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Efficient structural reliability including the effects of crystallographic texture on engineering-scale performance

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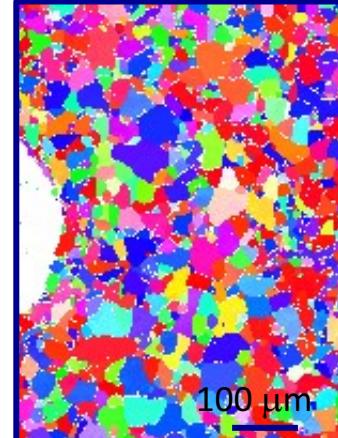
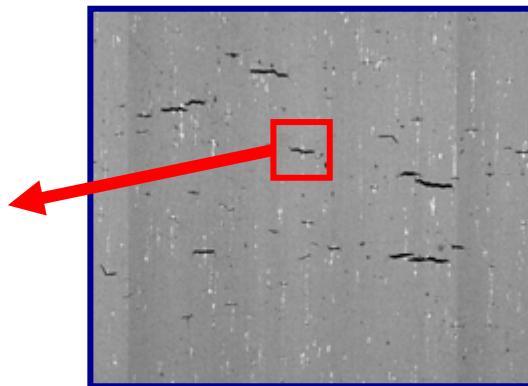
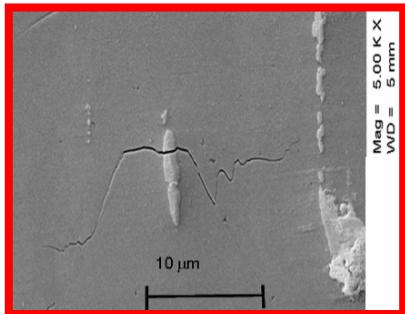
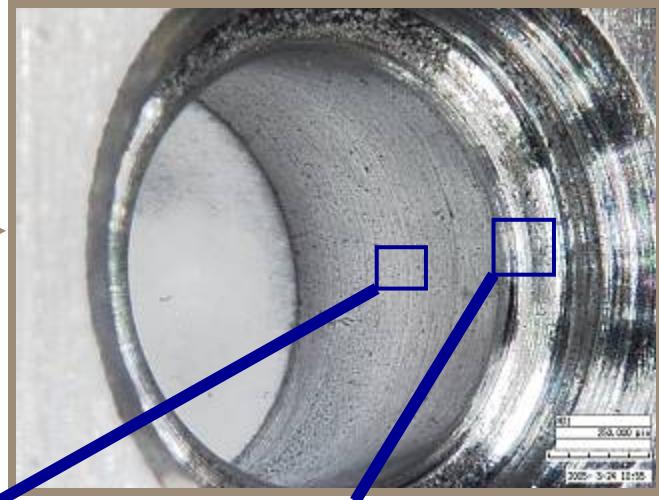
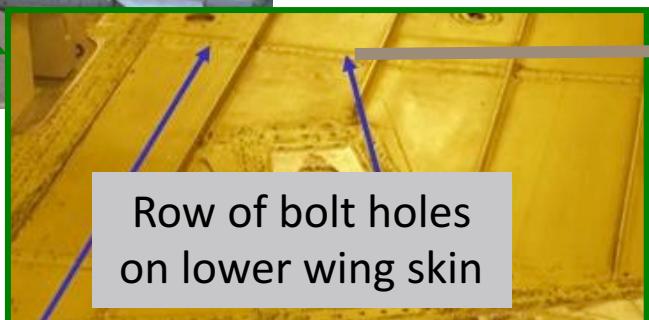
Outline

- Motivation & challenge
- Proposed algorithm for multiscale UQ
- Summary of engineering-scale UQ
- Mesostructural length scale focused on the effects of crystallographic orientation
 - Yield surfaces
 - Void nucleation
- Future work: bridging length scales
- (time permitting) Our Multiscale DIC developments
- Summary

Why do multiscale? Because structural reliability is dependent on **random** microstructure (among other sources of randomness)

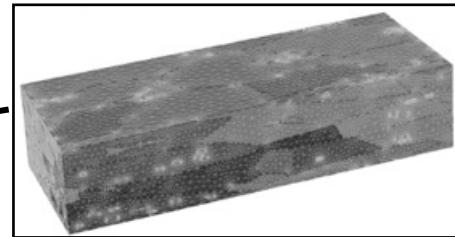
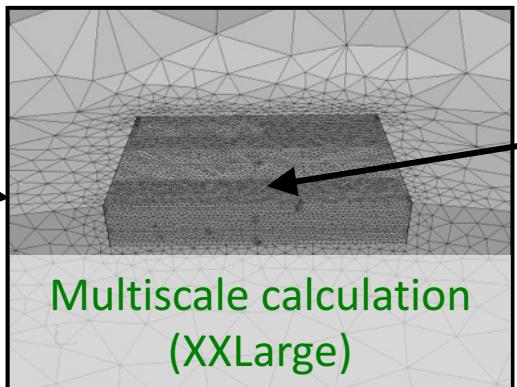
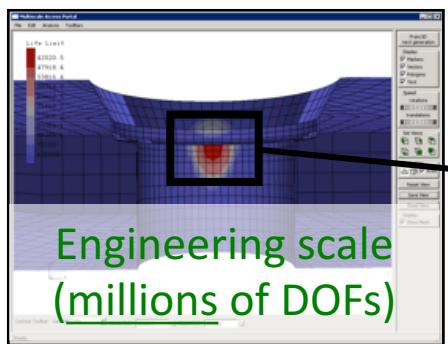


Engineering length scale (meters)

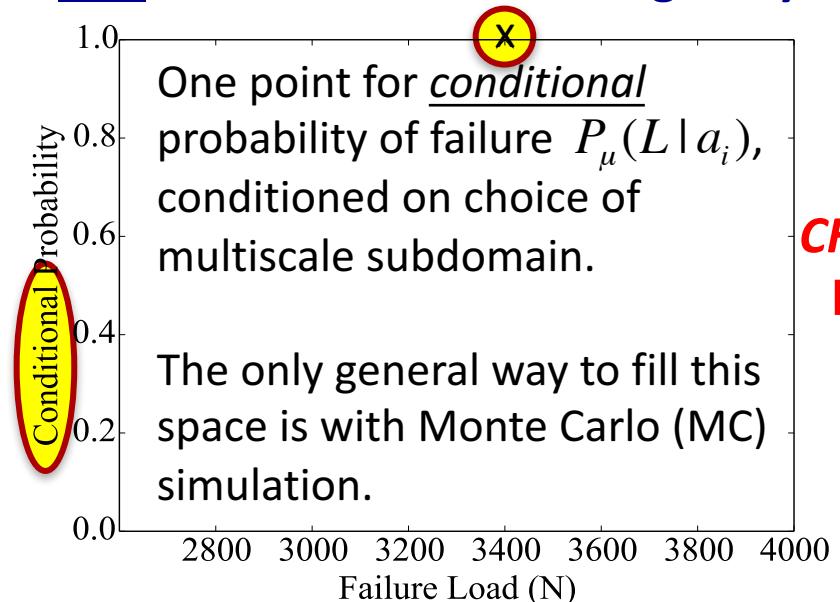


randomly distributed brittle particles embedded in randomly oriented, anisotropic matrix

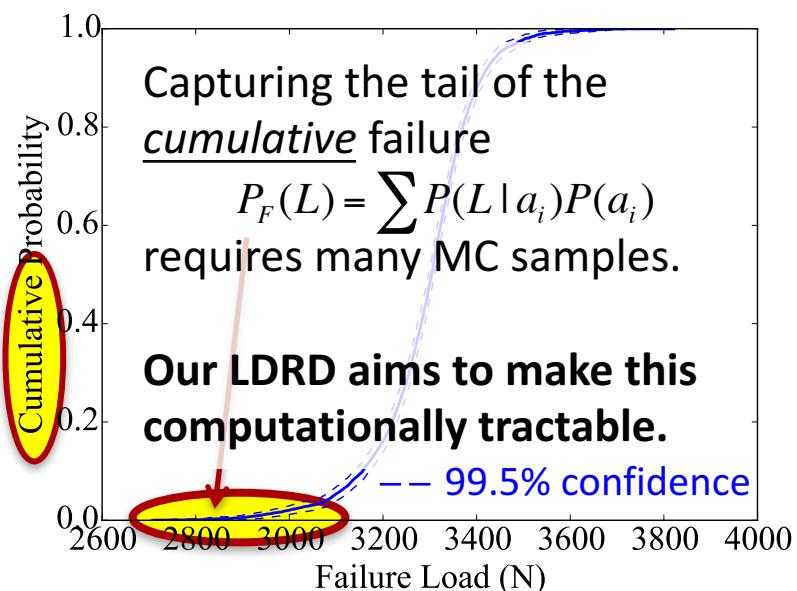
One multiscale calculation is necessary but not sufficient



One multiscale calculation gives you this:



But you set out to compute this:

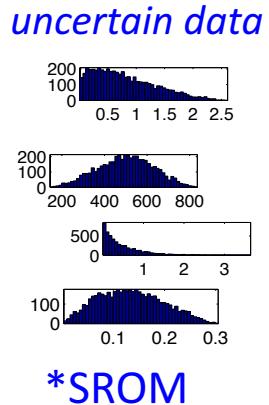


High level goal: tractably propagate fine-scale uncertainty through multiscale calculations

Why does Sandia care? Fracture is local and random, e.g., microstructure, and system/component reliability depends on phenomena occurring at various length scales.

Schematic of our novel hierarchical approach

Low fidelity



prior distribution

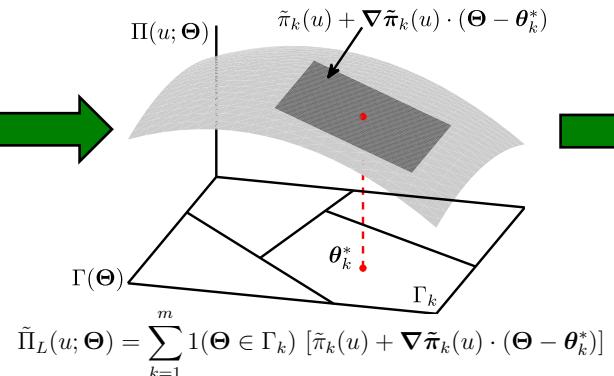
update

Higher fidelity

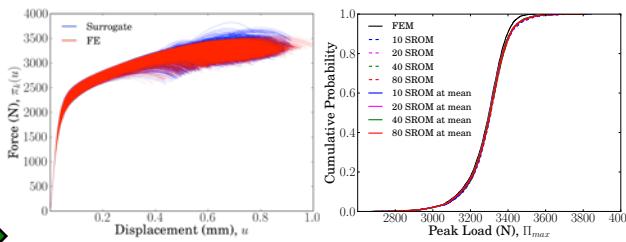
prior distribution of conditional failure

$P'_{\mu}(L|a_i)$

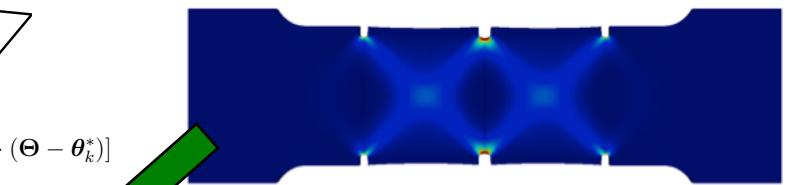
MCS of engineering-scale response via SROM-surrogate



Low-fidelity Probability of Failure



Hot-spot selection & prioritization



For hotspot i , iterate.
Repeat for all hotspots.

$i++$

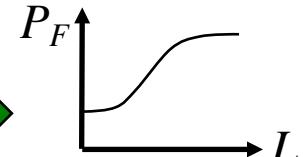
P''_{μ}

L

posterior distribution of conditional failure

$P''_{\mu}(L|a_i)$

$$P_F(L) = \sum_i^{hotspots} P(L|a_i)P(a_i)$$



Higher fidelity prediction

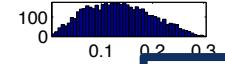
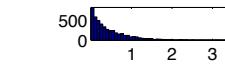
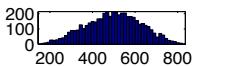
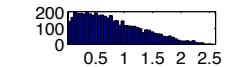
Multiscale calculation

**we assume hot-spots are independent for now

Schematic of our novel hierarchical approach

Low fidelity

uncertain data



*SRO

prior distribution

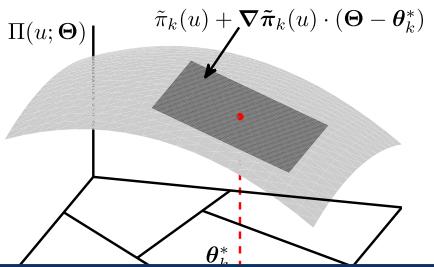
update

Higher fidelity

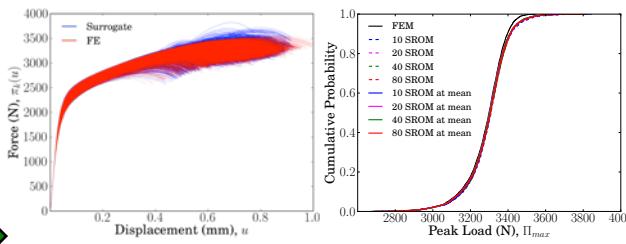
prior distribution of conditional failure

$P'_{\mu}(L|a_i)$

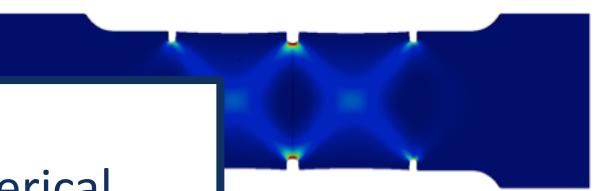
MCS of engineering-scale response via SROM-surrogate



Low-fidelity Probability of Failure



Hot-spot selection & prioritization

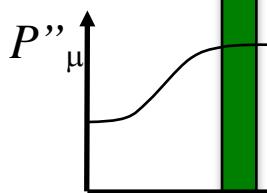
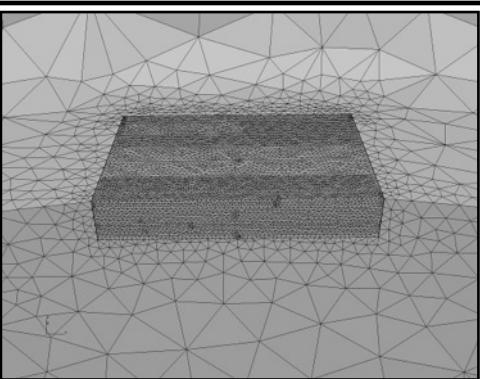


Comments:

1. Independent of the multiscale numerical method, e.g., use outcome from Foulk *et al.*
2. Could be applied to other multiscale physics.

