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Quantifying the Effects of Microstructure on Localization in Stainless Steel

PRESENTED BY

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Localization in Inelastic Deformation

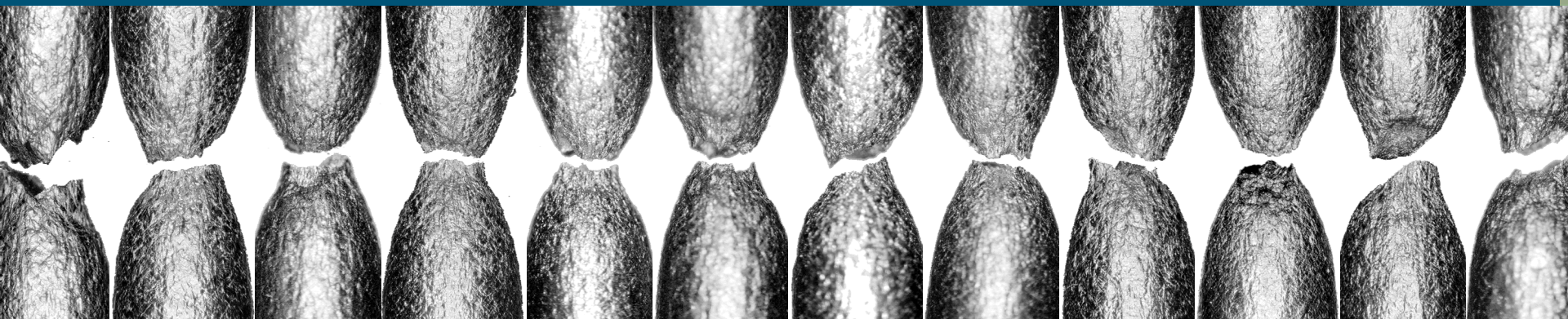
Goal: Understand (predict) localization leading to failure

Processing variables
- Alloying
- Forming
- Heat treatment

Property variables
- Microstructure
- Defect distribution

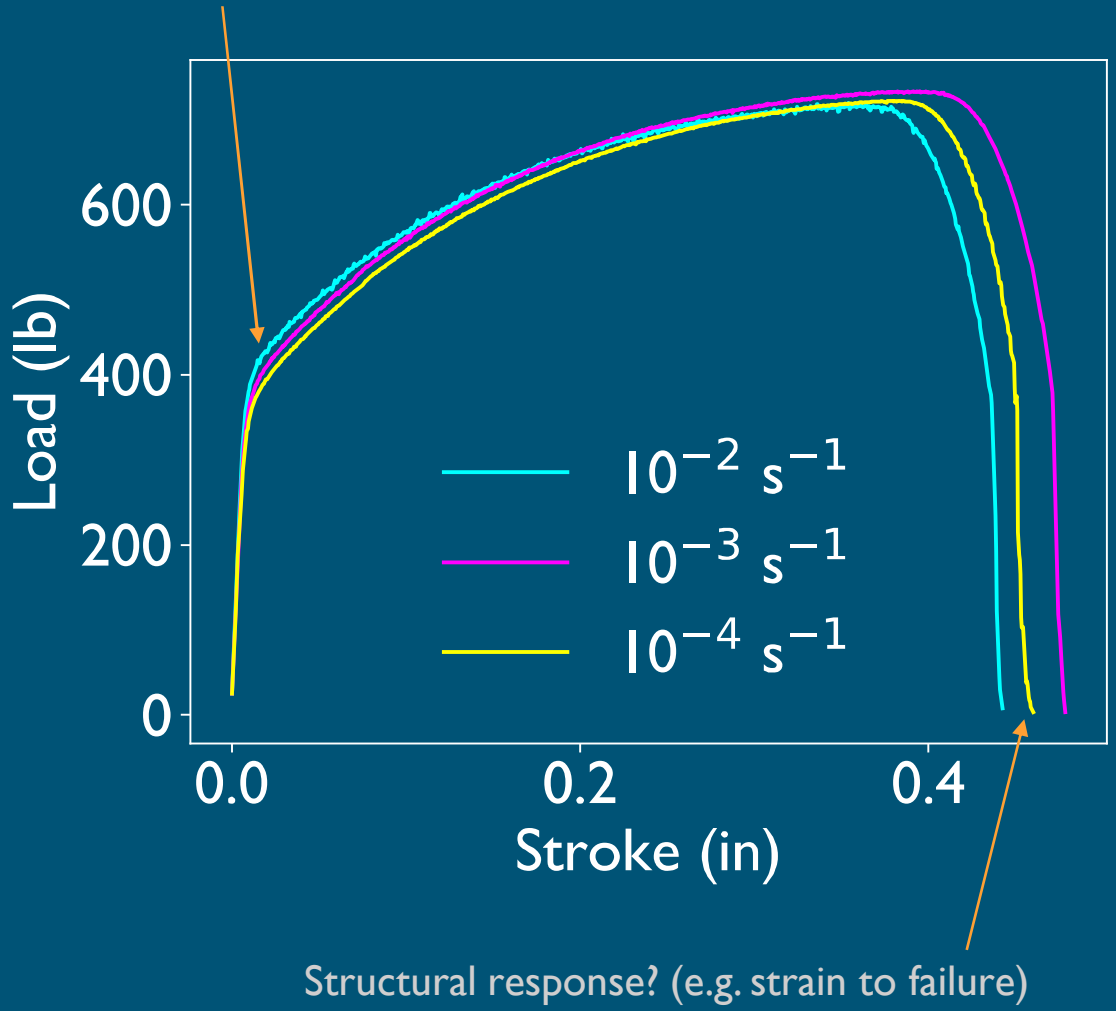
Predictor space
- Deformation rate
- Temperature
- Loading mode

Outcome space
- (An)isotropy
- Strength
- Ductility



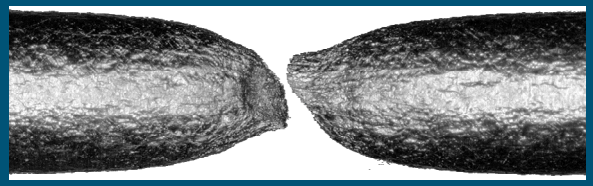
Rate sensitivity at the (micro)structural scale

Material response (e.g. yield strength)

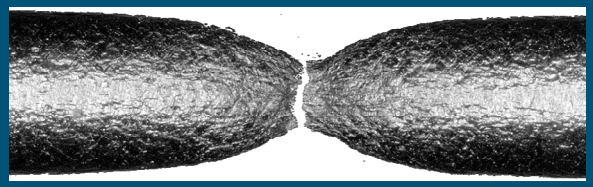


Structural response? (e.g. strain to failure)

