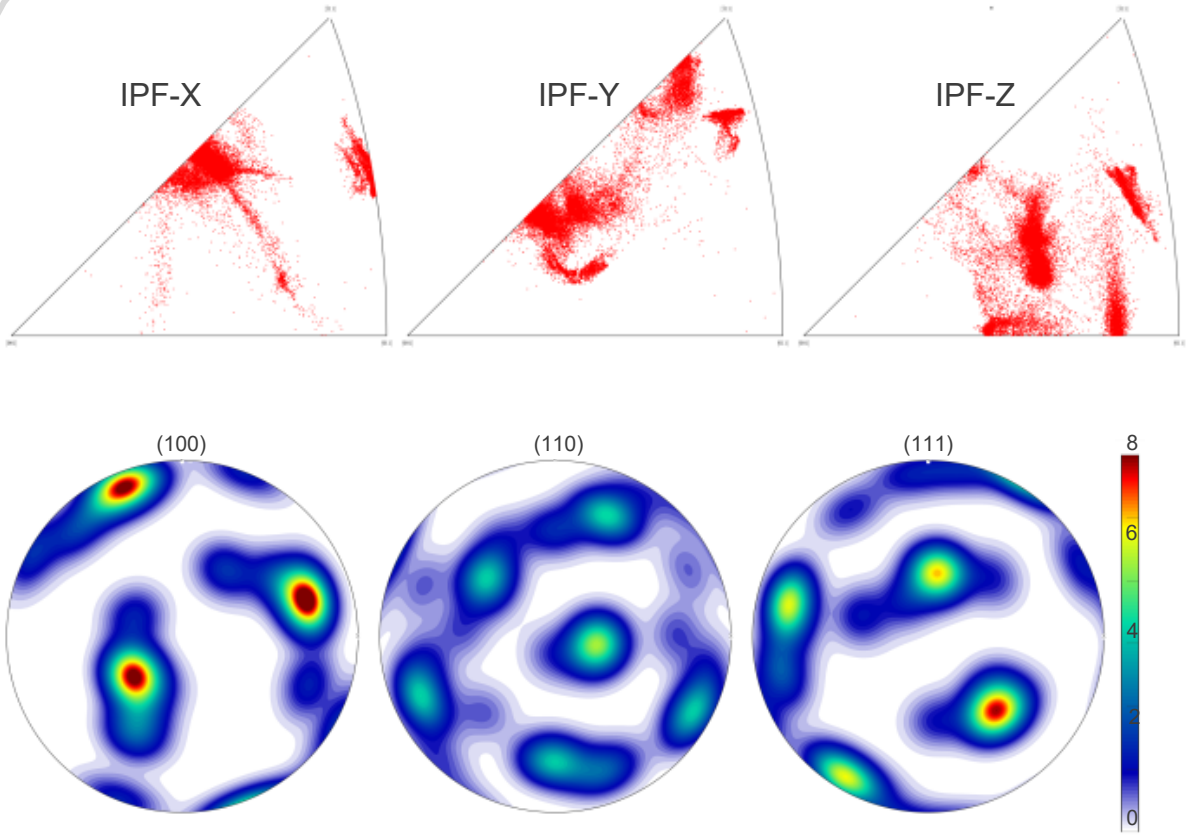
30%



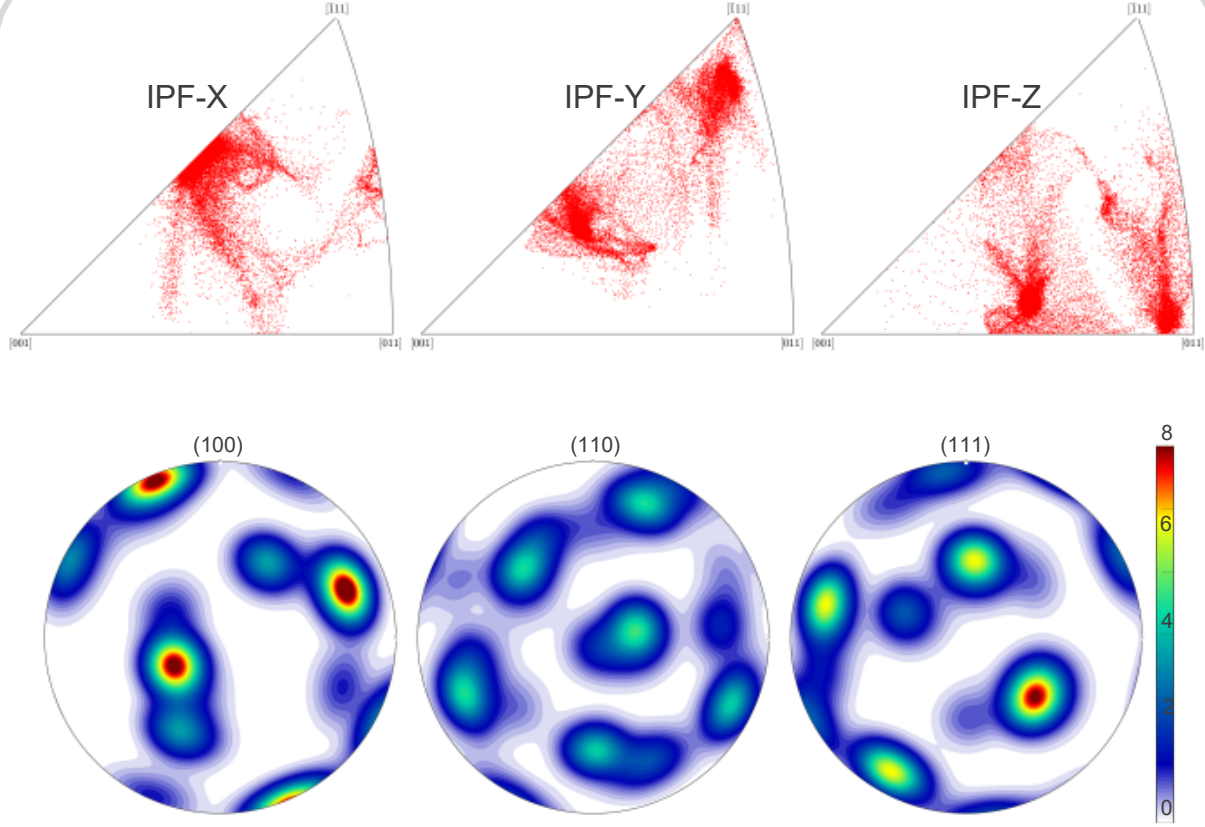
50%

Comparisons with experiments (50% deformation)