Repeat for all hot-spots

$$P_F(L) = \sum_i^{hotspots} P(L|a_i)P(a_i)$$



posterior distribution of conditional failure

$P''_{\mu}(L|a_i)$

Higher fidelity prediction

Multiscale calculation

Example objectives & uncertainties considered

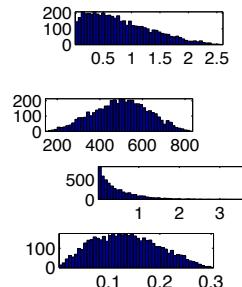
Example: low fidelity prediction of the probability of crack nucleation in an aluminum 6061-T6, engineering “component”

Low **fidelity**

Engineering scale constitutive model

- plasticity parameters
- damage parameters

uncertain data

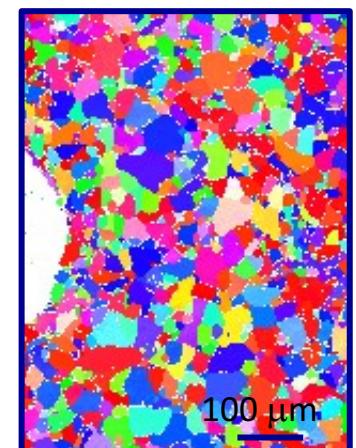


Example: build a probability model for crystal orientation and explore the effect of texture on the yield surface and void nucleation

Higher **fidelity**

Meso-scale plastic response

- texture = crystallographic orientation



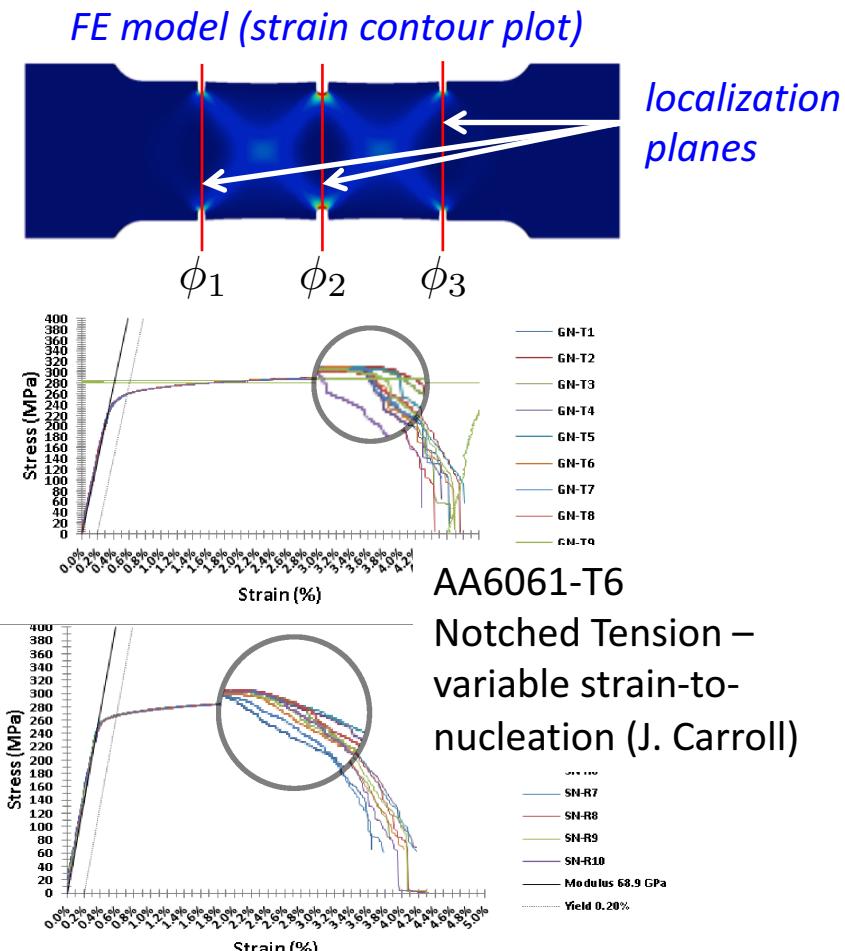
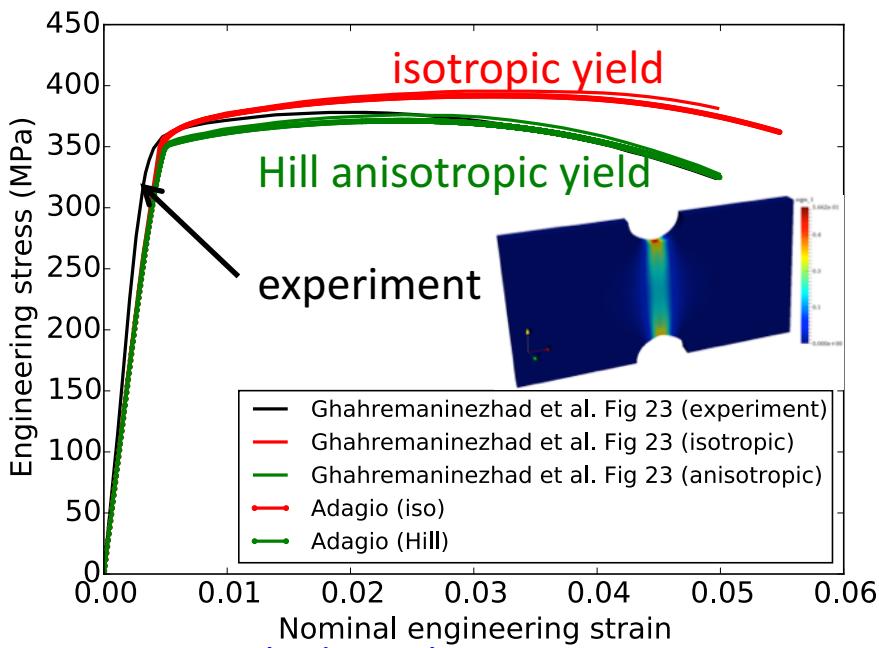
Engineering-scale model

- We use Hill anisotropic plasticity w/ damage and localization elements for numerical regularization on 3-planes (see figure). We use SROMs for uncertainty.
- Calibrate plasticity to tension data; calibrate damage to various notched-tension data.

damage:

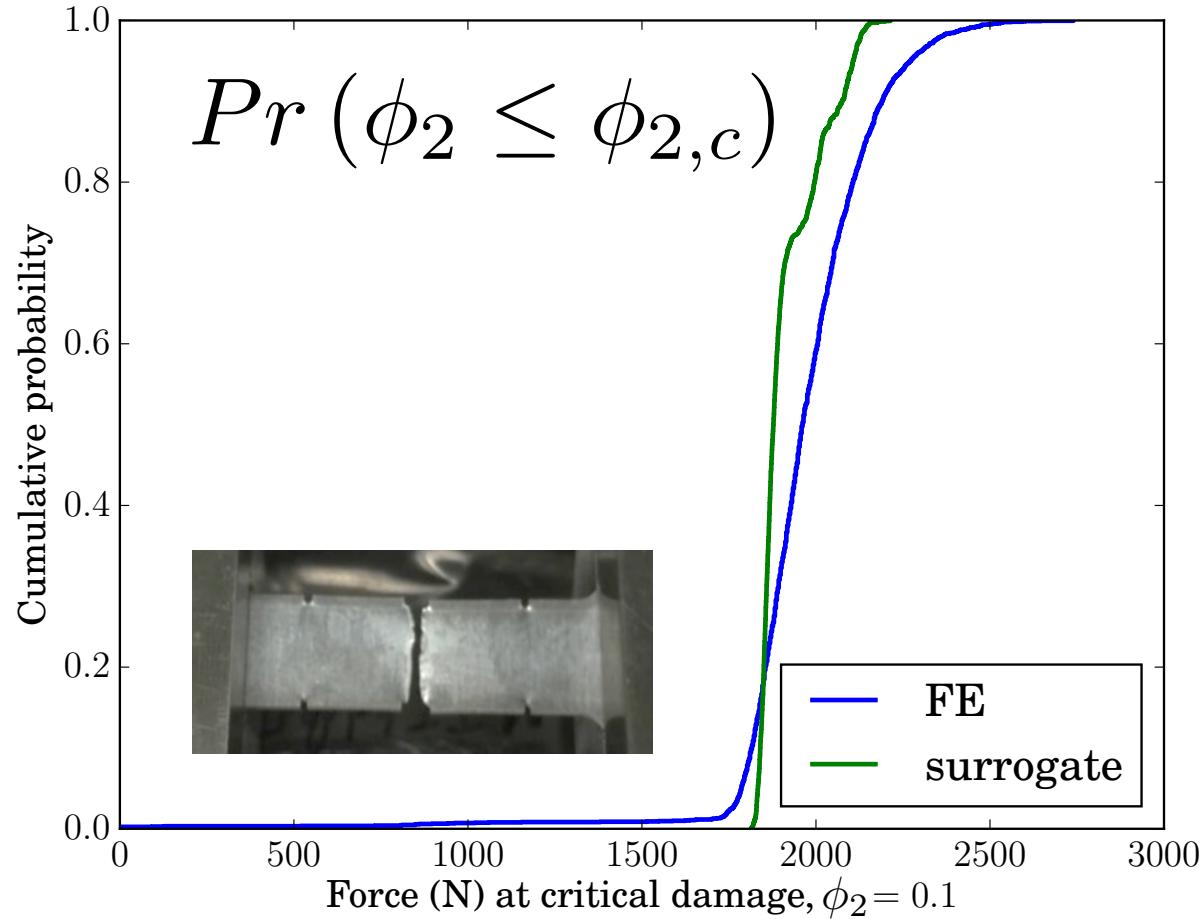
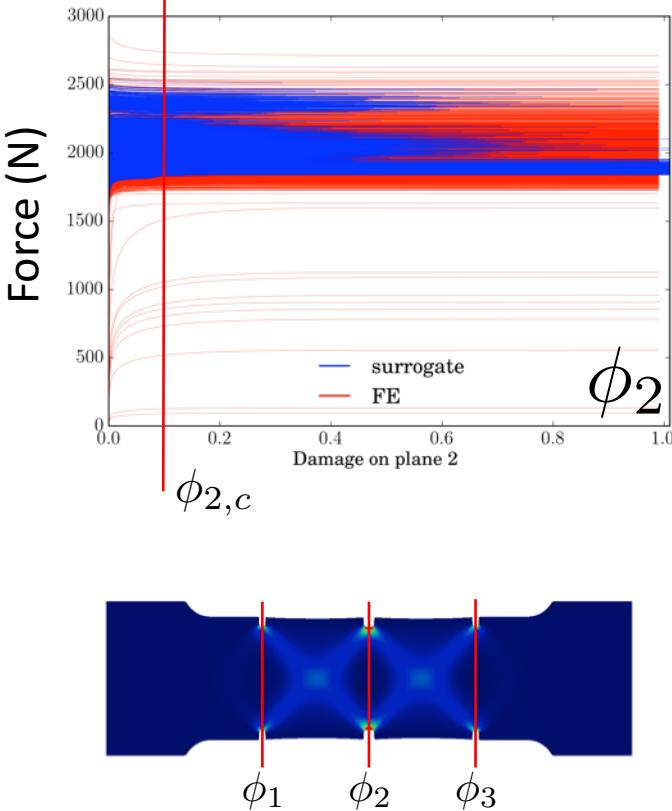
$$\dot{\phi} = \sqrt{\frac{3}{2}} \dot{\epsilon}_p \frac{1 - (1 - \phi)^{m+1}}{(1 - \phi)^m} \sinh \left[\frac{2(2m - 1)}{2m + 1} \frac{p}{\sigma_{vm}} \right]$$

$$\dot{\eta} = \eta \dot{\epsilon}_p \left[N \left\| \frac{I_1}{\sqrt{J_2}} \right\| \right]$$



Probability of nucleation for Low-fidelity predictions

- We construct a surrogate model for damage.
- Then, from damage, we can construct a CDF for failure load at some critical value of damage, *e.g.*, $\phi_{2,c} = 10\%$.