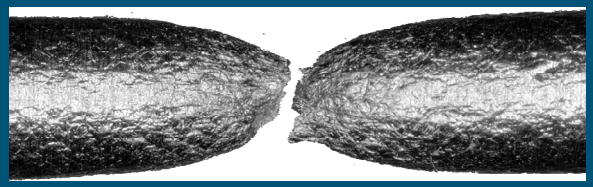
Tests at 200 °C



10^{-2} s^{-1}

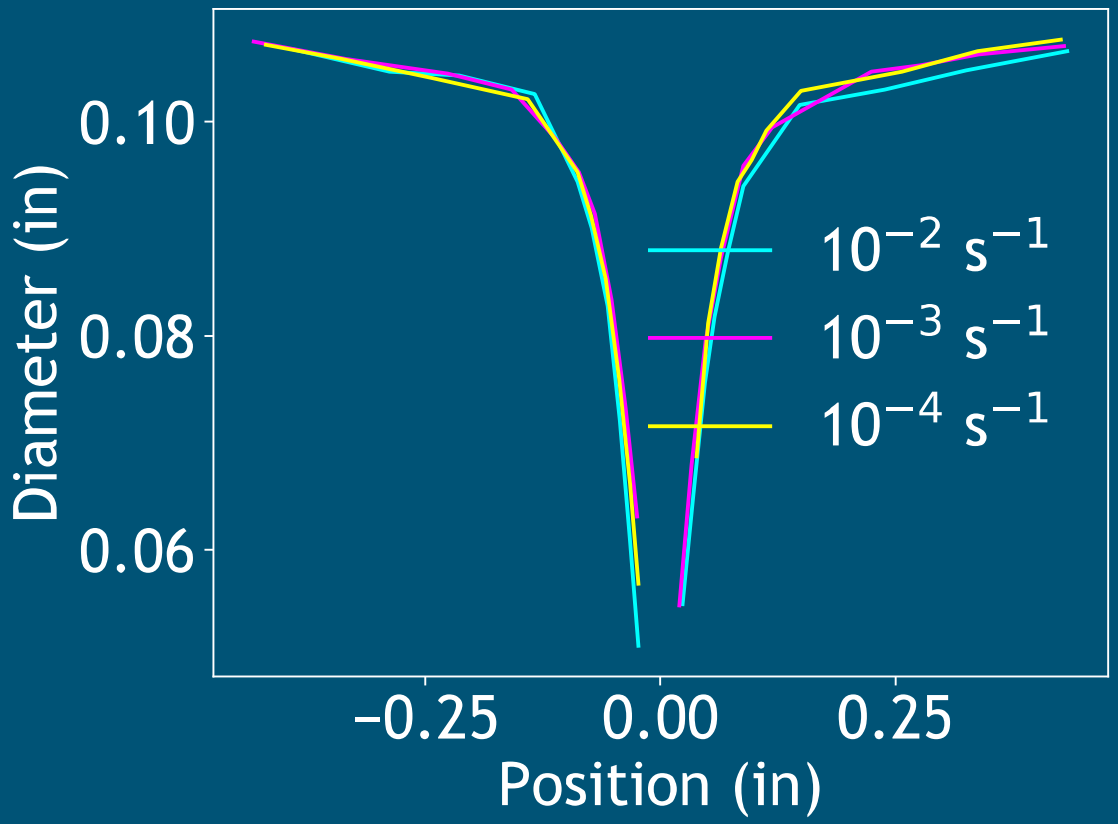


10^{-3} s^{-1}

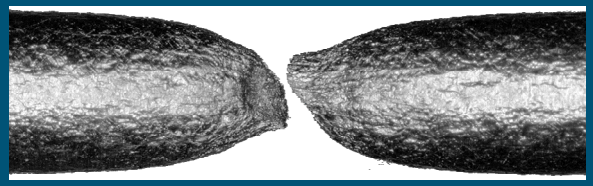


10^{-4} s^{-1}

Rate sensitivity at the structural scale



Tests at 200 °C



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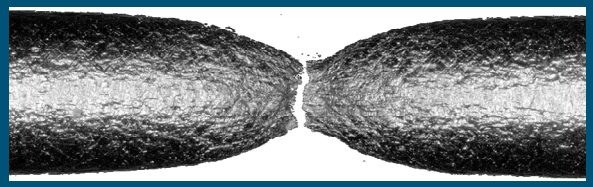
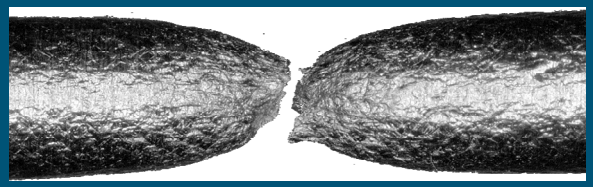


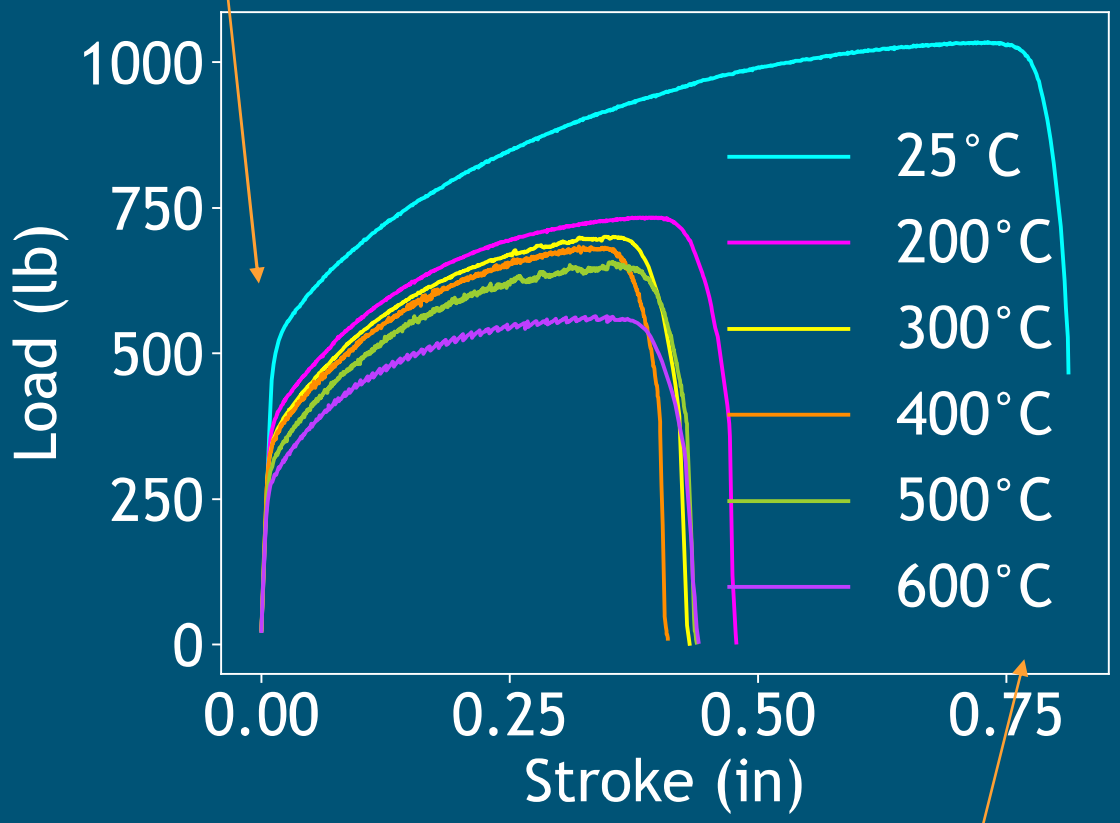
10^{-3} s^{-1}



10^{-4} s^{-1}

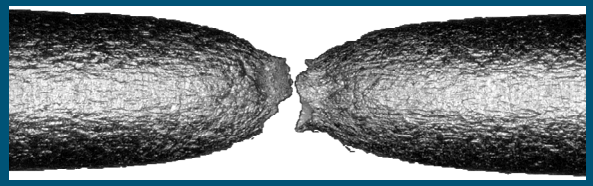
Temperature sensitivity at the (micro)structural scale

Material response (e.g. yield strength)

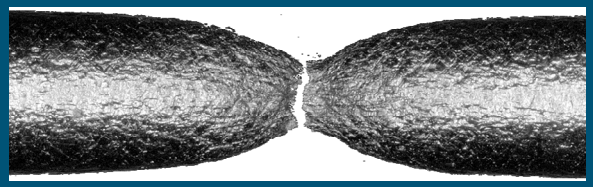


Structural response? (e.g. strain to failure)