EBSD



CP-FEM predictions

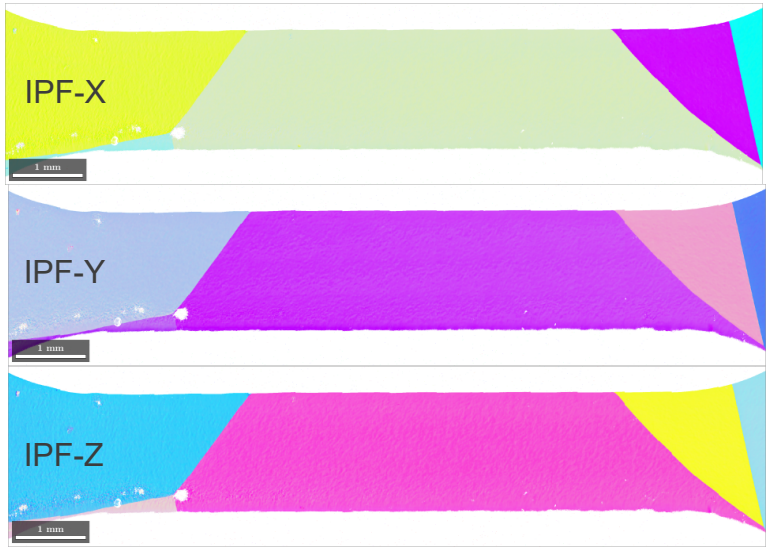


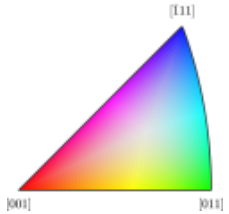
Texture predictions

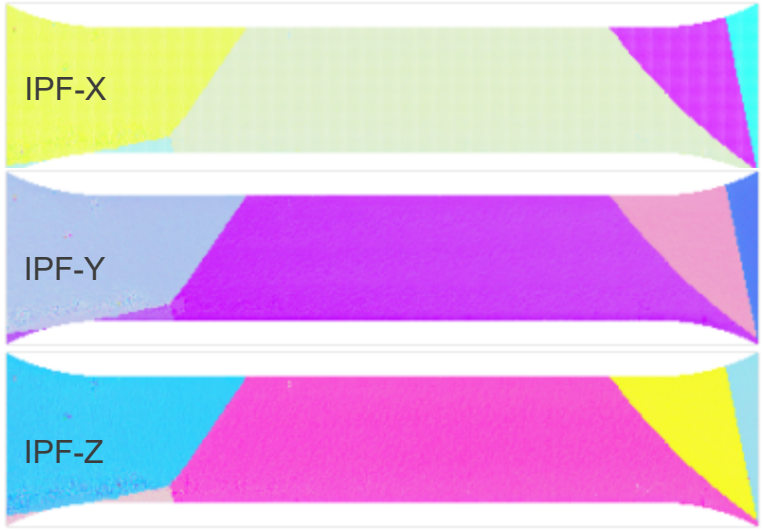
EBSD

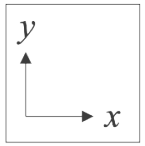
CP-FEM

Initial

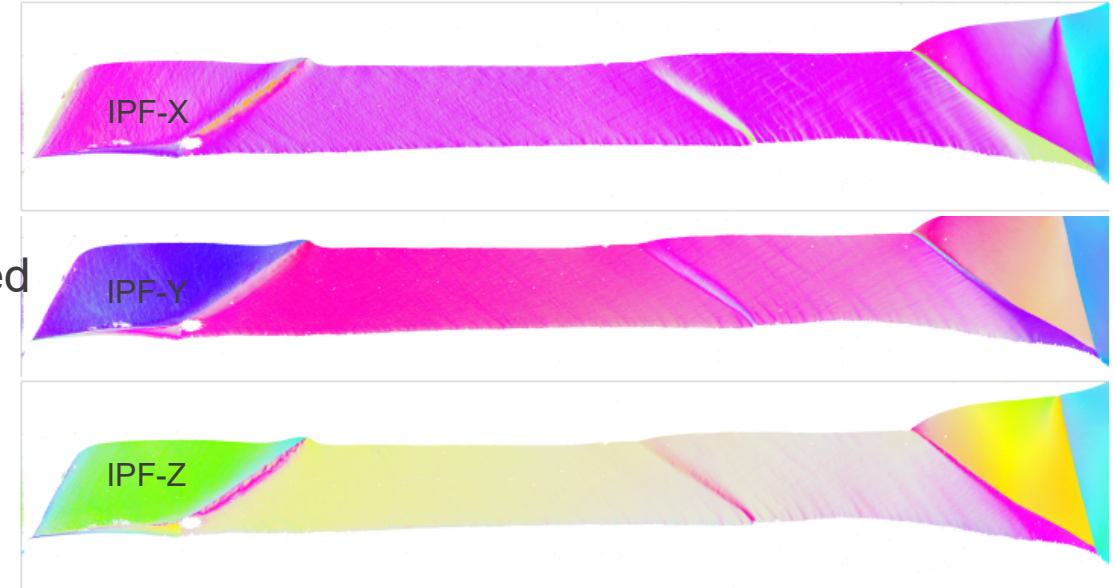


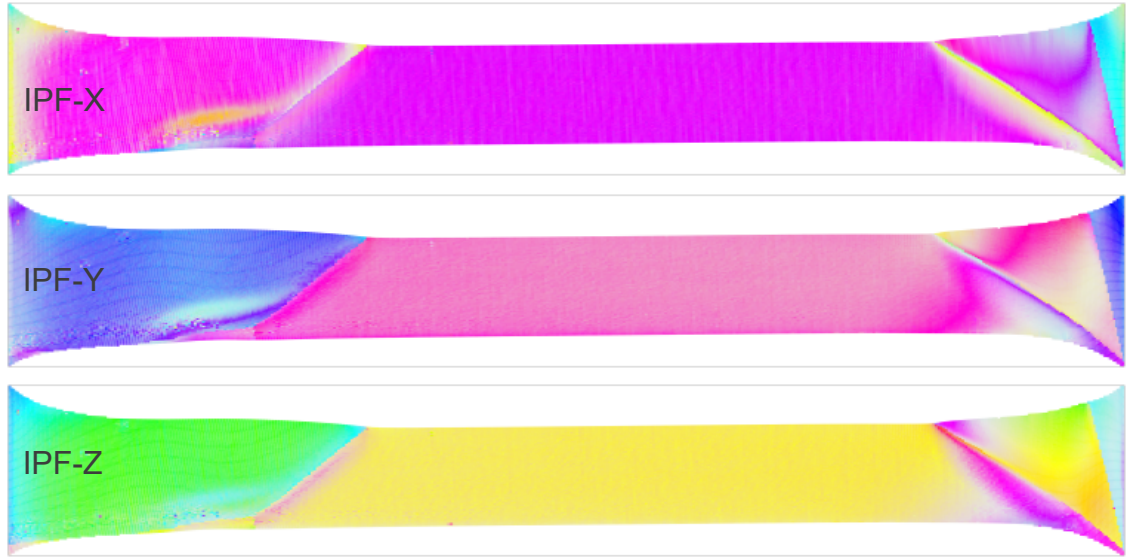