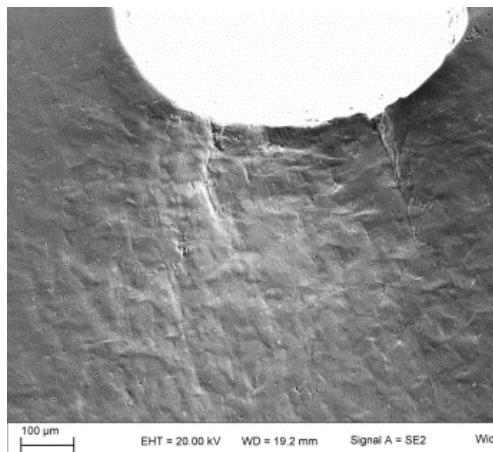
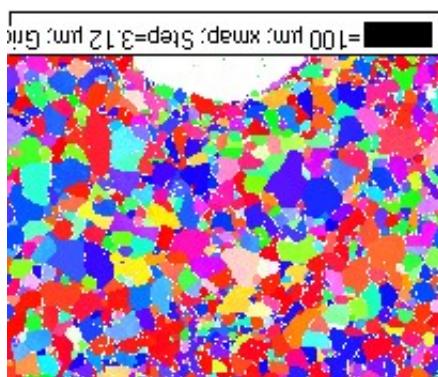
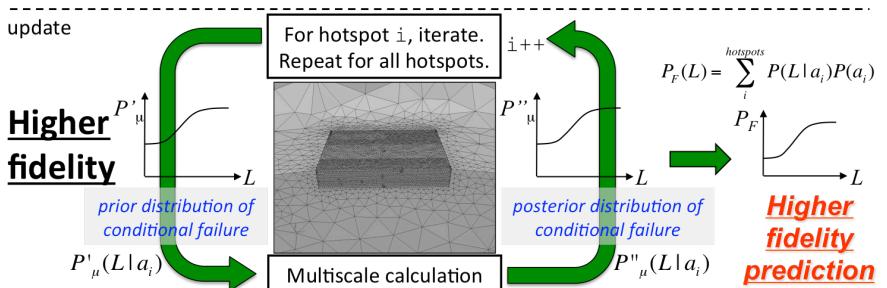


Higher fidelity – focused on texture

Build a probability model for crystal orientation and explore the effect of texture on the yield surface and embedded second-phase particles

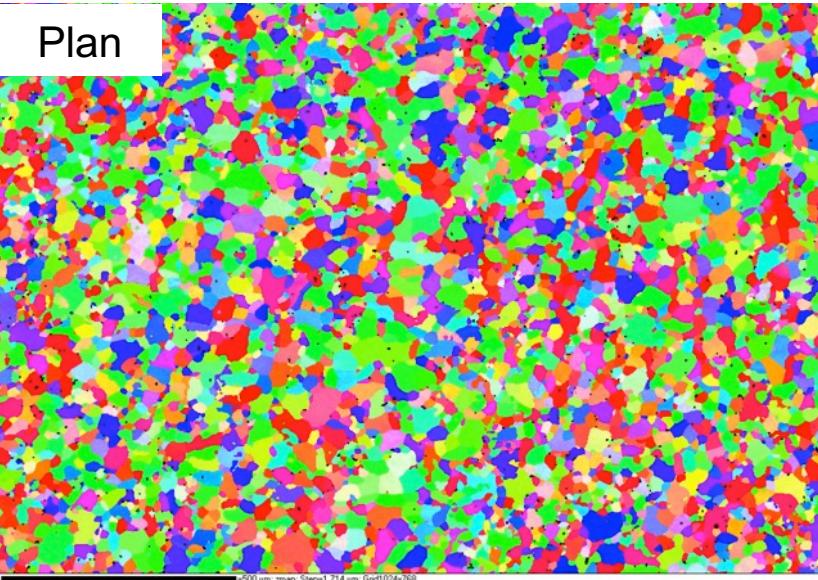
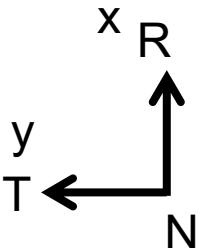
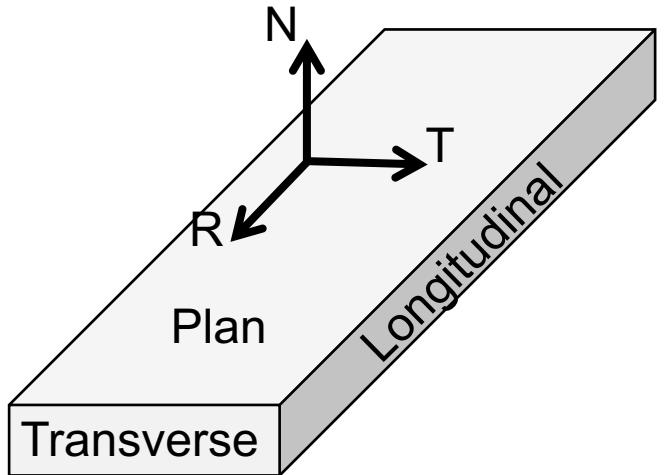
Things we need:

- Data to support fine scale uncertainty – we focus on crystallography and use EBSD measurements of crystallographic orientation
- Computational microstructure: morphology; mesh; & texture models



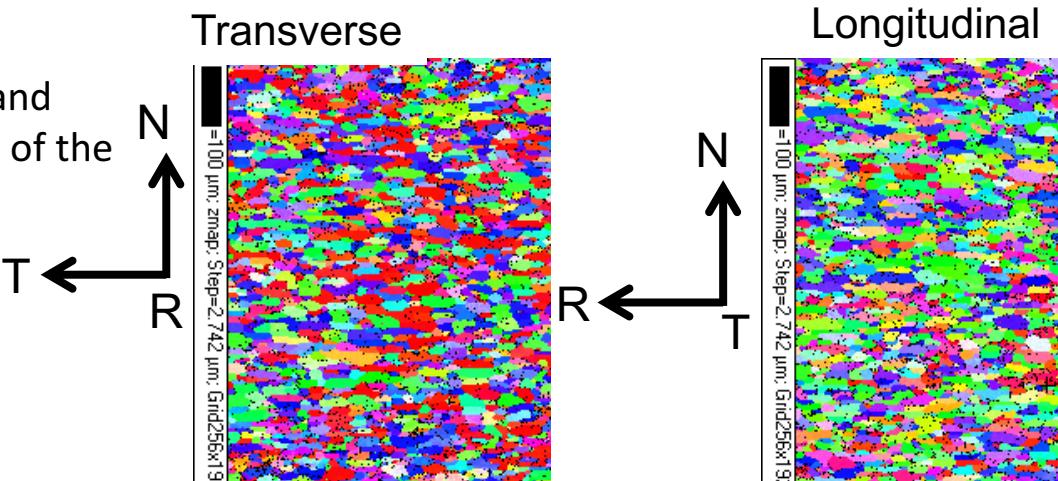
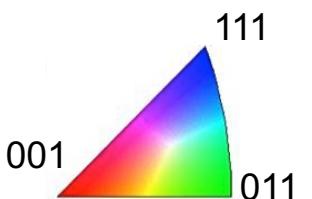
AA 6061-T6 – EBSD measurements/images at a notch tip

AA6061-T6 EBSD on three planes shows pancake-shaped grains with mild texture



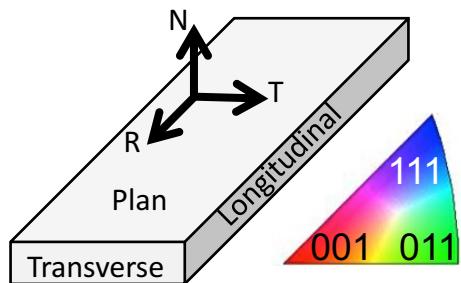
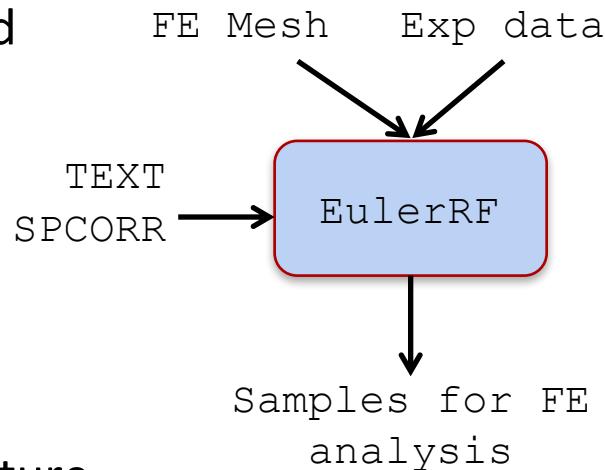
From Ghahremaninezhad & Ravi-Chandar, and confirmed for our material, mean grain size of the rolled 6061 microstructure:

y-z mean 15 μm
x-z mean 14 μm
x-y mean 39 μm

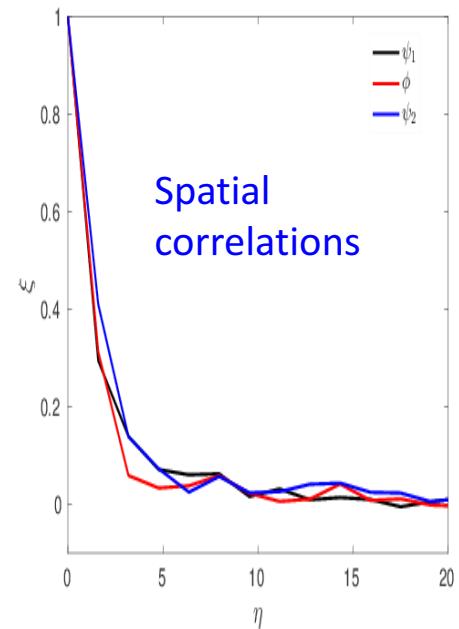
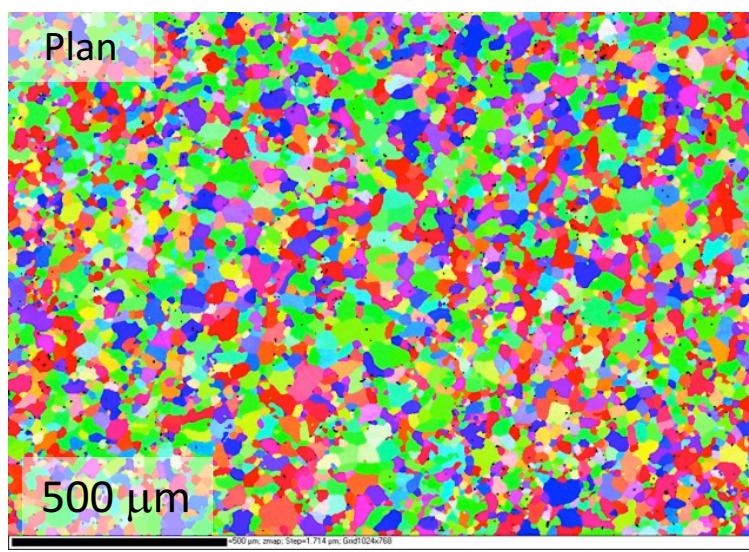


“EulerRF” Code

- Code to generate samples of Euler angle random field model for FE meshes, implemented in MATLAB
- Input:
 - Finite element mesh (grain centroids)
 - Texture data (EBSD data – AA6061 below)
 - User options
- Output: samples of no texture, macro- and micro-texture



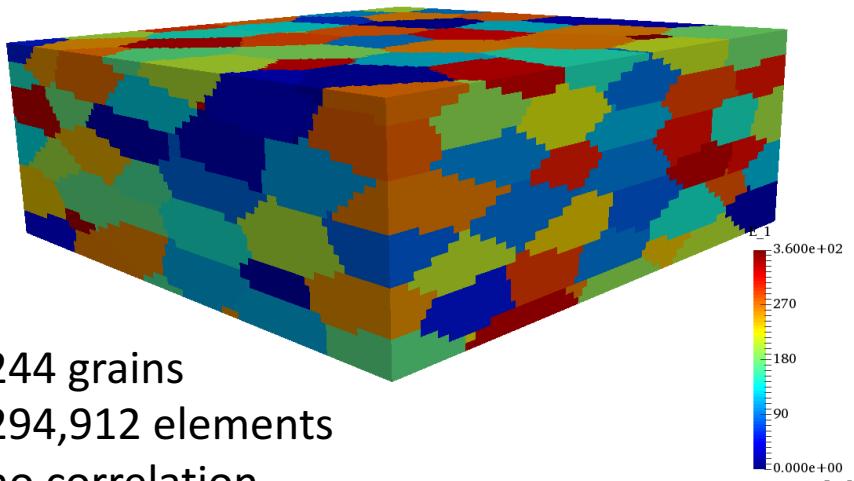
Ghahremaninezhad *et al.*,
mean grain size:
y-z mean 15 μm
x-z mean 14 μm
x-y mean 39 μm