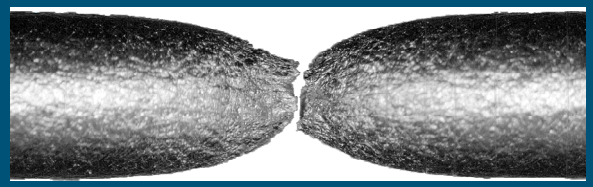
Tests at 10^{-3} s^{-1}



25 °C

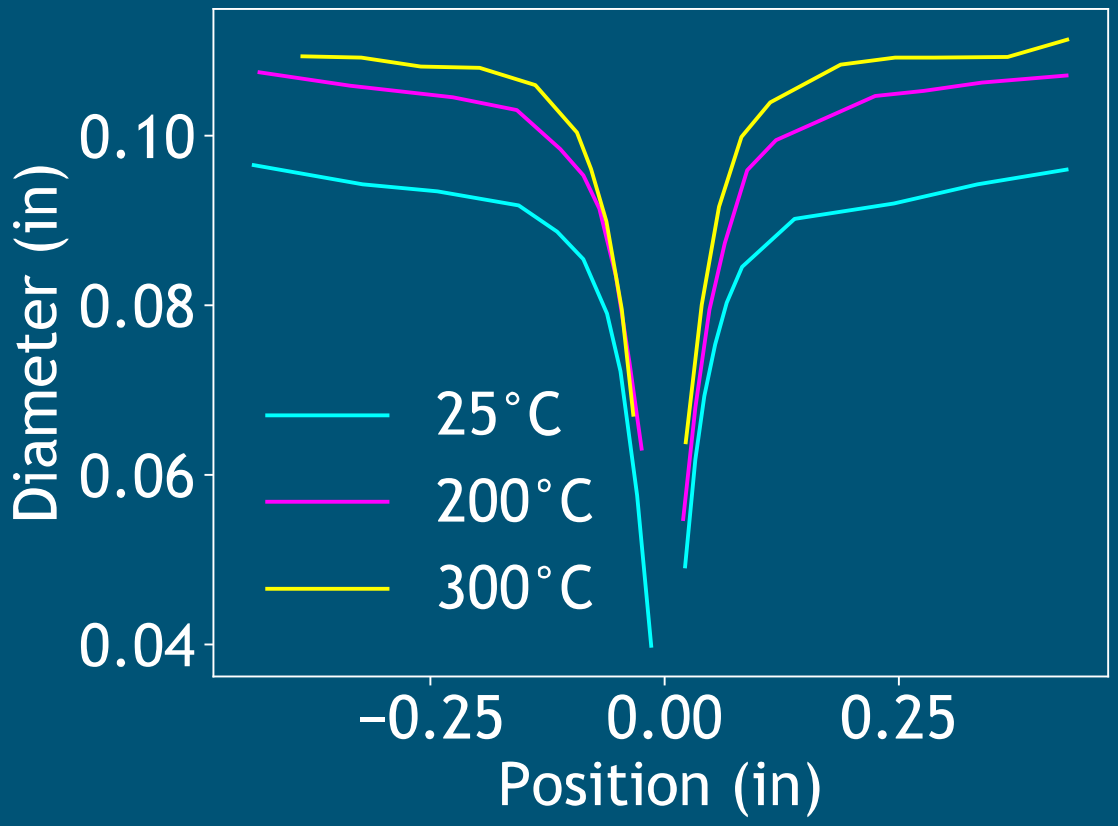


200 °C

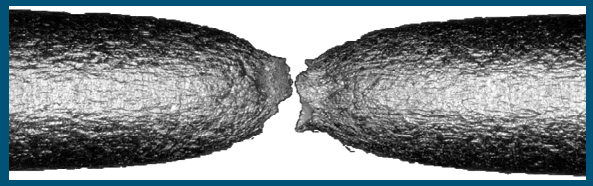


300 °C

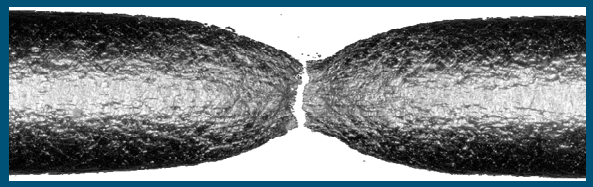
Temperature sensitivity at the structural scale



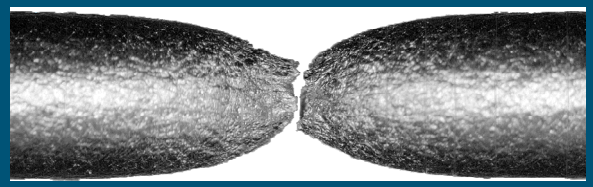
Tests at 10^{-3} s^{-1}



25 °C



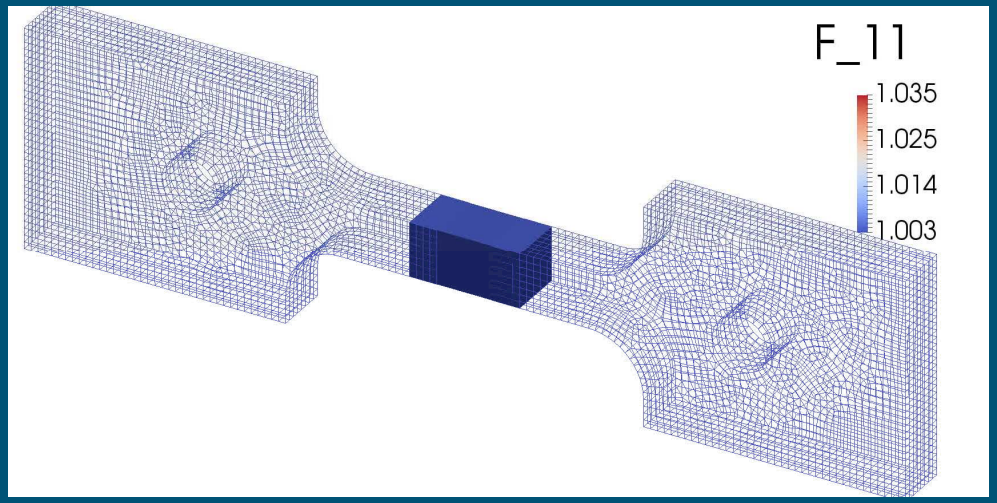
200 °C

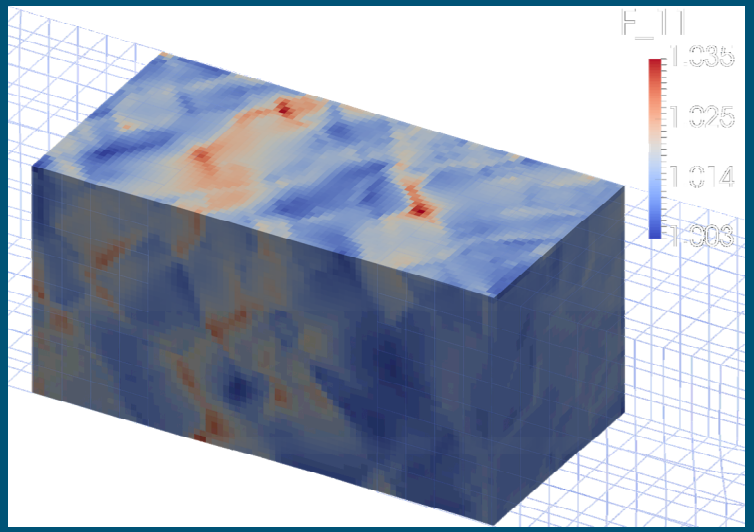


300 °C

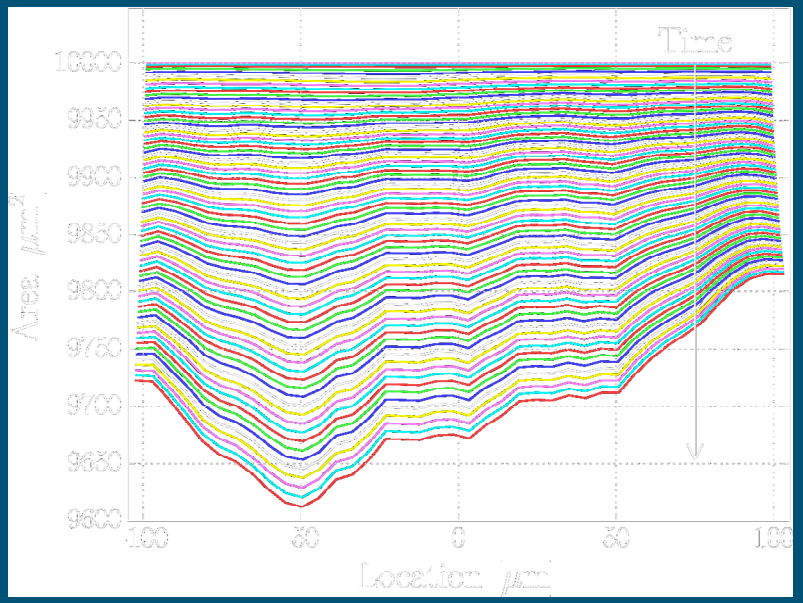
Performance: Necking Localization

Heterogeneity and localization in plasticity



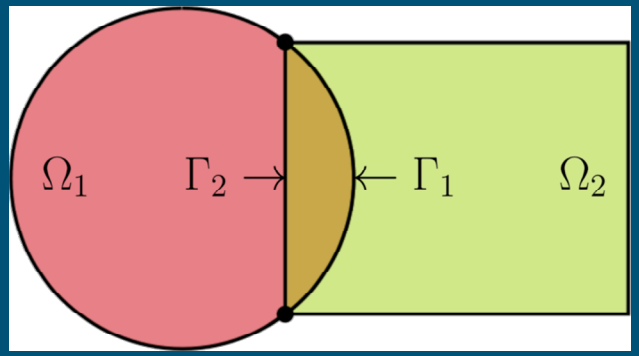


Reduction in area over time



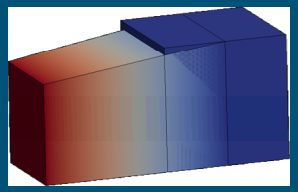
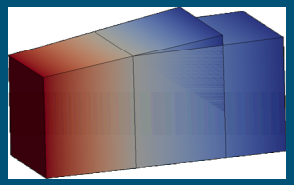
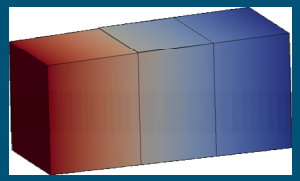
C. Alleman et. al., Comp. Mech., 61(1-2), 2018.

Concurrent Coupling: Schwarz Method



Concept of solution scheme

- Solve on Ω_1 using initial guess for BCs on Γ_1.
- Solve on Ω_2 using BCs on Γ_2 interpolated from Ω_1.
- Solve on Ω_1 with BCs on Γ_1 interpolated from Ω_2.