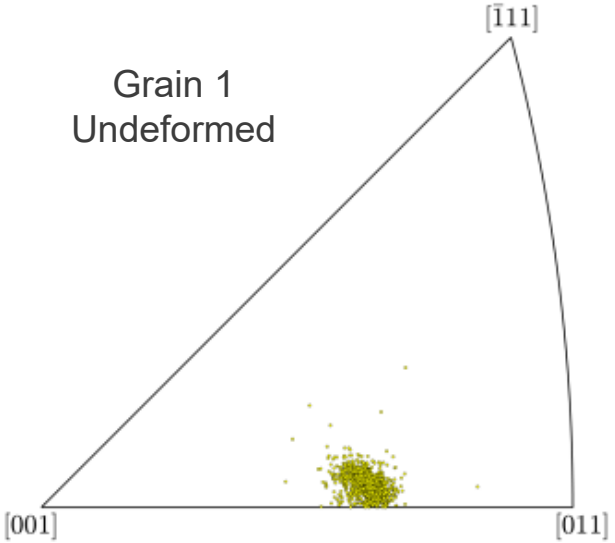


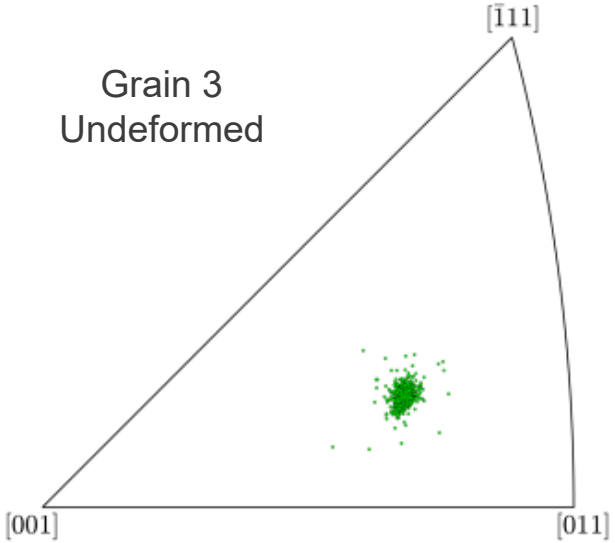
Deformed

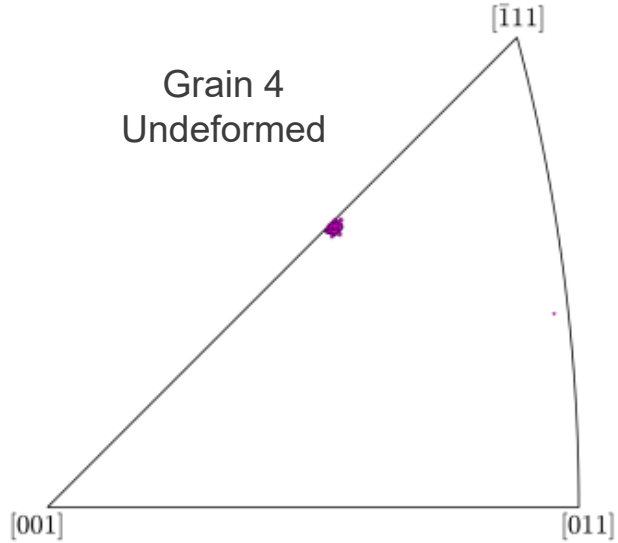


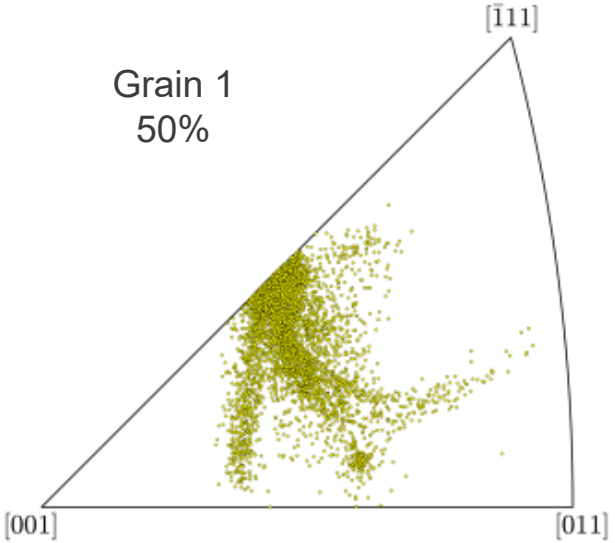


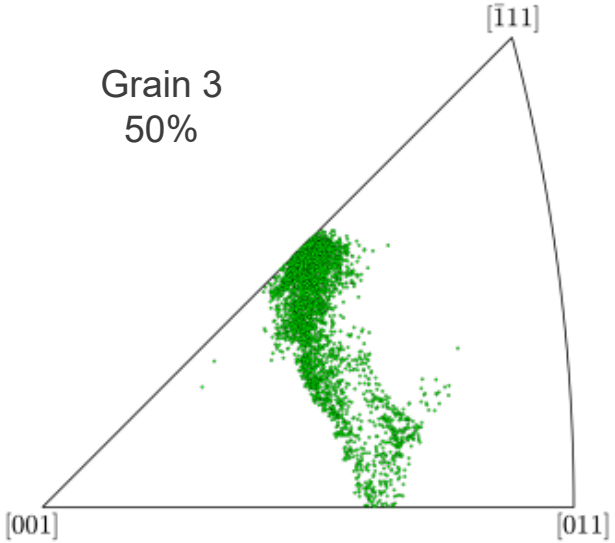
Crystal rotations – per grain analysis

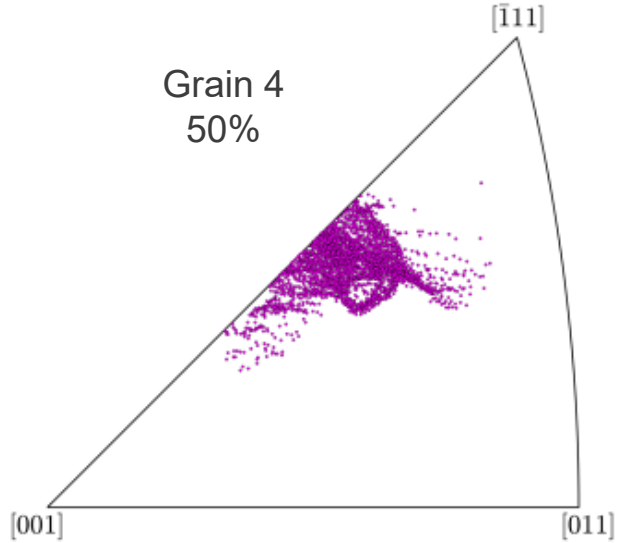




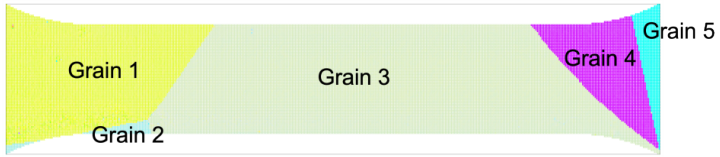