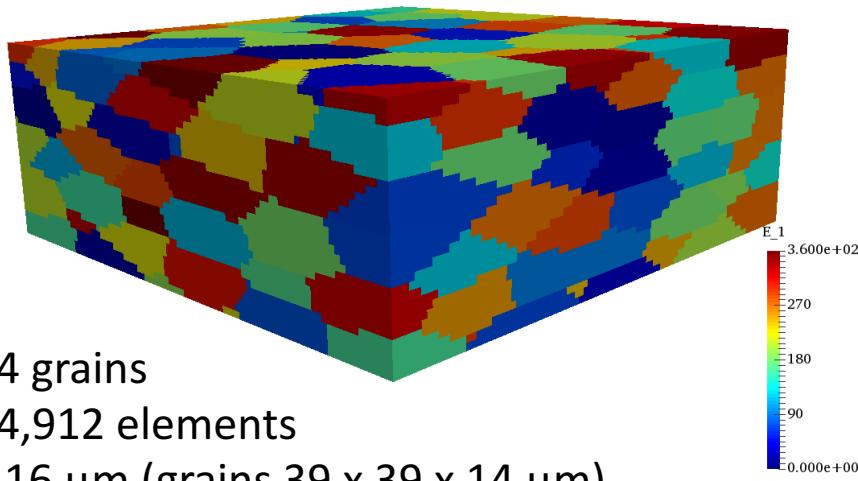
3D Samples for AA 6061 T6 rolled sheet

- 2 samples each macro-texture (left) & micro-texture (right)

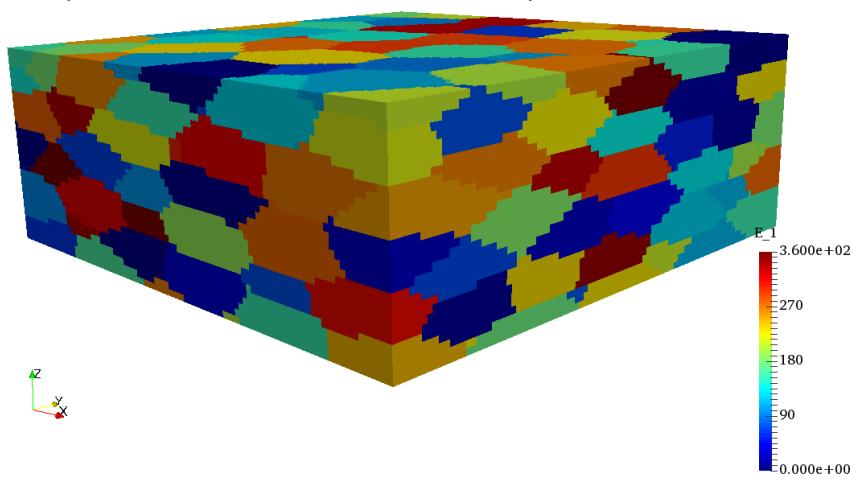
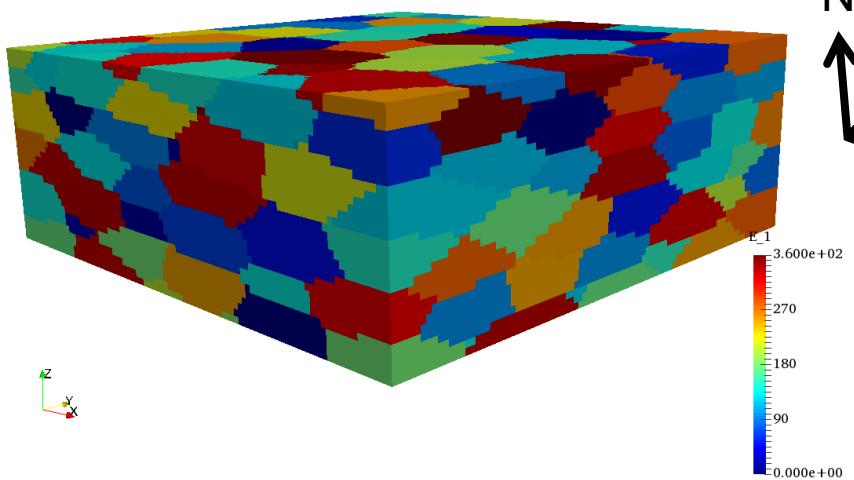
“Macro” texture



“Micro” texture

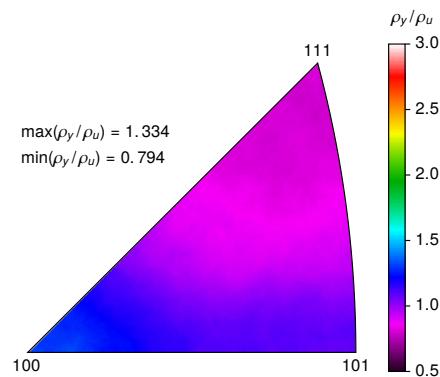
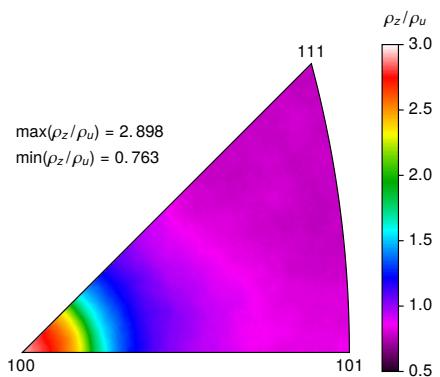
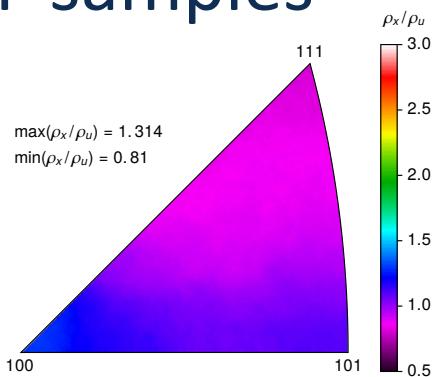


N
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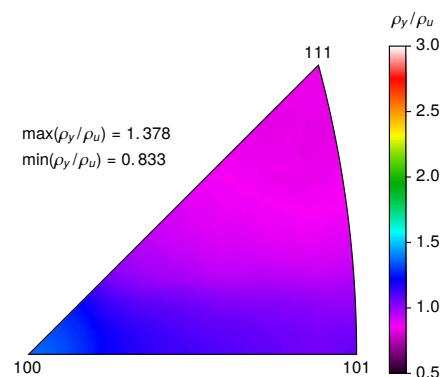
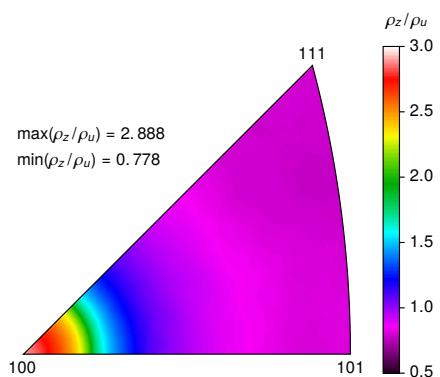
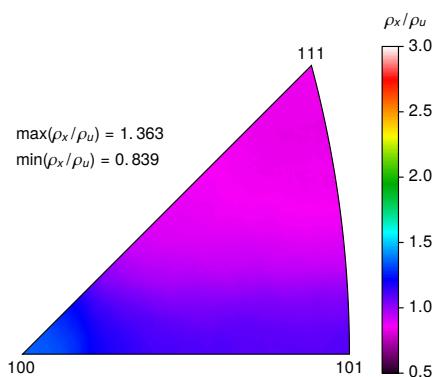


Inverse pole figure (IPF) comparing EBSD to eulerRF samples

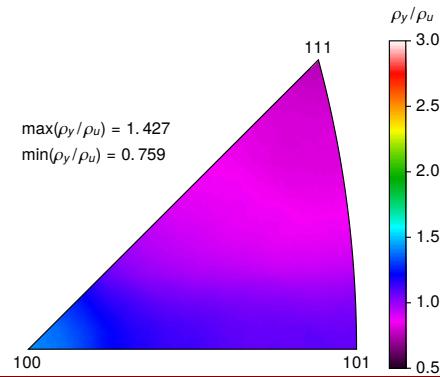
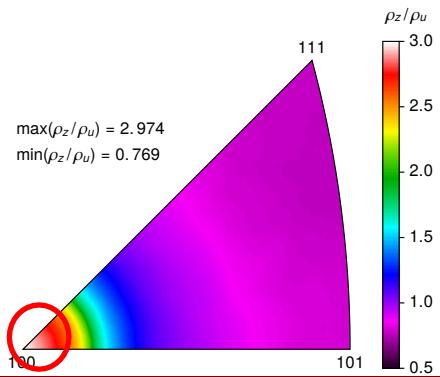
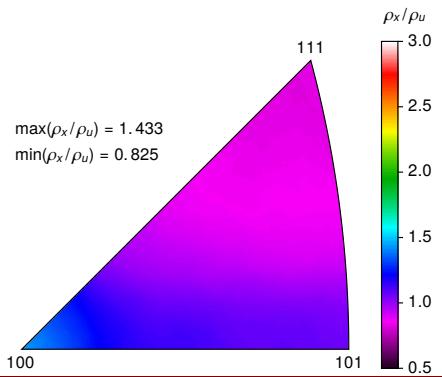
measured
EBSD data



macro-
texture



micro-
texture



Crystal plasticity formulation

- Here we use a simple crystal plasticity formulation following Matous and Maniatty 2004 :

$$\mathbf{L}^p = \sum_{\alpha=1}^{12} \dot{\gamma}^\alpha \mathbf{P}^\alpha$$

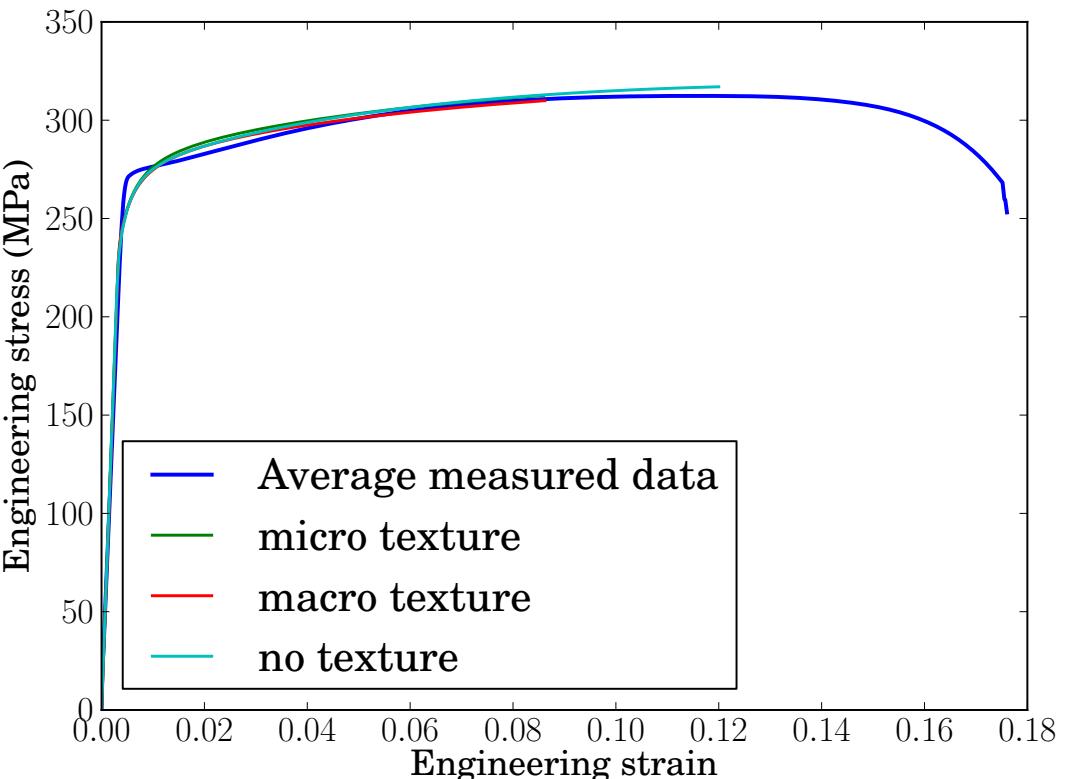
$$\mathbf{P}^\alpha = \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha$$

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{g^\alpha} \right|^{1/m} \text{sign}(\tau^\alpha)$$