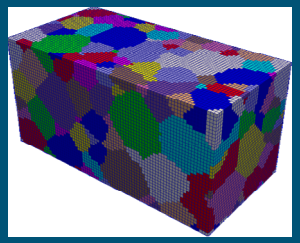
- Mathematical proof of convergence for solid mechanics problem
- Allows coupling of nonconforming domains with different element types and levels of refinement
- Information is exchanged concurrently among two or more subdomains
- Different solvers can be used for each subdomain
- Different material models can be coupled provided that they are compatible

A. Mota, I. Tezaur, C. Alleman, CMAME, 319(1), 2017.

Performance: Local/Global Response

Mesoscale

voxelated microstructure derived from Kinetic Monte Carlo evolution (F. Abdeljawad)



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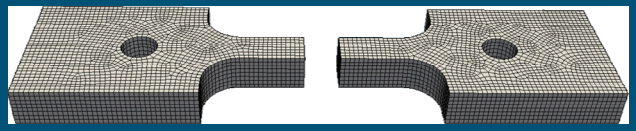
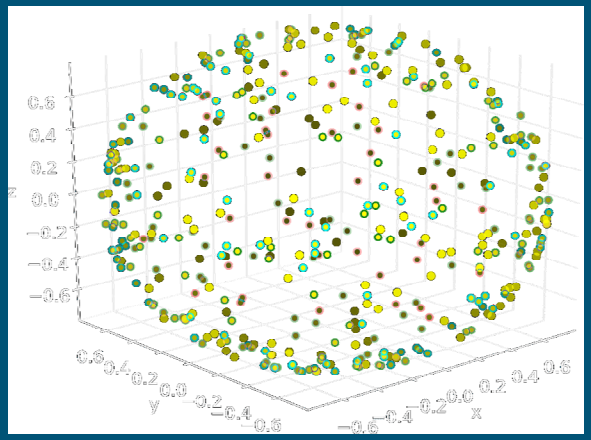
Macroscale

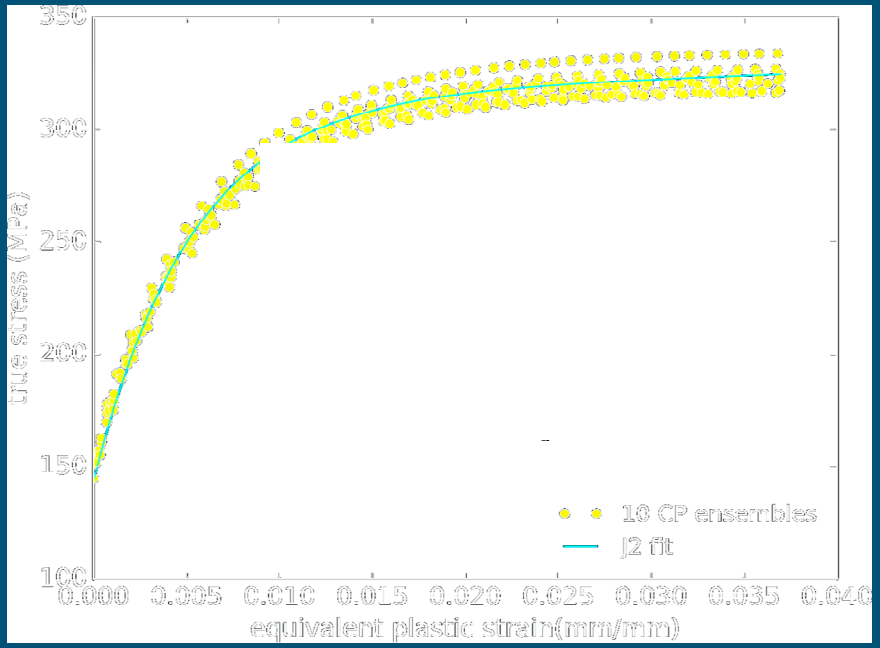


- Load microstructural ensembles in uniaxial stress
- Fit flow curves with a macroscale J_2 plasticity model

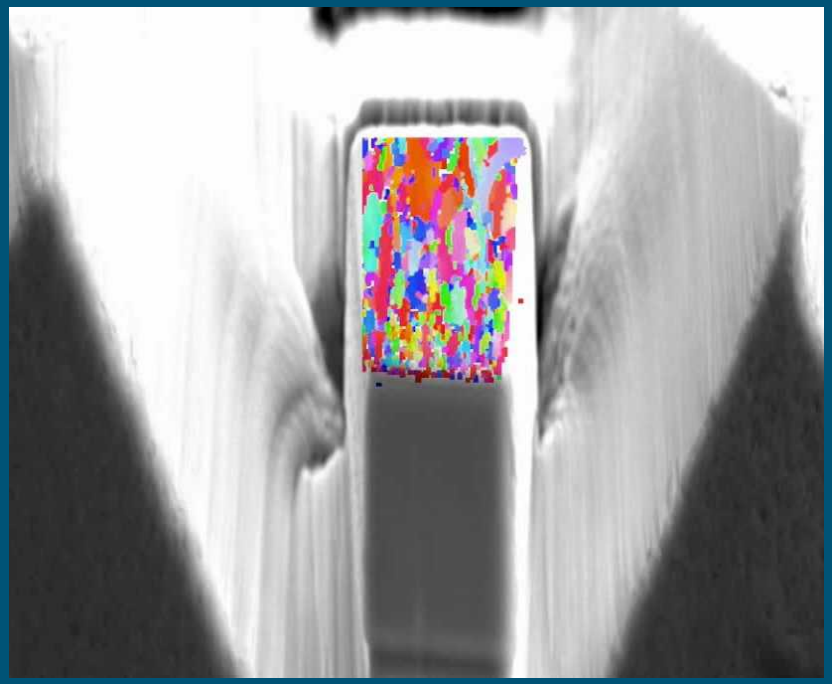
Fix microstructure, investigate ensembles



151 axial vectors from 3 of the 10 ensembles of random rotations



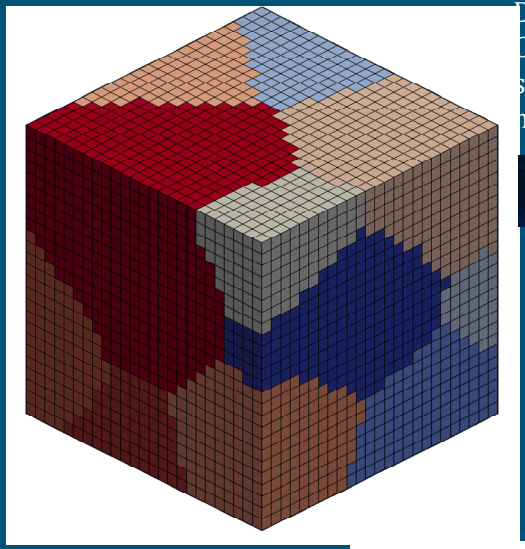
Property: Microstructure



Sugar, 2017

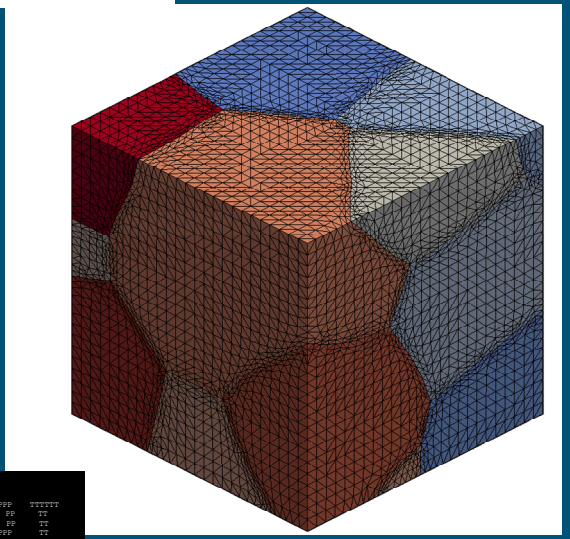
Serial sectioning characterization experiment

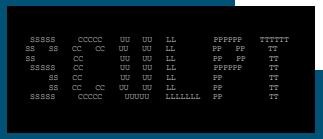
Demonstration on Ni sample



DREAM.3D
Compute microstructure statistics, output voxelized microstructure

SCULPT
Input: voxel orientations
Output: conformal mesh





Single Crystal Physics

Kinematics

Multiplicative elastic-plastic decomposition

$$\mathbf{F}^e = \mathbf{F} \cdot (\mathbf{F}^p)^{-1}$$

Crystal elasticity

Linear elastic constitutive relation

$$\mathbf{T}^* = \mathbb{L}^c : \mathbf{E}^e$$

Elastic Lagrangian strain

$$\mathbf{E}^e = \frac{1}{2}[(\mathbf{F}^e)^{\mathrm{T}}\mathbf{F}^e - \mathbf{I}]$$

Crystal Plasticity

Evolution of plastic deformation gradient

$$\dot{\mathbf{F}}^p = \mathbf{L}^{p*} \cdot \mathbf{F}^p$$

Plastic part of the velocity gradient

$$\mathbf{L}^{p*} = \sum_\alpha \dot{\gamma}^\alpha \mathbf{m}_0^\alpha \otimes \mathbf{n}_0^\alpha$$

Resolved shear stress

$$\tau^\alpha = [(\mathbf{F}^e)^{\mathrm{T}} \cdot \mathbf{F}^e \cdot \mathbf{T}^*] : \mathbf{m}_0^\alpha \otimes \mathbf{n}_0^\alpha$$

Hardening

- Linear w/ recovery

$$\dot{g}^\alpha = (H - R_d g^\alpha)|\dot{\gamma}^\alpha|$$

- Saturation

$$\dot{g}^\alpha = \dot{g}_0 \left(\frac{g_s - g^\alpha}{g_s - g_0}\right) H^{\alpha\beta} |\dot{\gamma}^\beta|$$