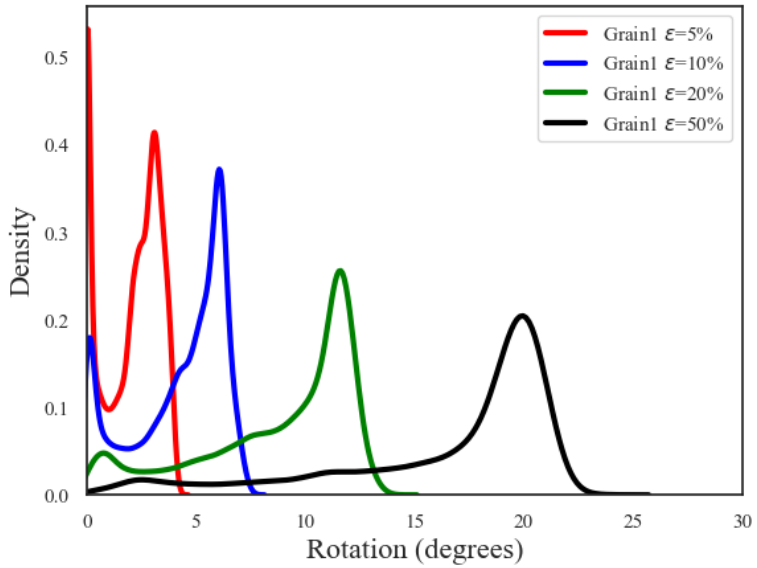


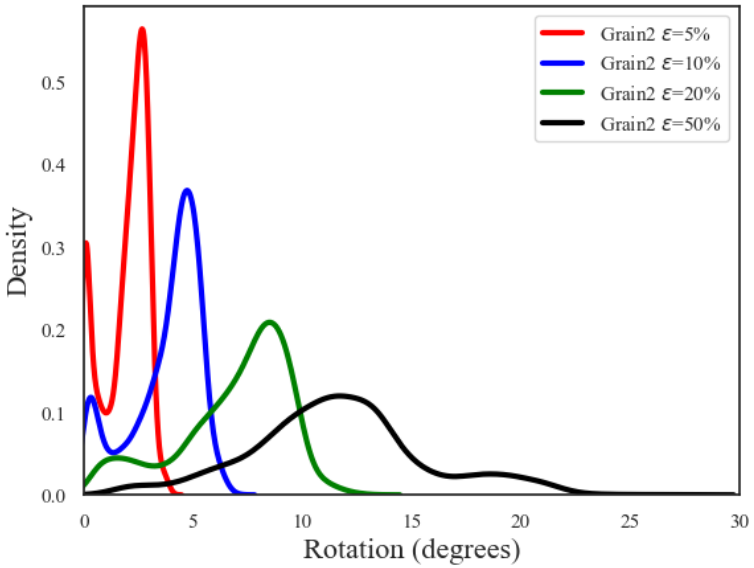


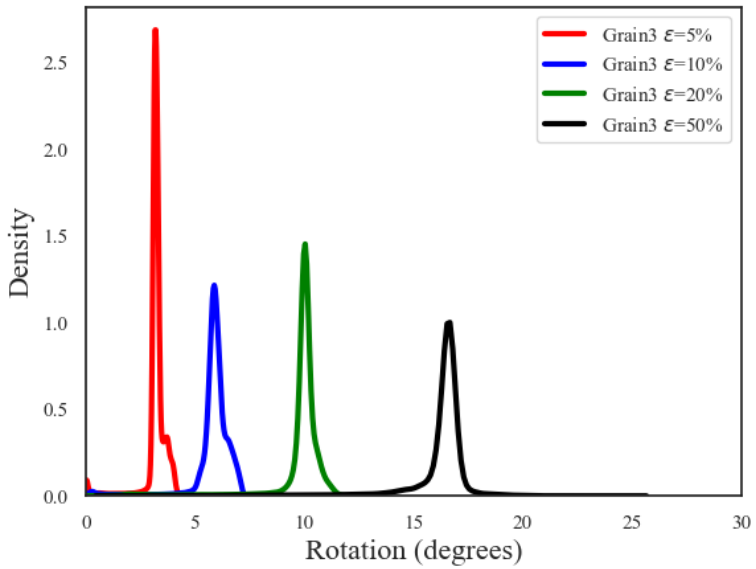


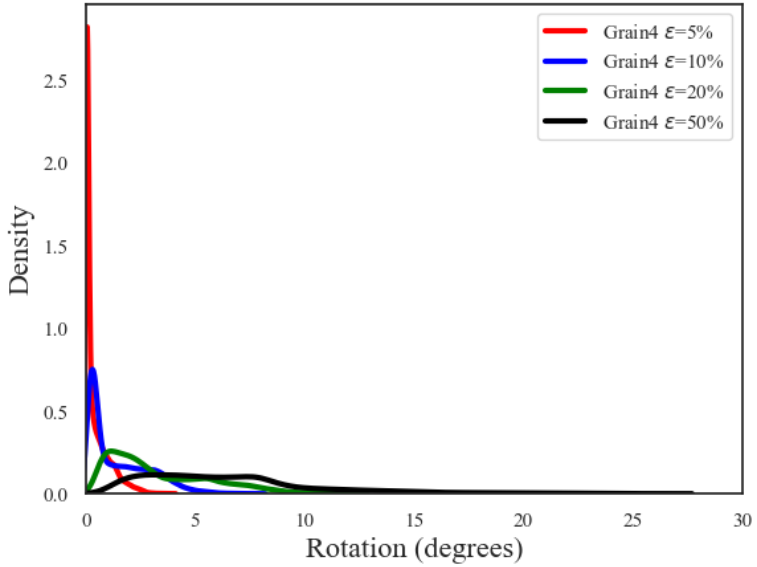
Crystal rotations – per grain analysis

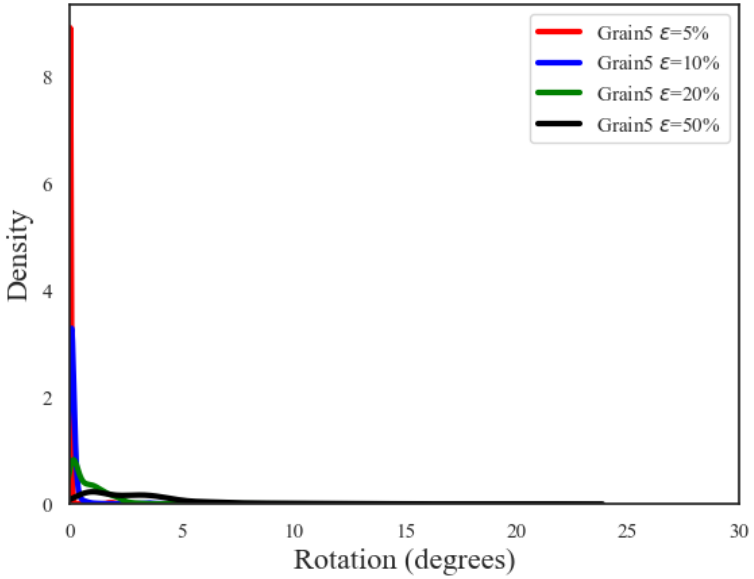




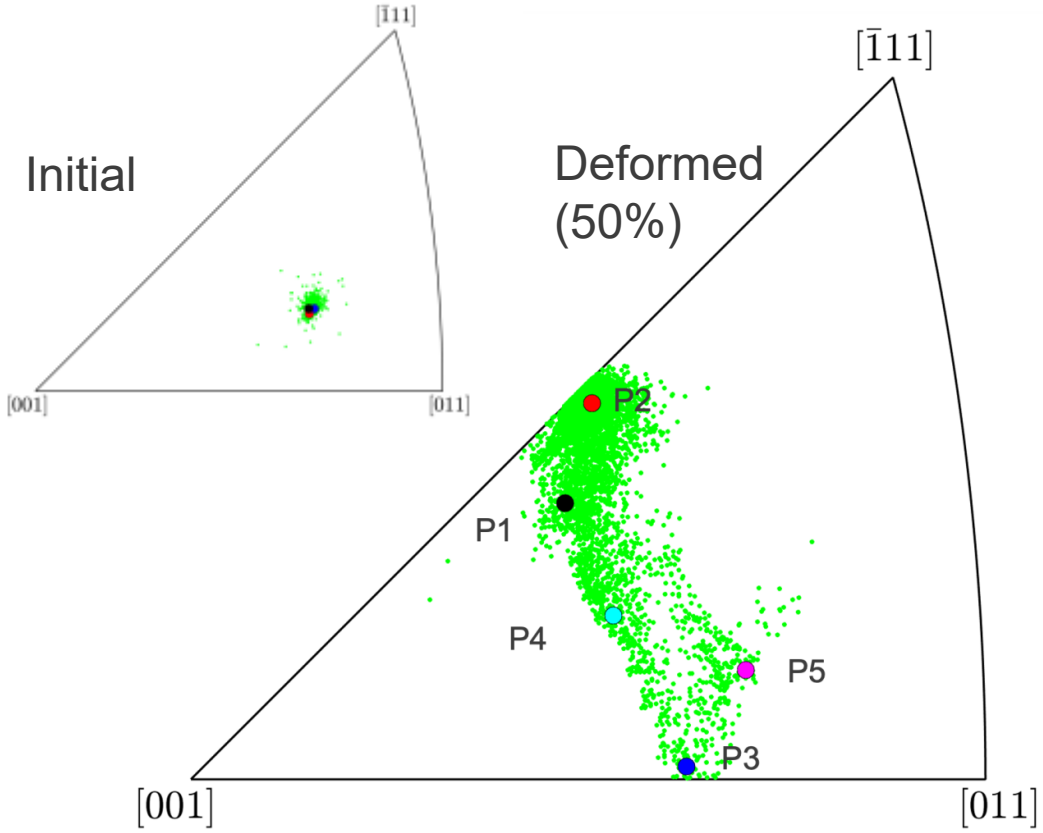




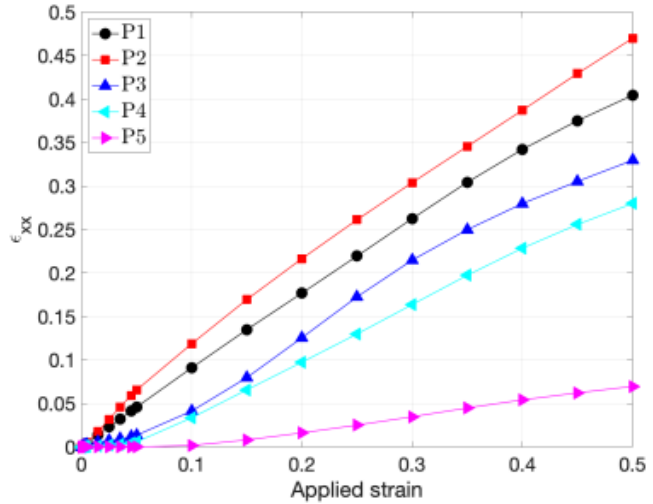