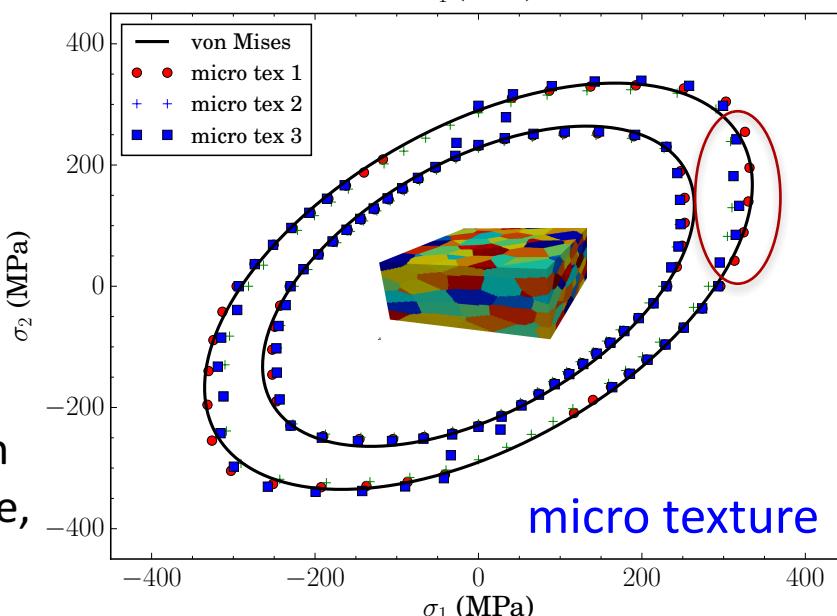
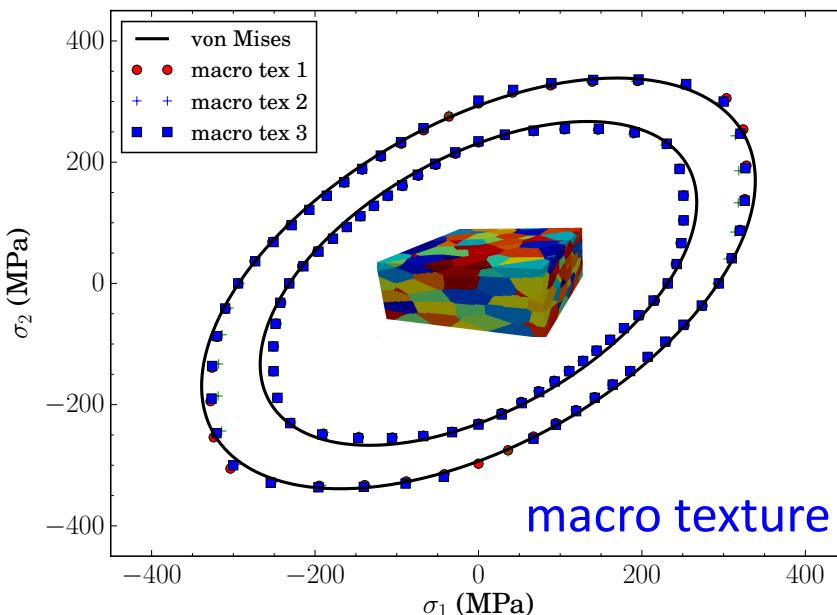
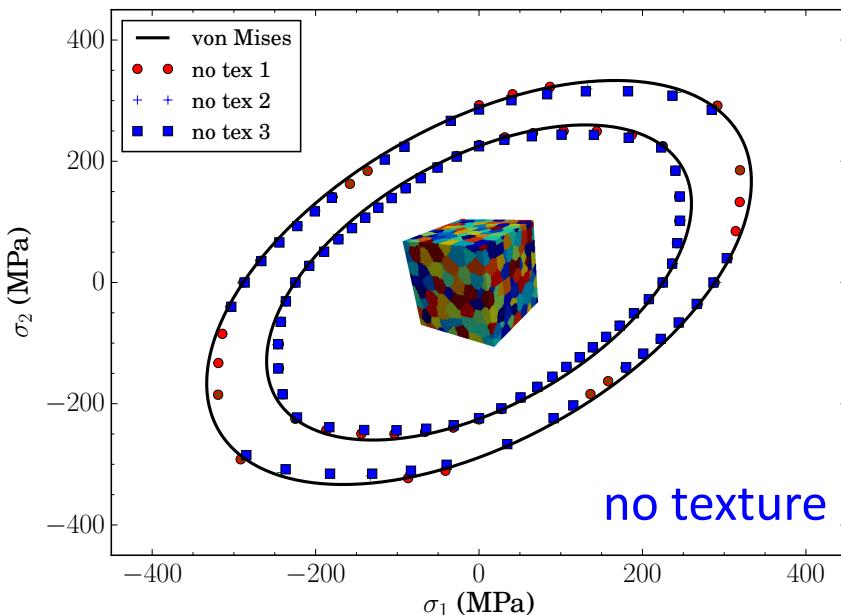
$$\dot{g} = G_0 \left(\frac{g_{s_0} - g}{g_{s_0} - g_0} \right) \dot{\gamma}$$

$$\dot{\gamma} = \sum_{\alpha=1}^{12} |\dot{\gamma}^\alpha|$$

	no texture	micro texture	macro texture
g_0	110.6	114.0	115.2
g_{s_0}	169.4	172.8	174.7
G_0	116.6	116.6	116.6
m	0.01	0.01	0.01



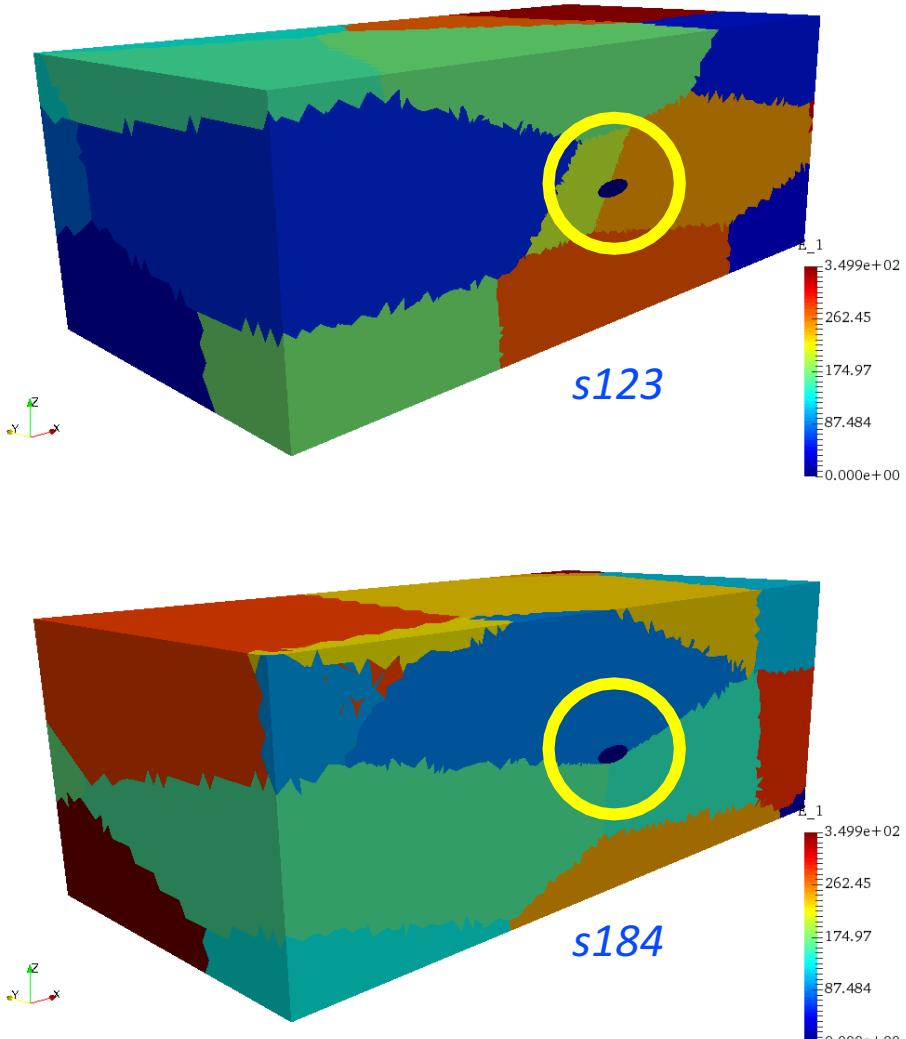
Yield surfaces recovered from simulations w/ various textures



- Using a simple crystal plasticity constitutive model for each texture
- Plotting yield surface at 0.2% and 2.0% offset assuming small strains
- We observe greater heterogeneity in micro texture (“super grain” – need a larger RVE?)
- There are subtle differences from the von Mises yield surface for all forms of texture, may be amplified at higher strains

Void nucleation at brittle second phase

- Embed an ellipsoidal particle, 5 μm x 1.8 μm
- Coherent mesh at particle/matrix interface, grains by overlay method
- 2 morphologies w/ \sim 27 grains, s123 & s184
- 200 samples of macro-texture & 55 samples of micro-texture
- Assumed elastic mechanical properties for particle (pure iron)
 - $E = 211 \text{ GPa}$, $\nu = 0.29$
 - Strength 540 MPa
- Assumed perfect and rigid particle/matrix interface bond



Cross-sections through major-axis of ellipsoid

Quantify particle fracture with mean, first-principal stress

Assuming elastic and brittle, monitor the mean first-principal stress in the particle.

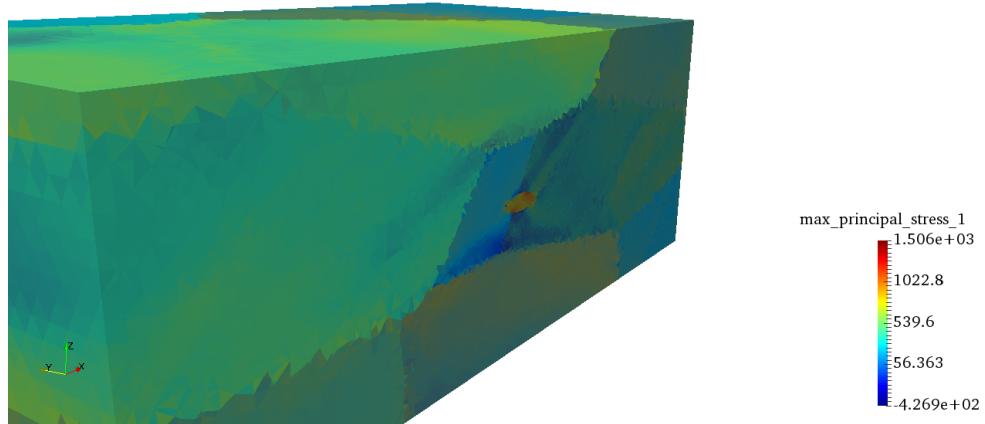
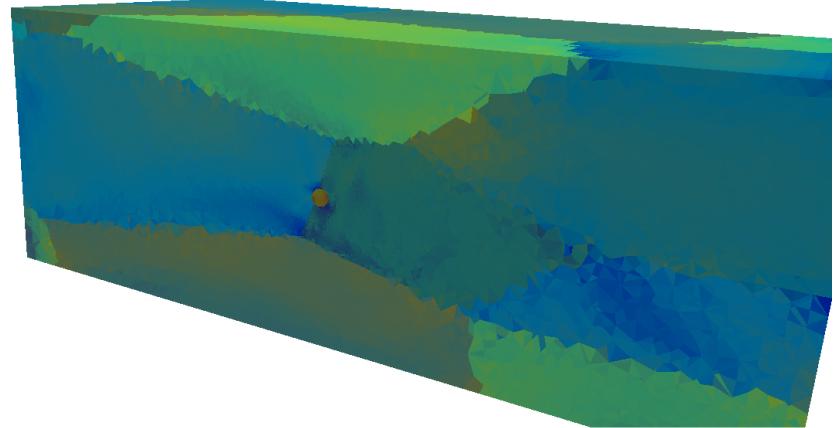
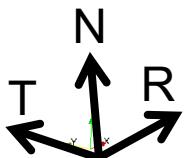
$$Pr(\bar{\epsilon}_{RVE} \in S)$$