- Dislocation density

$$g^\alpha = \sqrt{H^{\alpha\beta}\rho^\beta}, \dot{\rho}^\alpha = \left(\kappa_1 \sqrt{\sum \rho^\beta} - \kappa_2 \rho^\alpha\right)|\dot{\gamma}^\alpha|$$

Plastic flow

- Power law

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left|\frac{\tau^\alpha}{g^\alpha}\right|^m sign(\tau^\alpha)$$

- Dislocation drag

$$\dot{\gamma}^\alpha = D \frac{\tau^\alpha}{g^\alpha}$$

- Thermal activation

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \exp\left(-\frac{F_0}{k_B \theta}\left[1 - \left(\frac{\tau^\alpha - g^\alpha}{\tau_0}\right)^p\right]^q\right)$$

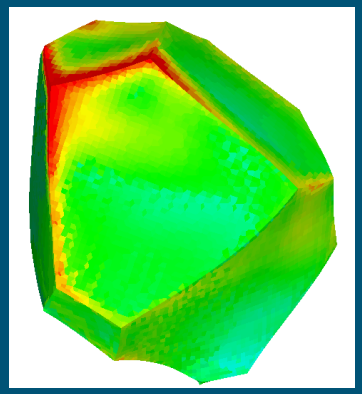
Performance: Crystal Plasticity

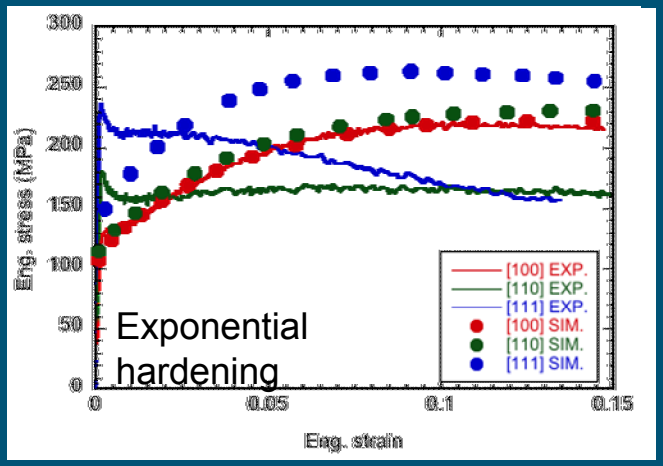
Linear hardening w/ recovery

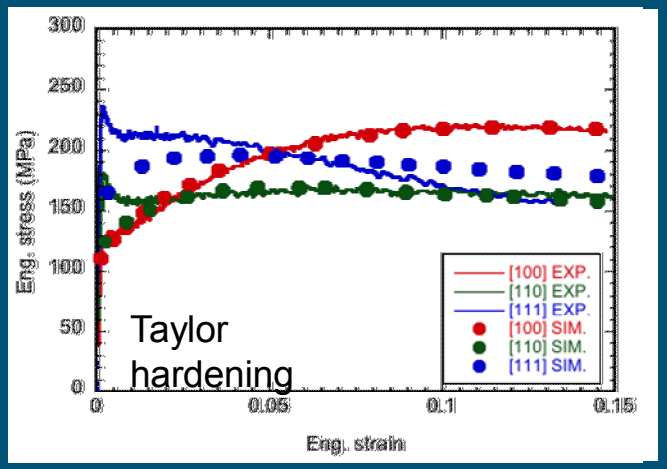
$$\dot{g}^{\alpha} = (H - R_d g^{\alpha})|\dot{\gamma}^{\alpha}|$$

Taylor (dislocation density) hardening

$$g^{\alpha} = \sqrt{H^{\alpha\beta}\rho^{\beta}}, \qquad \dot{\rho}^{\alpha} = \left(\kappa_1\sqrt{\Sigma\rho^{\beta}} - \kappa_2\rho^{\alpha}\right)|\dot{\gamma}^{\alpha}|$$



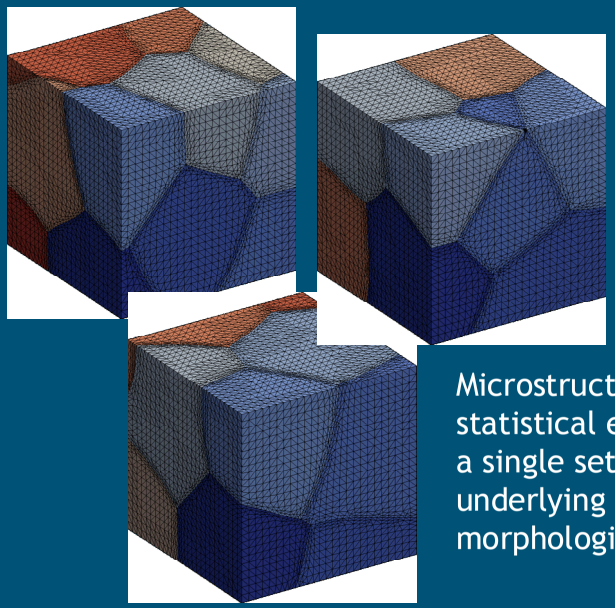




Lim, 2016

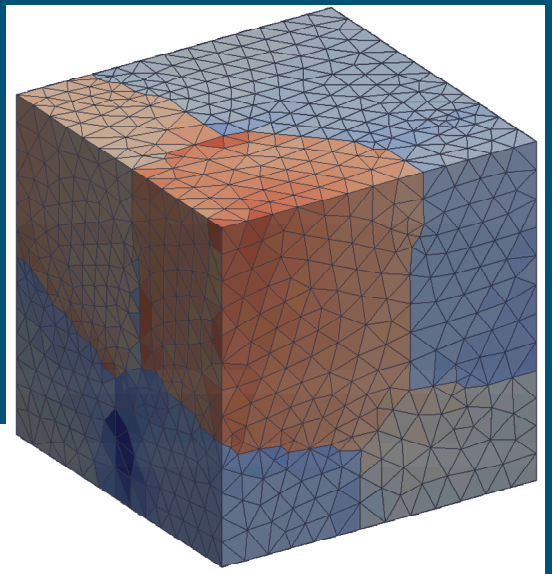
- Parameterize through [100] Ta single crystal experiments
- Predict [110] and [111] response.
- *Dislocation density based Taylor hardening model* most accurately reflects anisotropy.

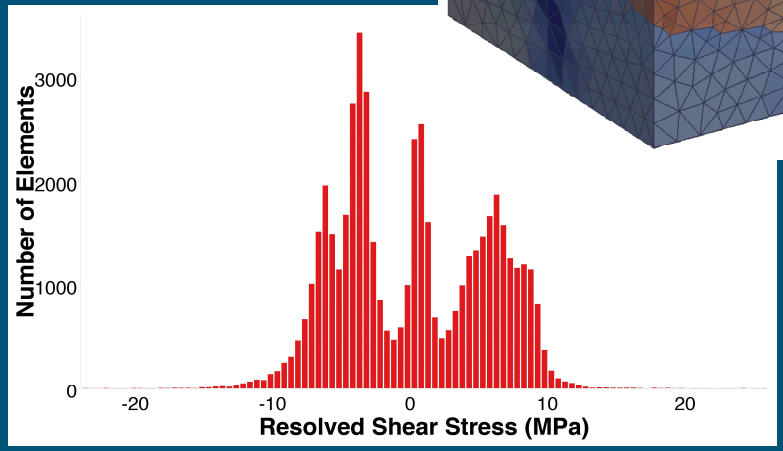
Microstructural Parametrization

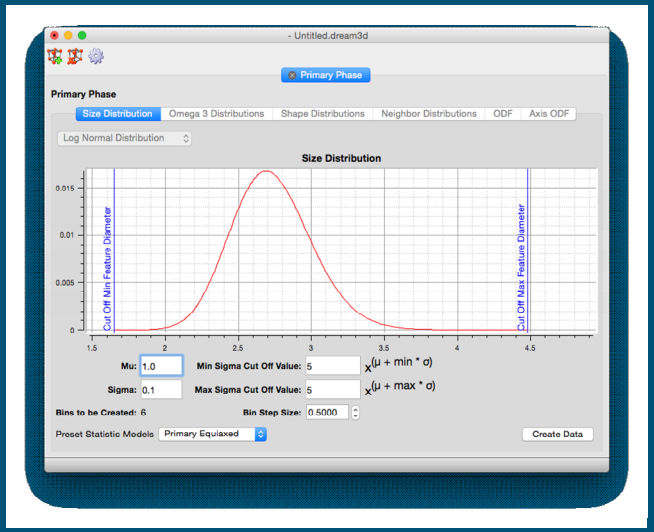


Microstructure statistical equivalence: a single set of underlying morphological statistics

Microstructure performance equivalence: metrics for mechanical response?