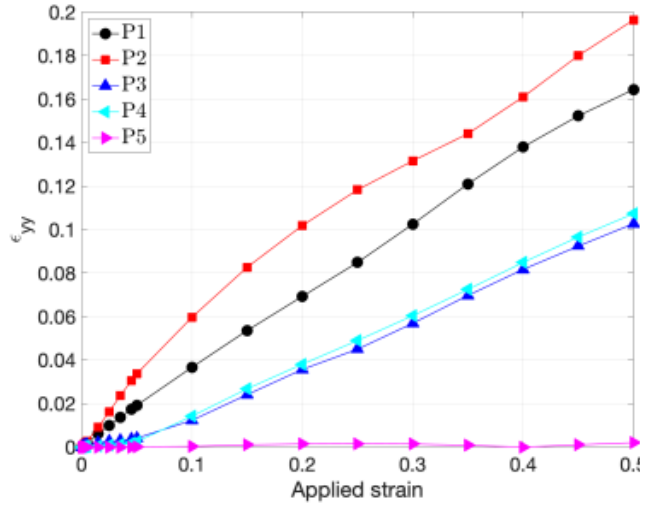


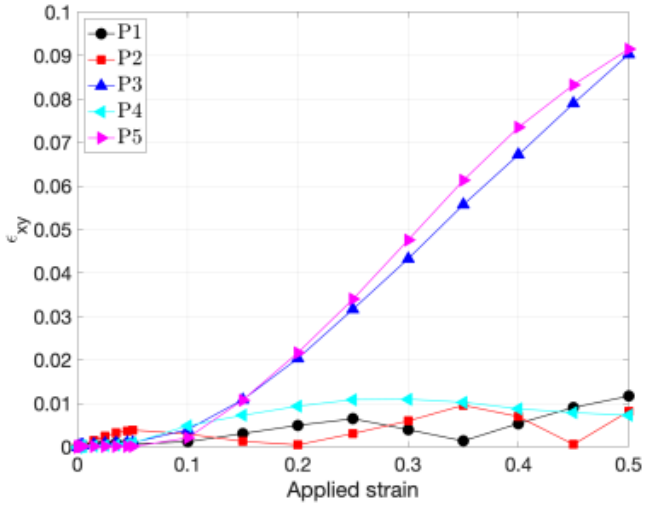
Intragranular rotation



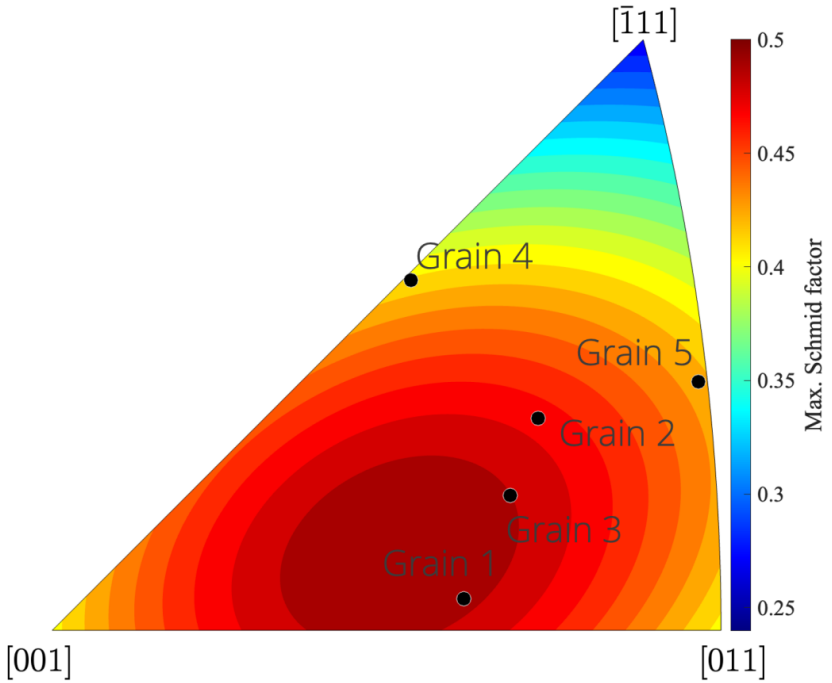
Local strain fields



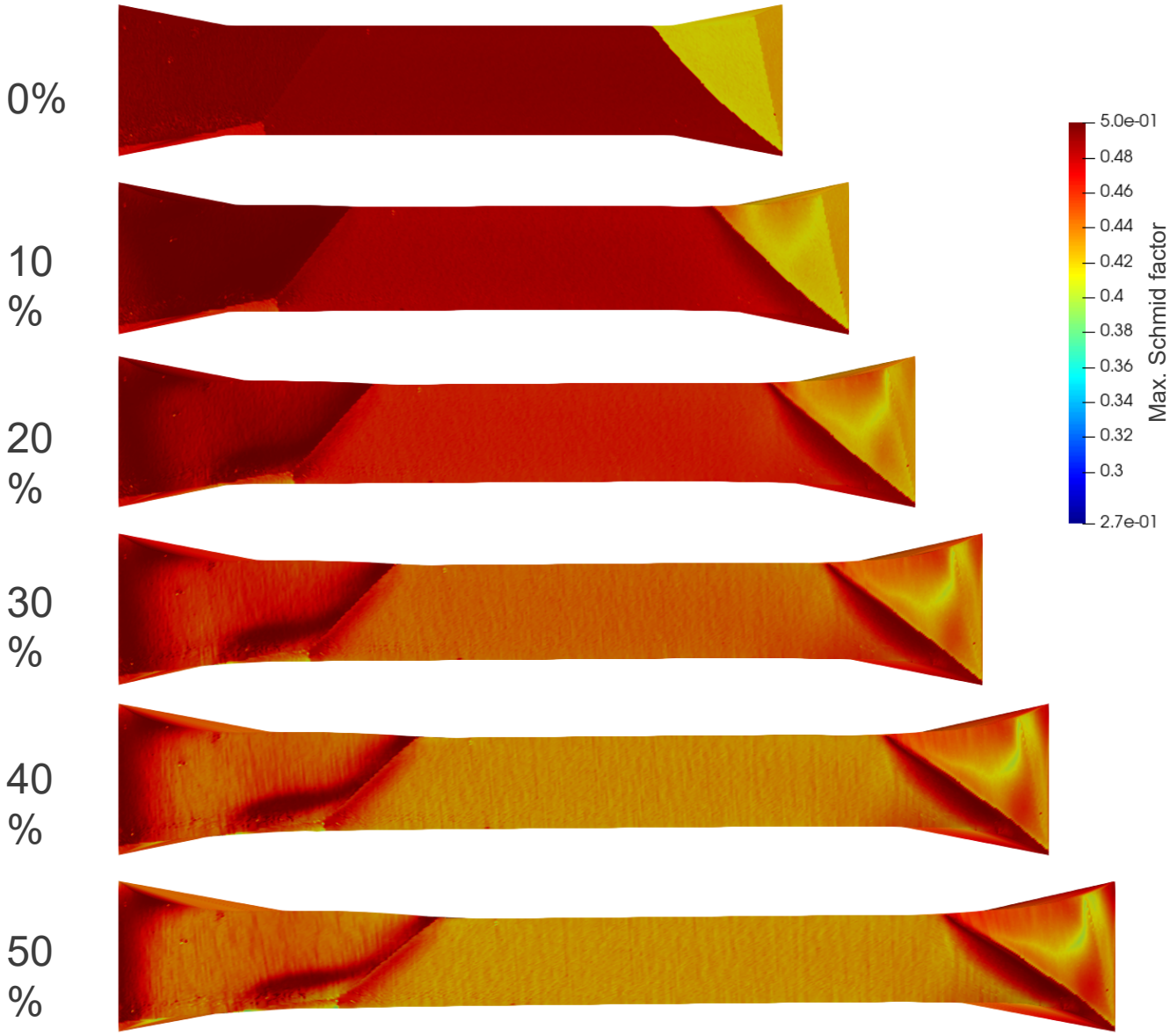




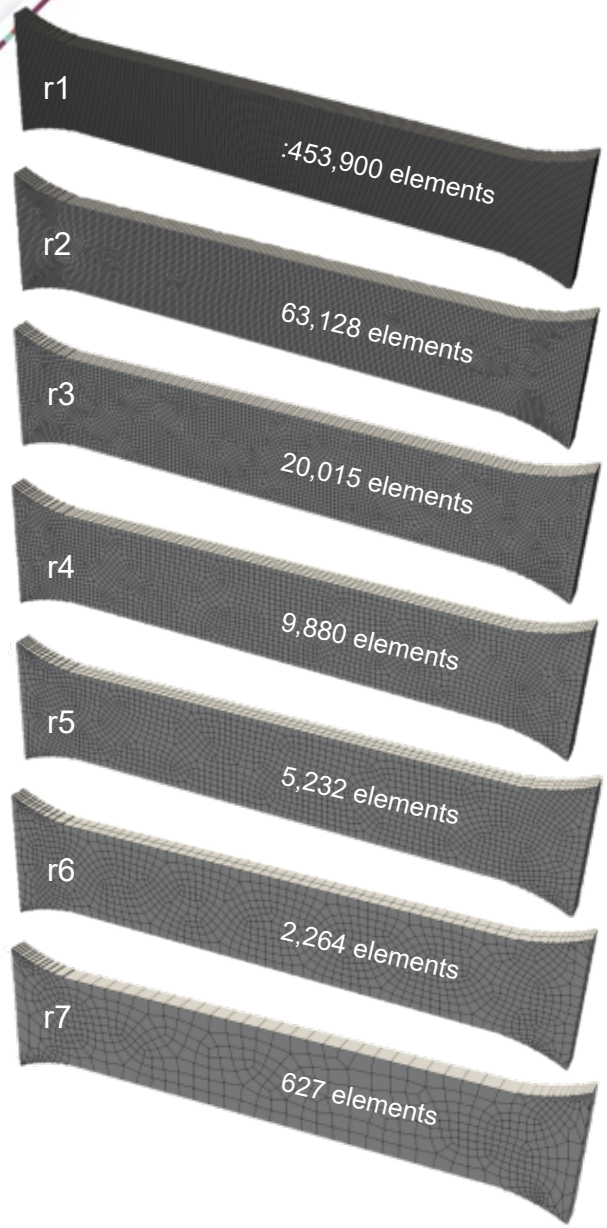
Evolution of Schmid factors

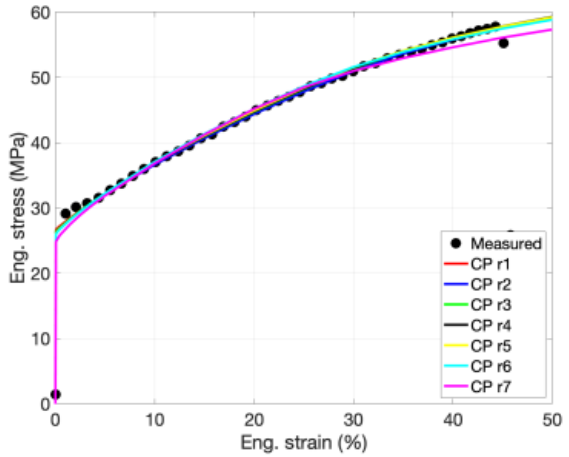