$$S = \{\bar{\epsilon}_{RVE} \in \mathbb{R} : g(\bar{\epsilon}_{RVE}) \leq 0\}$$

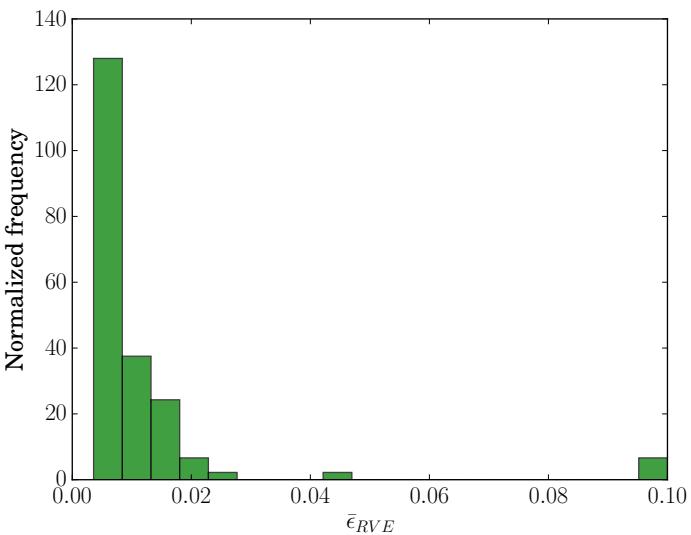
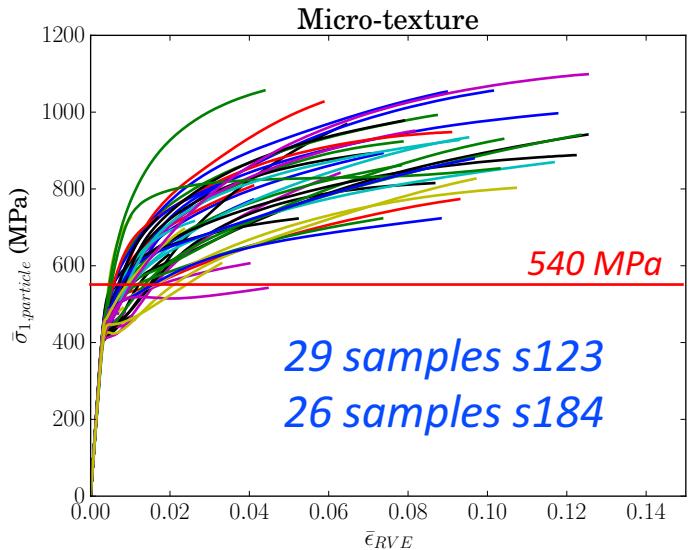
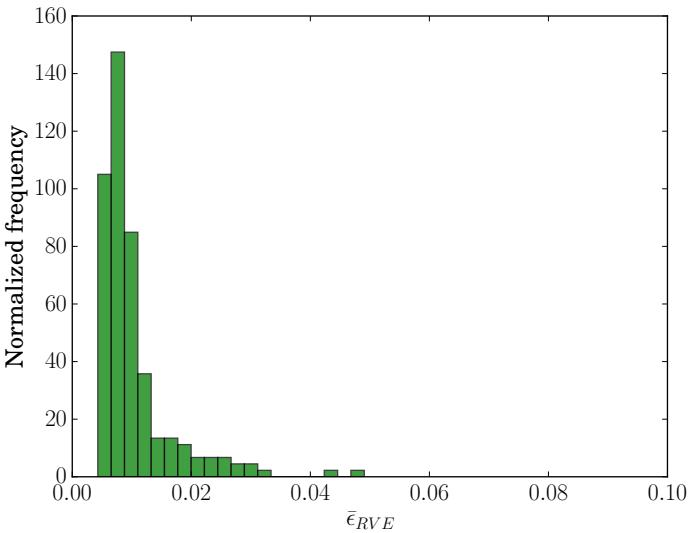
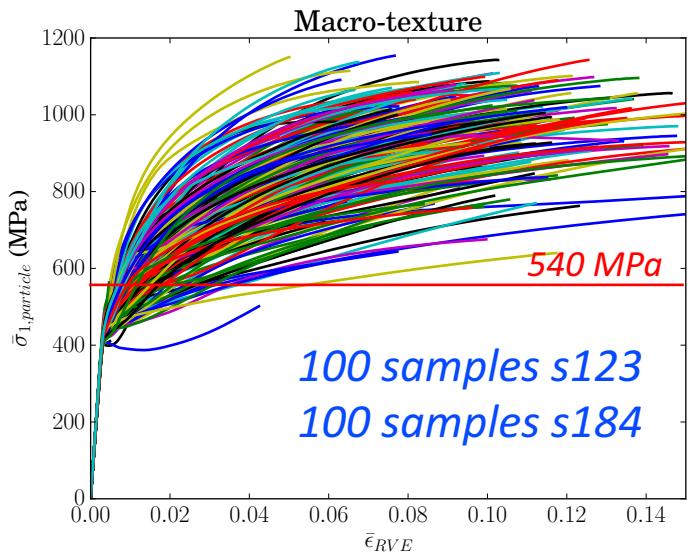
$$g(\bar{\epsilon}_{RVE}) = \bar{\sigma}_{p,cr} - \bar{\sigma}_p(\bar{\epsilon}_{RVE})$$

$$\bar{\sigma}_{p,cr} = 540 \text{ MPa}$$

Maximum principal stress contour plot for s123 (showing two, orthogonal cross-sections)



Mean max principal stress in particle

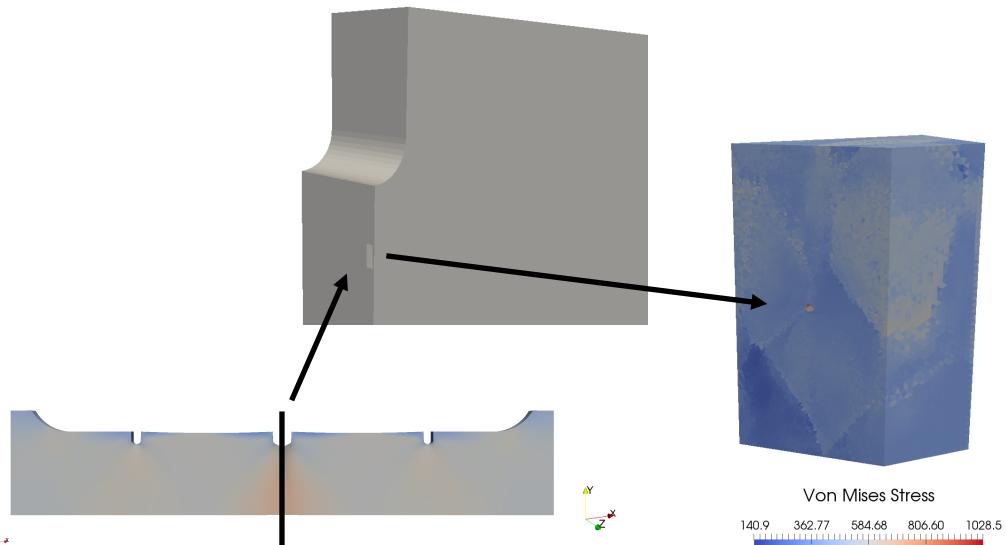


Bridging length scales

- We are pursuing three strategies and will contrast them:
 - Submodeling
 - Concurrent coupling with a Schwarz-based algorithm (Foulk, Alleman, & Mota)
 - Direct numerical simulation

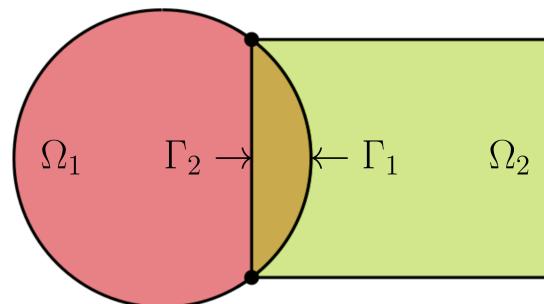
Submodeling:

- Mesh through region where submodel will exist
- Run engineering-scale model
- Map displacements from engineering-scale model onto boundaries of meso-scale model

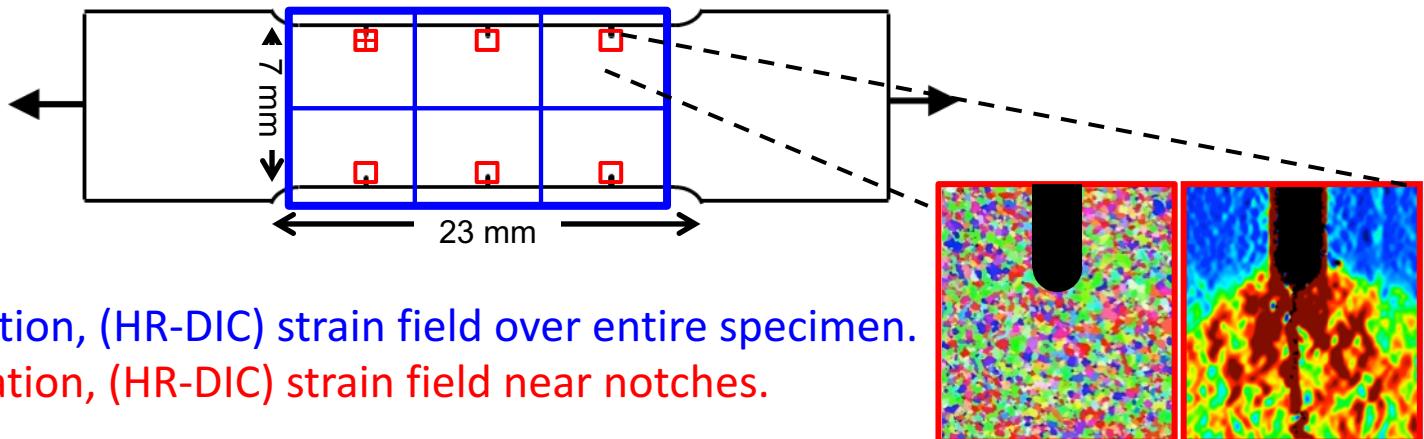


Schwarz-based solution scheme:

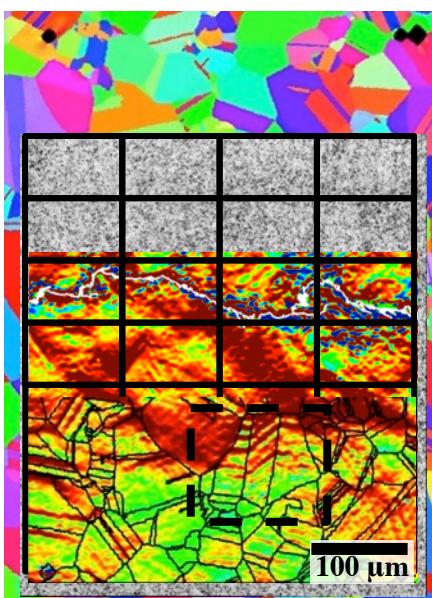
- Solve PDE by any method on Ω_1 using an initial guess for Dirichlet BCs on Γ_1 .
- Solve PDE by any method (can be different than for Ω_1) on Ω_2 using Dirichlet BCs on Γ_2 that are the values just obtained for Ω_1 .
- Solve PDE using Dirichlet BCs on Ω_1 that are the values just obtained for Ω_2 .
- Mathematically proved to converge for solid mechanics problems.



Multiscale DIC for experimental validation



- Low magnification, (HR-DIC) strain field over entire specimen.
- High magnification, (HR-DIC) strain field near notches.

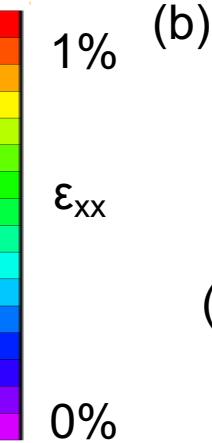
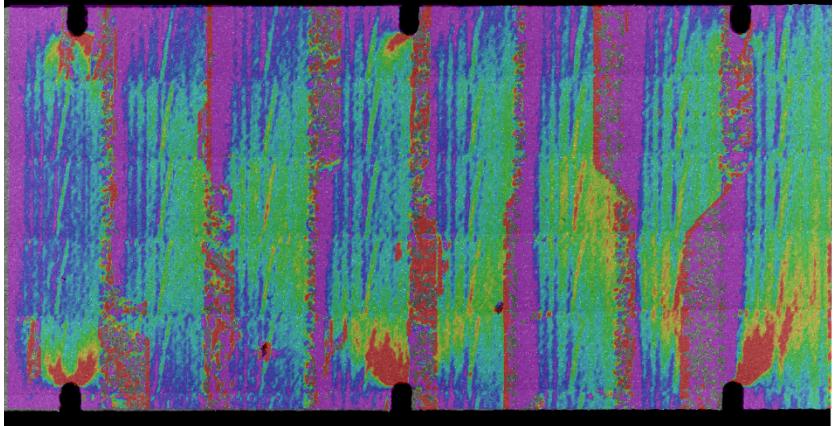


1. EBSD: microstructure
2. Capture reference images
3. Load specimen
4. Capture deformed images
5. DIC on each image location.
6. Stitch DIC results into large field of view
7. Overlay Microstructure

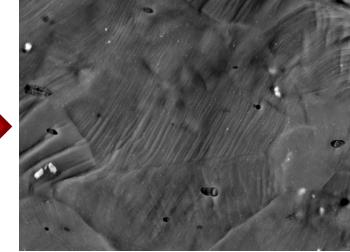
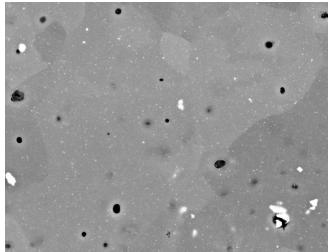
Requires a multi-resolution speckle pattern

DIC near each notch tip and throughout entire specimen using HR-DIC

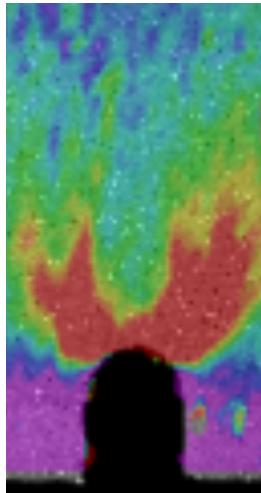
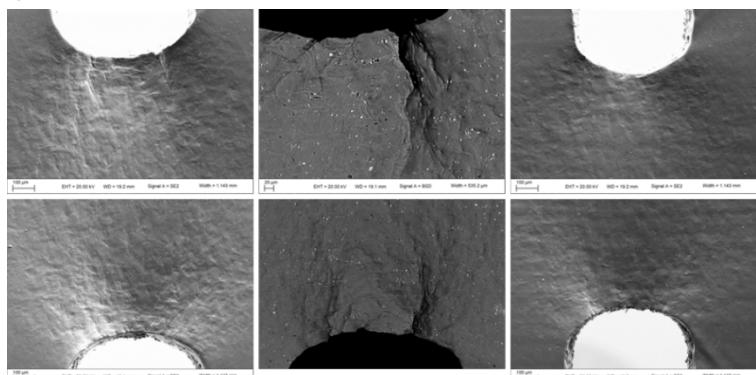
(a)