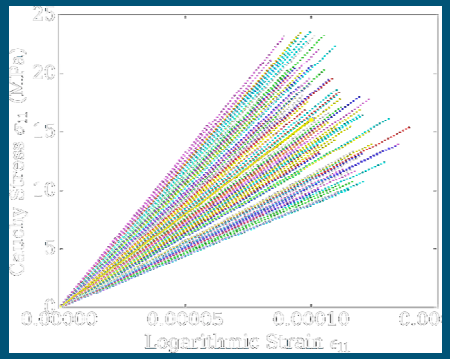


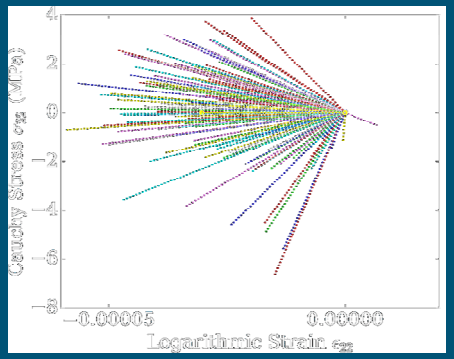


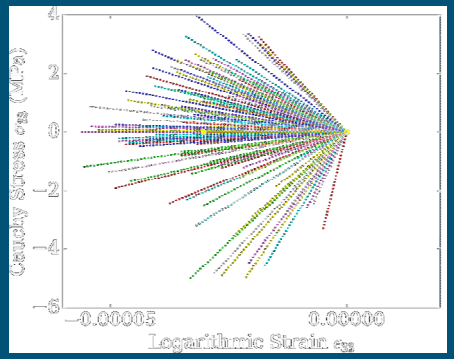
Microstructure - Performance Links

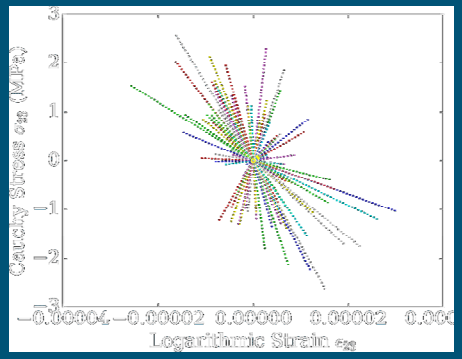
Grain orientation - Anisotropy
Grain size - Yield strength
Grain neighborhood - *Localization*