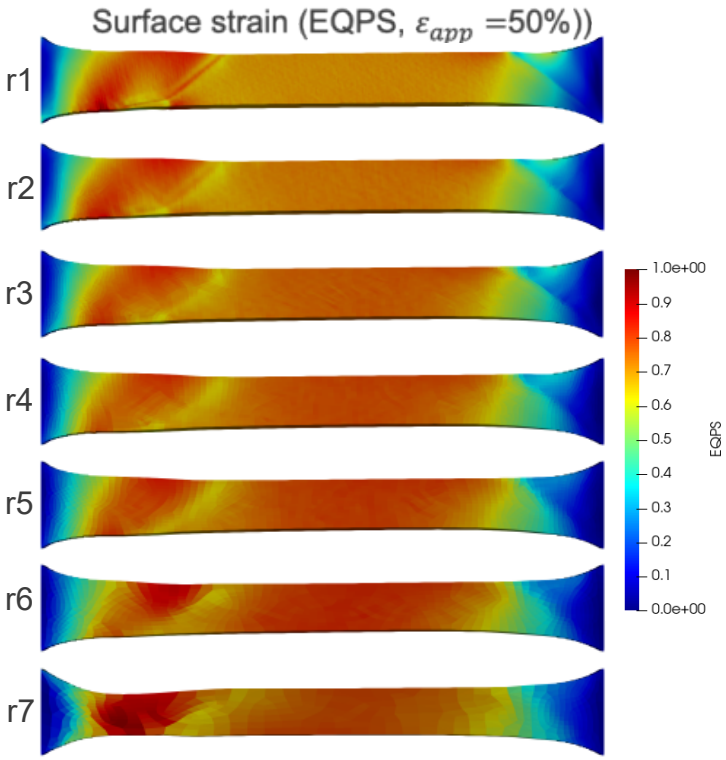
Grain ID	φ_1	Φ	φ_2	M
Grain 1	138.39	46.09	29.22	0.4923
Grain 2	327.87	26.50	63.36	0.4730
Grain 3	337.93	24.13	52.19	0.4893
Grain 4	242.60	26.49	3.90	0.4150
Grain 5	335.85	39.56	63.50	0.4284

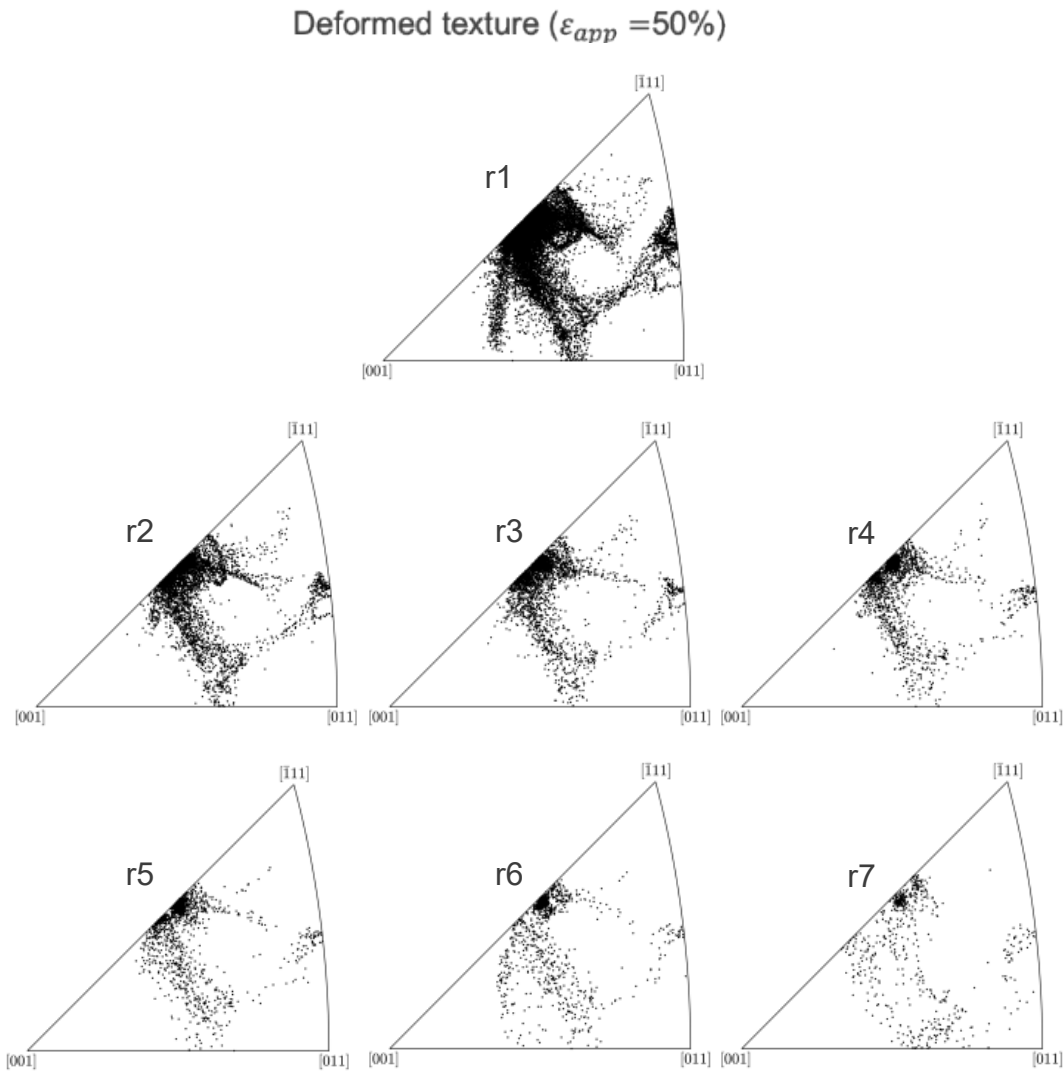


Mesh sensitivity test (Clone 2.1)









Summary

- Microstructural clones – nearly identical multi-crystal, 2D microstructures
  - Novel experimental technique to investigate the stochasticity and repeatability of microstructures
- Clones demonstrate repeatable deformation response and sensitivity of microstructural/ geometrical features on local stress/strain localization
- Coordination of microstructural clones and computational crystal plasticity to improve models and mechanism understandings
  - CP provides qualitatively accurate strain localization and texture predictions
  - Heterogeneous intragranular fields are captured
  - Clones highlight limitations of CP

THANK YOU !

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