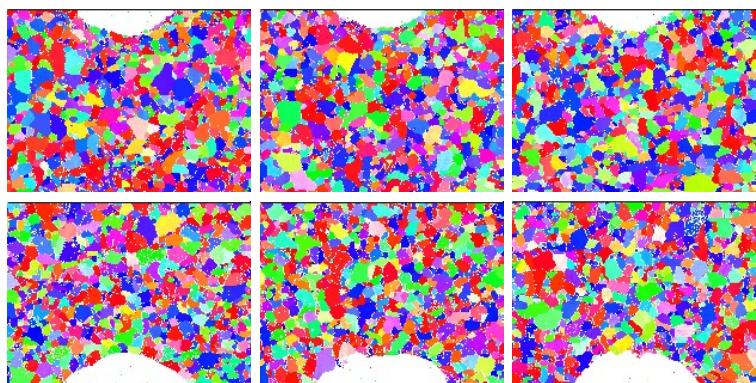
(b)



(c)

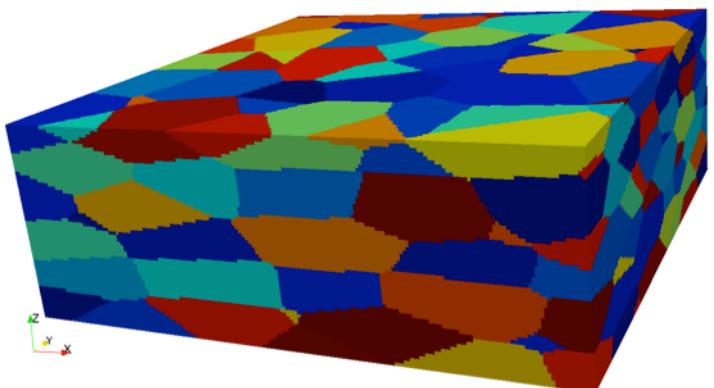
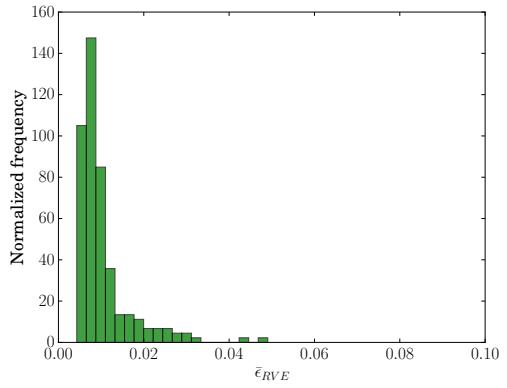
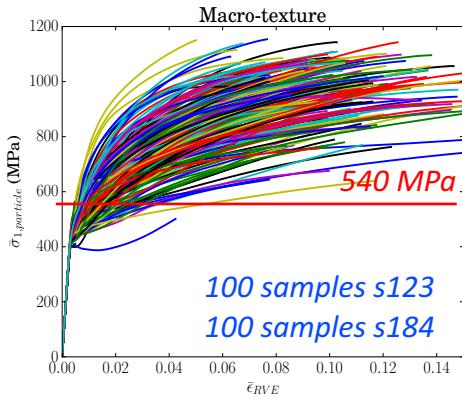


- (a) Learning to correct or eliminate lens distortion for low magnification SEM images.
- (b) Need to capture more images throughout loading because the material looks so different near failure.
- (c) Natural speckles lose contrast at high load levels we are interested in.



Summary

- Structural reliability is a function of *random* microstructure and multiscale numerical methods are necessary for predictive simulation *but they are not sufficient*. One multiscale simulation is insufficient to predict reliability.
- We summarized our hierarchical approach for tractable multiscale UQ.
- We briefly summarized the engineering-scale calculations.
- We demonstrated calculations for meso-scale void nucleation prediction with various models for texture.





May I answer your questions?

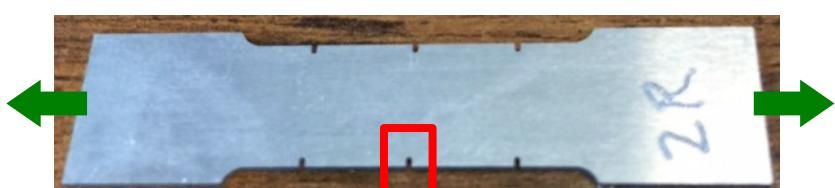
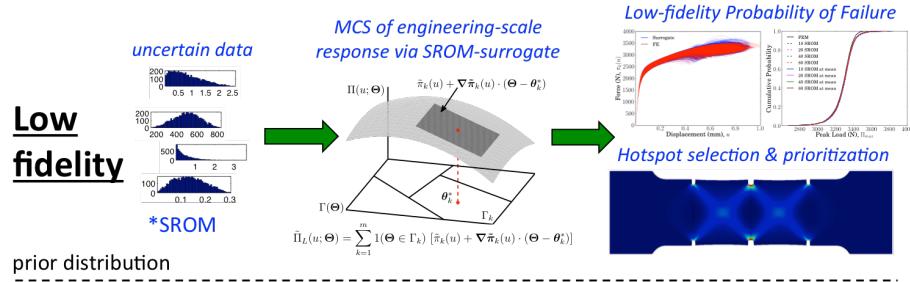
- Intentionally blank

Details needed for low fidelity simulation

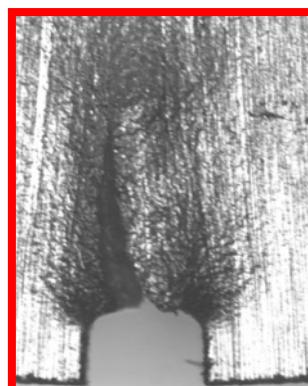
Example: low fidelity prediction of the probability of crack nucleation in an aluminum 6061-T6, engineering “component”

Things we need:

1. Engineering-scale model
2. Method for uncertainty propagation – we use stochastic reduced-order models (SROM)
3. Engineering-scale failure metric (quantity of interest) for hot-spot selection

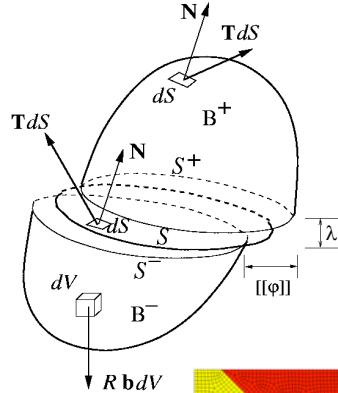


*predict nucleation for AA6061-T6
“component” in monotonic loading*



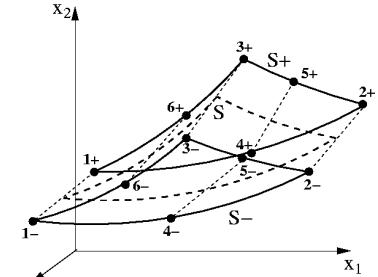
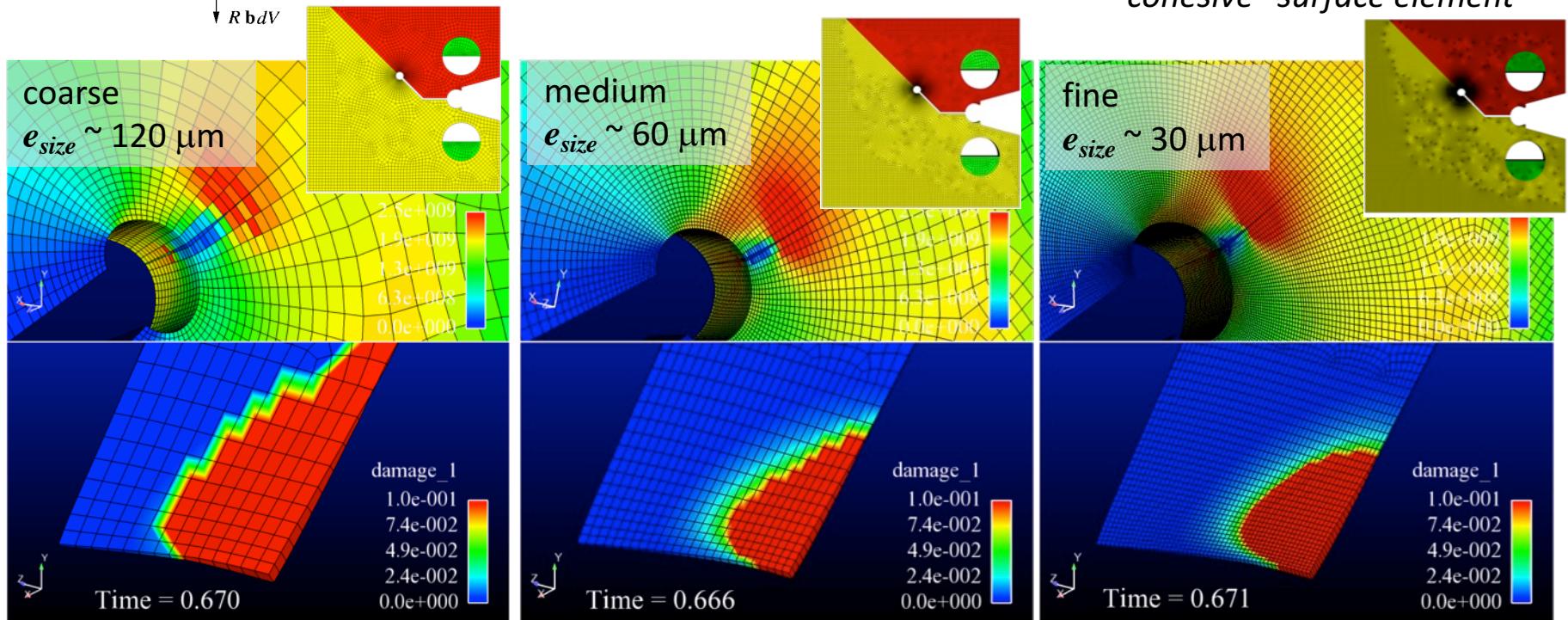
Localization elements to regularize

Capture localization processes with mesh convergence. Localization elements construct a deformation gradient (use existing constitutive models).

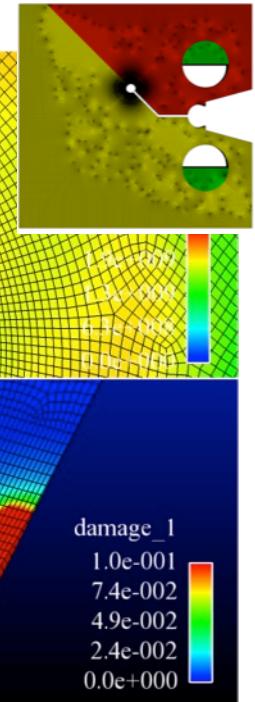


$$\begin{aligned}
 \mathbf{F} &= \mathbf{F}^{\parallel} \mathbf{F}^{\perp} \\
 \mathbf{F}^{\parallel} &= \mathbf{g}_i \otimes \mathbf{G}^i \quad \mathbf{F}^{\perp} = \mathbf{I} + \frac{[\![\lambda]\!]}{l} \otimes \mathbf{N} \\
 \mathbf{F} &= \mathbf{F}^{\parallel} + \frac{[\![\lambda]\!]}{l} \otimes \mathbf{N}
 \end{aligned}$$

l = band thickness (user specified)



Topologically the same as
"cohesive" surface element



Stochastic reduced-order model (SROM)

To develop a model that optimally represents the uncertainty in the input we choose a discrete random variable $\tilde{\Theta}$. The SROM is then defined by the collection $(\tilde{\theta}_k, \tilde{p}_k)$ $k = 1, \dots, n$ that minimizes an objective function of the form:

$$\max_{1 \leq r \leq \bar{r}} \max_{1 \leq s \leq d} \alpha_{s,r} |\tilde{\mu}_s(r) - \hat{\mu}_s(r)| + \max_x \max_{1 \leq s \leq d} \beta_s |\tilde{F}_s(x) - \hat{F}_s(x)| + \zeta_{s,t} \max_{s,t} |\tilde{c}(s,t) - \hat{c}(s,t)|$$


moments **cumulative distribution** **correlation**

Estimates of SROM statistics given SROM sample size n

$$\tilde{\mu}_s(r) = \mathbf{E}[\tilde{\Theta}_s^r] = \sum_{k=1}^n p_k (\tilde{\theta}_{k,s})^r$$

$$\tilde{F}_s(x) = \Pr(\tilde{\Theta}_s \leq x) = \sum_{k=1}^n p_k \mathbf{1}(\tilde{\theta}_{k,s} \leq x)$$

$$\tilde{c}(s, t) = \mathbb{E}[\tilde{\Theta}_s \tilde{\Theta}_t] = \sum_{k=1}^n p_k \tilde{\theta}_{k,s} \tilde{\theta}_{k,t}$$