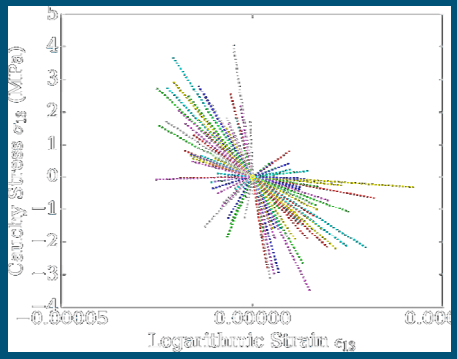
Performance: Crystal Elasticity

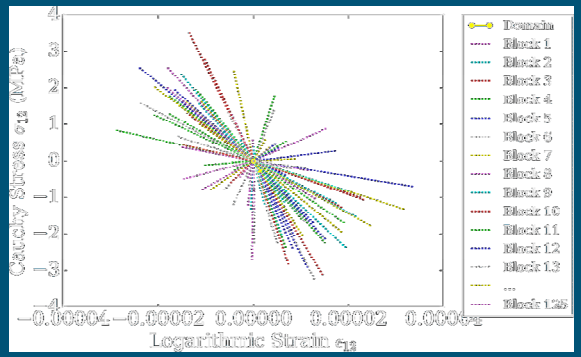


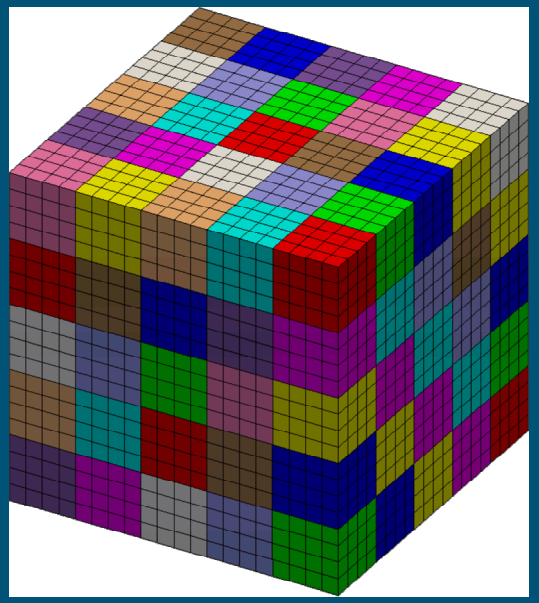




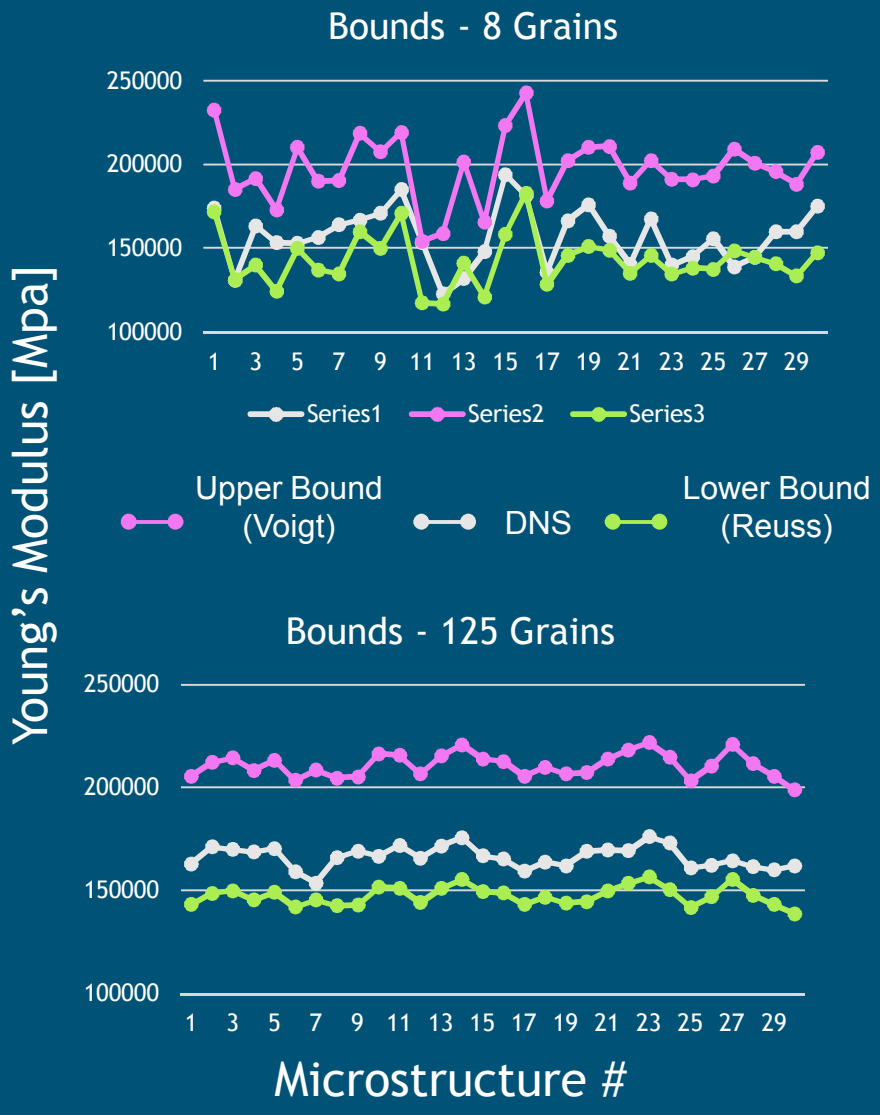


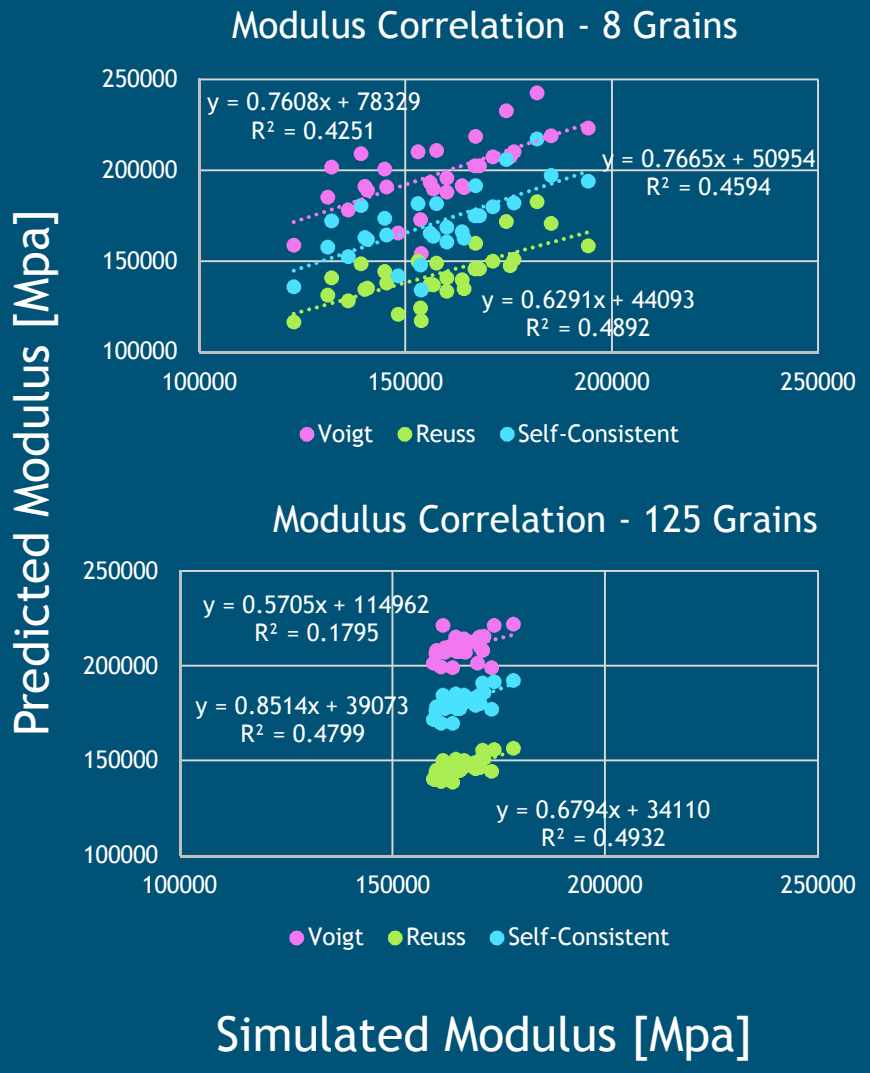




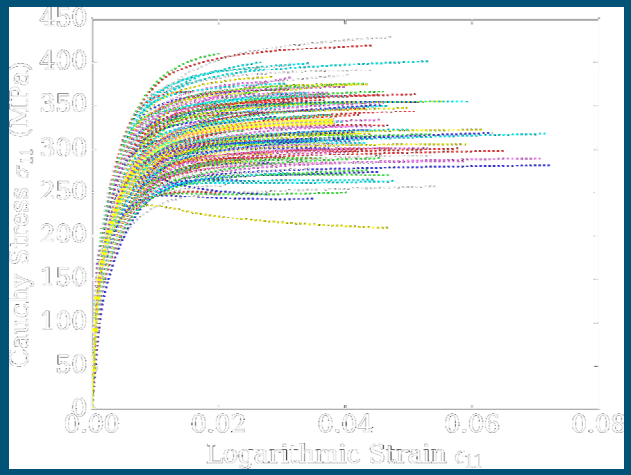


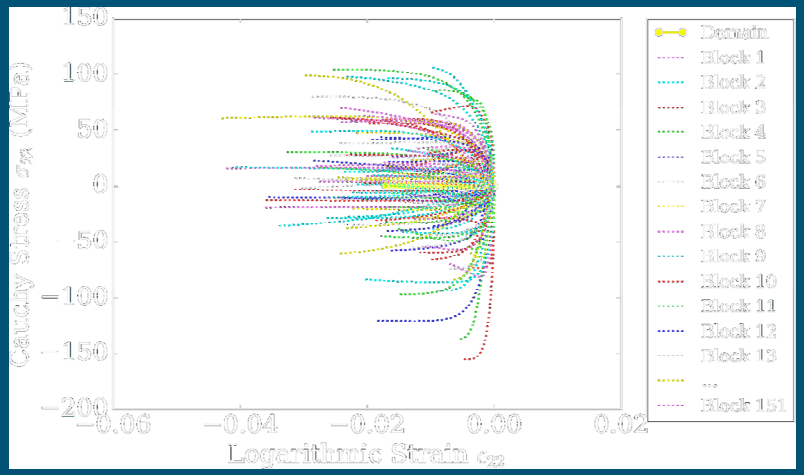
Performance: (An)isotropic Elasticity

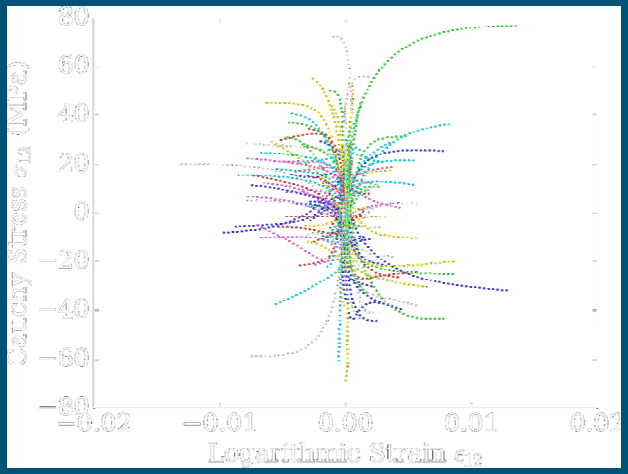




Performance: Upscaling Plasticity

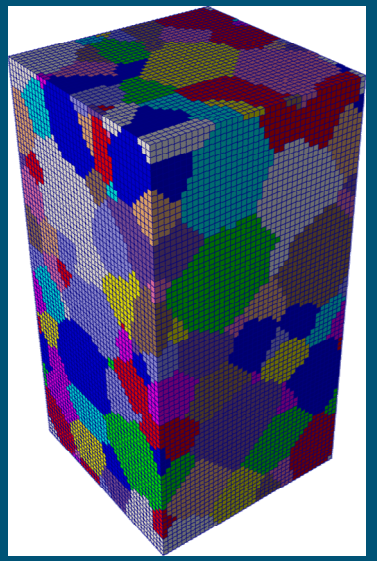






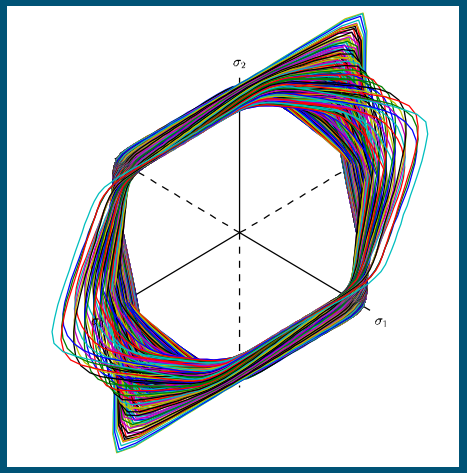
<u>Predict performance from properties:</u>

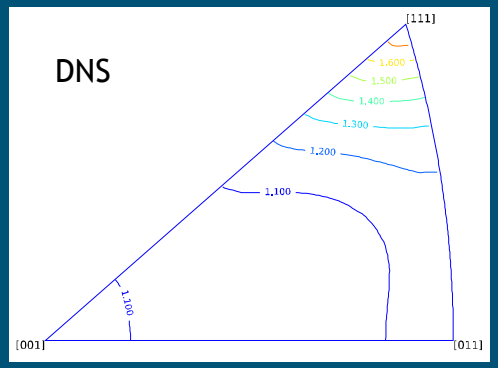
- Property Metrics
  - Beyond average grain size
  - → Grain neighborhood character
- Response Metrics
  - Characterize heterogeneity
  - → Locally triaxial stress state, but globally uniaxial
  - → Isotropic macroscale; anisotropic mesoscale
- Mapping from property metrics to response metrics
  - Framework to upscale response



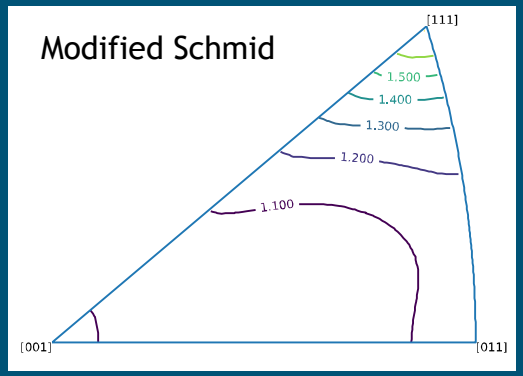
Single crystal yield strength and macroscale response

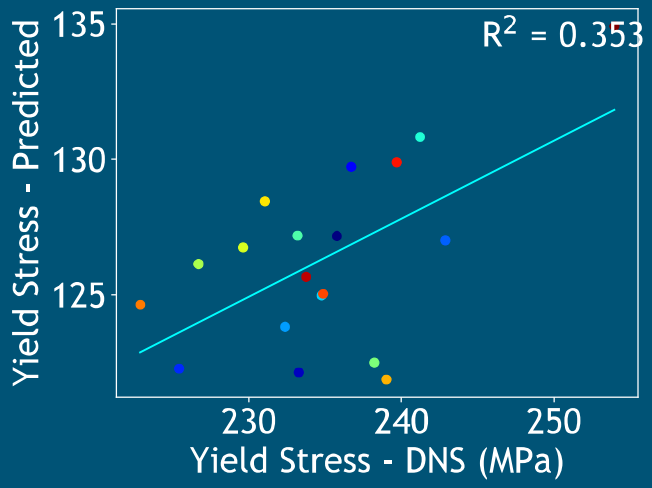
Yield loci for anisotropic single crystals oriented throughout the orientation space.





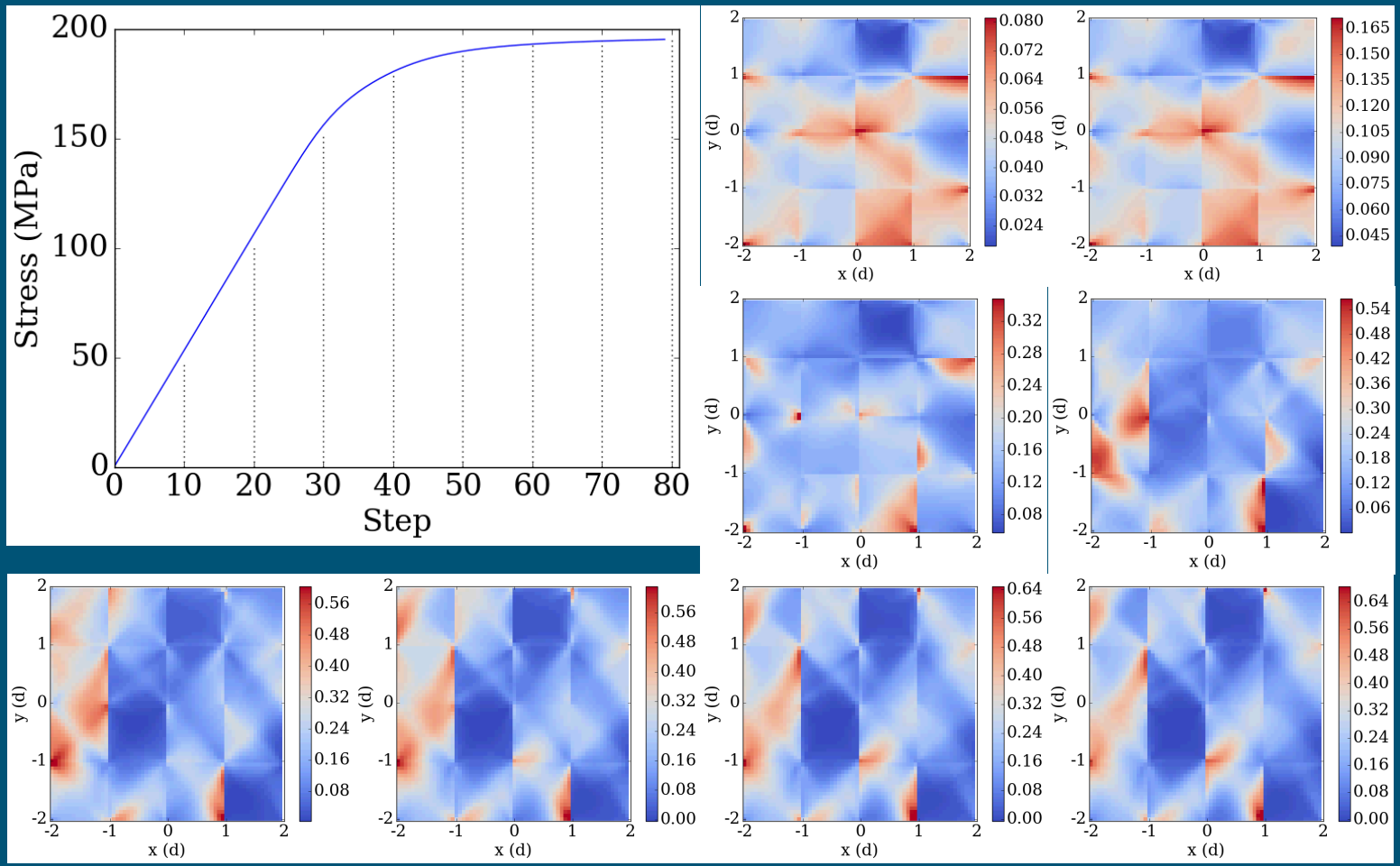
Uniaxial tensile yield strengths for anisotropic single crystals oriented throughout the orientation space.



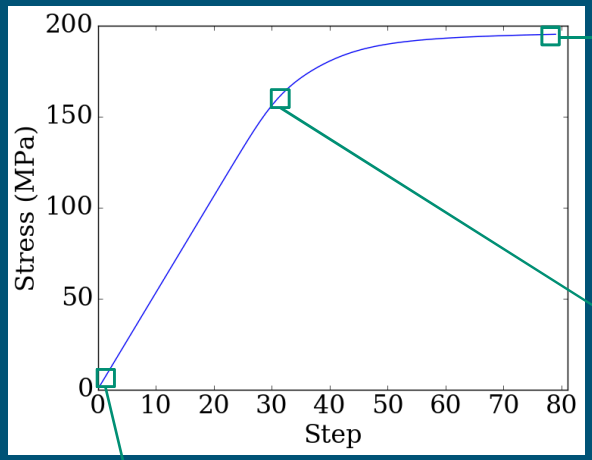


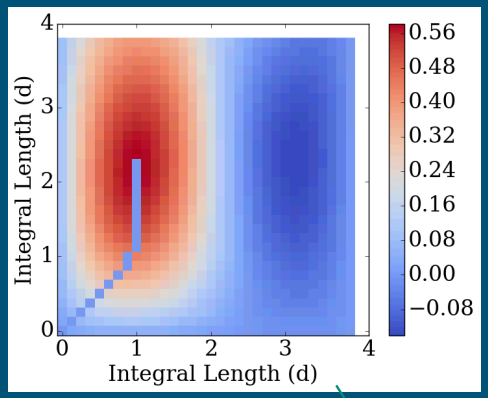
Crystal Plasticity

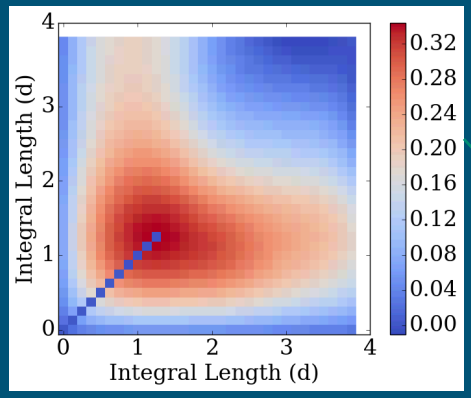
Total Power, $\underline{\underline{\sigma}} : \underline{\underline{L}}$

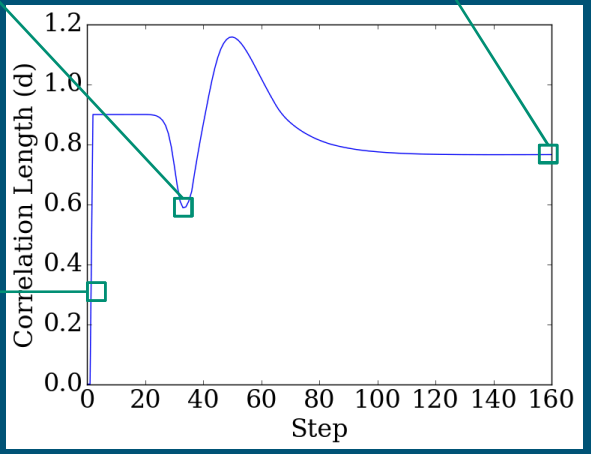


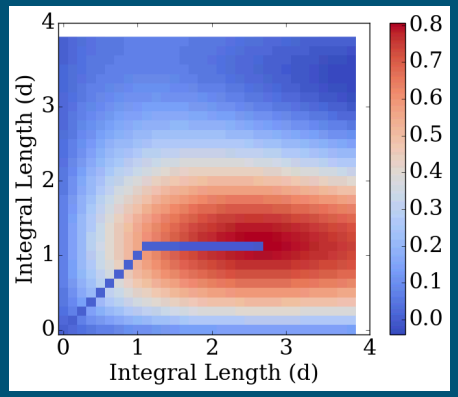
Correlation Length: Total Power









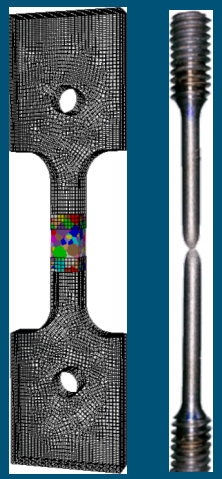


Progress and Future Work

Goal: Understand (predict) localization leading to failure

Modeling

- Structure-microstructure coupling (Schwarz)
- Investigating effects of microstructural physics



Coupling to characterization and mechanical testing

- Realistic microstructures
- Rate and temperature dependence
- Identifying/discovering mechanisms of deformation

Thank you

Additional questions to callema@sandia.gov