Estimates of sample statistics given q samples of Θ

$$\hat{\mu}_s(r) = \sum_{i=1}^r (1/q)(\theta_{i,s})^r$$

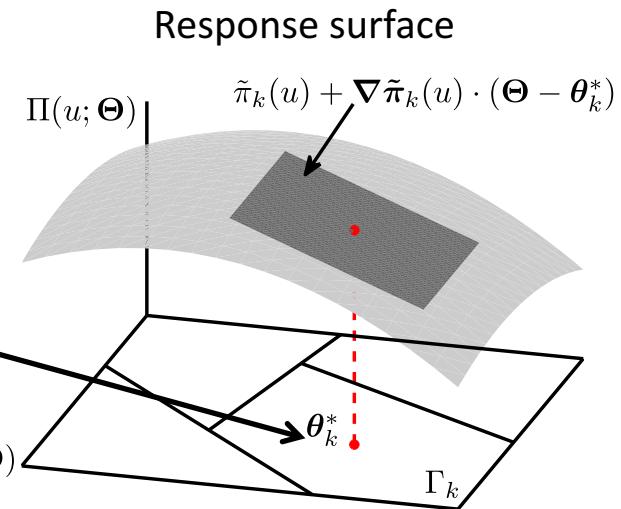
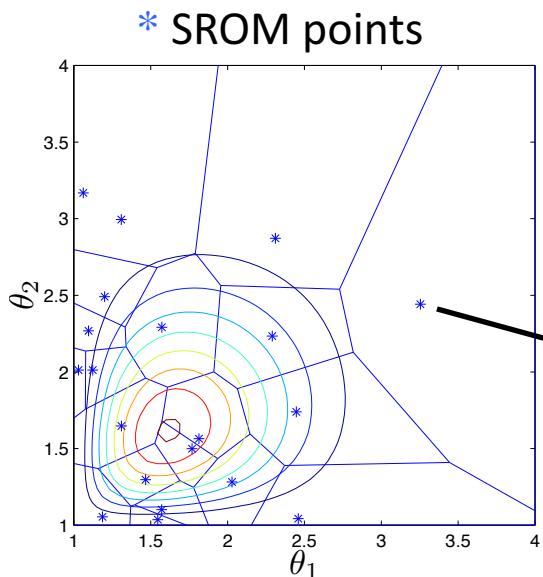
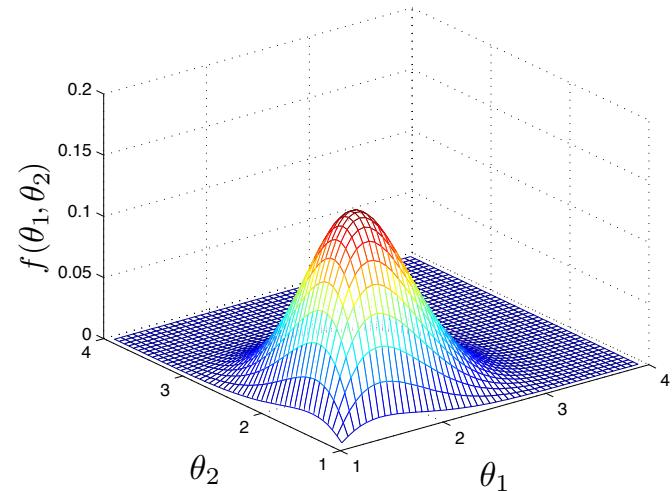
$$\hat{F}_s(x) = \sum_{i=1}^q (1/q) \mathbf{1}(\theta_{i,s} \leq x)$$

$$\hat{c}(s, t) = \sum_{i=1}^q (1/q) \theta_{i,s} \theta_{i,t}$$

with $n \ll q$ and $\alpha, \beta, \zeta > 0$ are weights and subject to probabilities $\tilde{p}_k \geq 0$ and $\sum_k \tilde{p}_k = 1$.

Construction of SROM-based surrogate

Example 2D probability density



- A response surface is constructed for the structural response of the component, $\Pi(u; \Theta)$
- The surface is a series of hyper-planes described with a first-order Taylor approximate of the structural response

$$\tilde{\Pi}_L(u; \Theta) = \sum_{k=1}^n \mathbf{1}(\Theta \in \Gamma_k) [\tilde{\pi}_k(u) + \nabla \tilde{\pi}_k(u) \cdot (\Theta - \theta_k^*)]$$

- The SROM samples are used as the expansion points θ_k^* and the domain Γ_k are determined by the Voronoi tessellation of the uncertain parameters
- Requires $n*(d+1)$ FE calculations

Assumes the quantity of interest is differentiable.

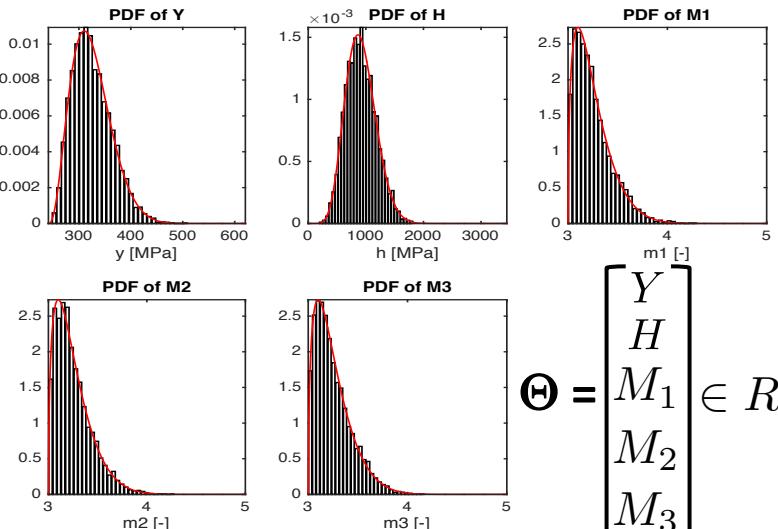
Calculations demonstrating progress toward the goal

- Plasticity parameters, y and h , calibrated to 10 smooth tensile tests for AA 6061-T6 sheet.
- Damage exponent, m , calibrated to 20 notched tensile specimens w/ two notch radii for a range of triaxiality

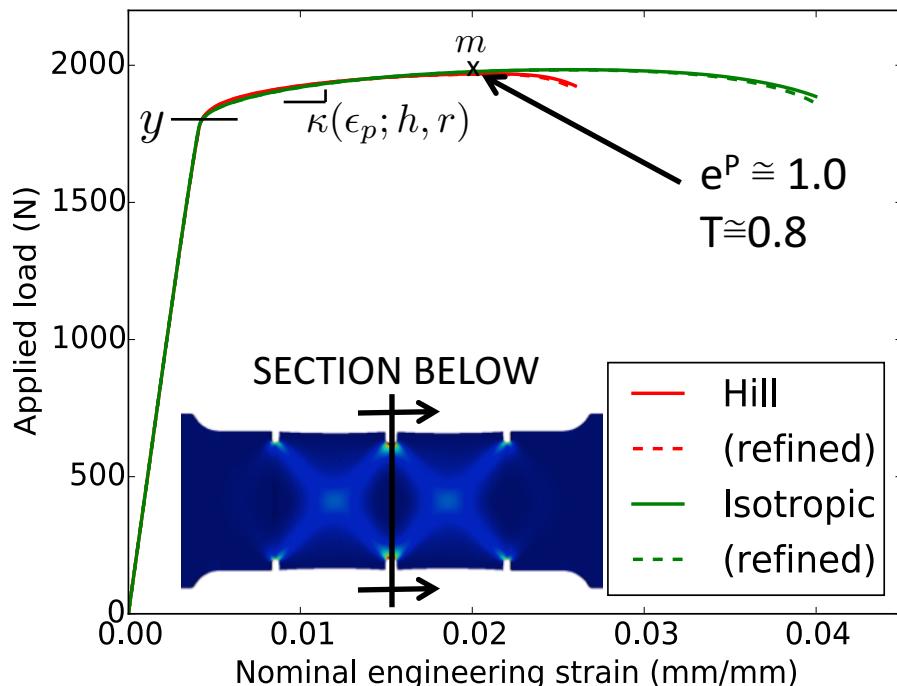
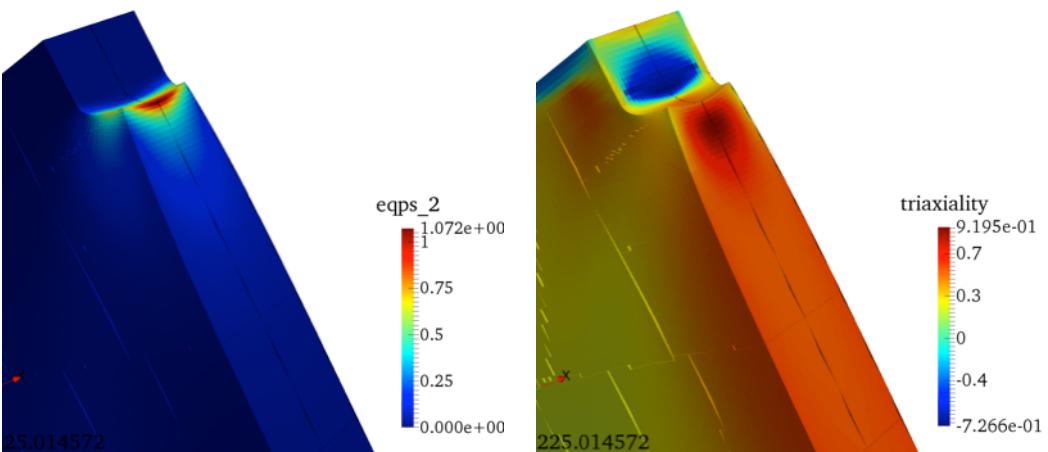
$$\dot{\phi} = \sqrt{\frac{3}{2}} \dot{\epsilon}_p \frac{1 - (1 - \phi)^{m+1}}{(1 - \phi)^m} \sinh \left[\frac{2(2m-1)}{2m+1} \frac{p}{\sigma_{vm}} \right]$$

$$\sigma_y = y + \kappa \quad \kappa(\epsilon_p) = \frac{h}{r} [1 - \exp(-r\epsilon_p)]$$

- We use available data and previous experience and expert judgment to approximate model parameter uncertainty.

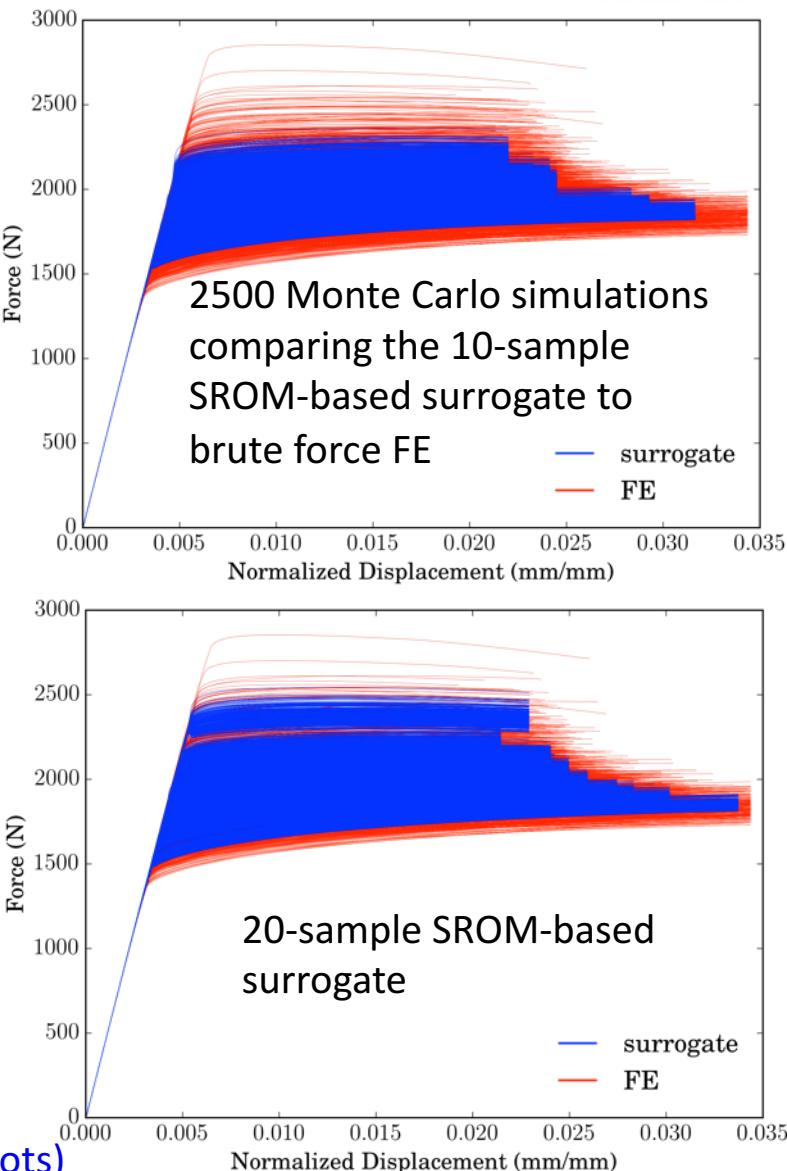
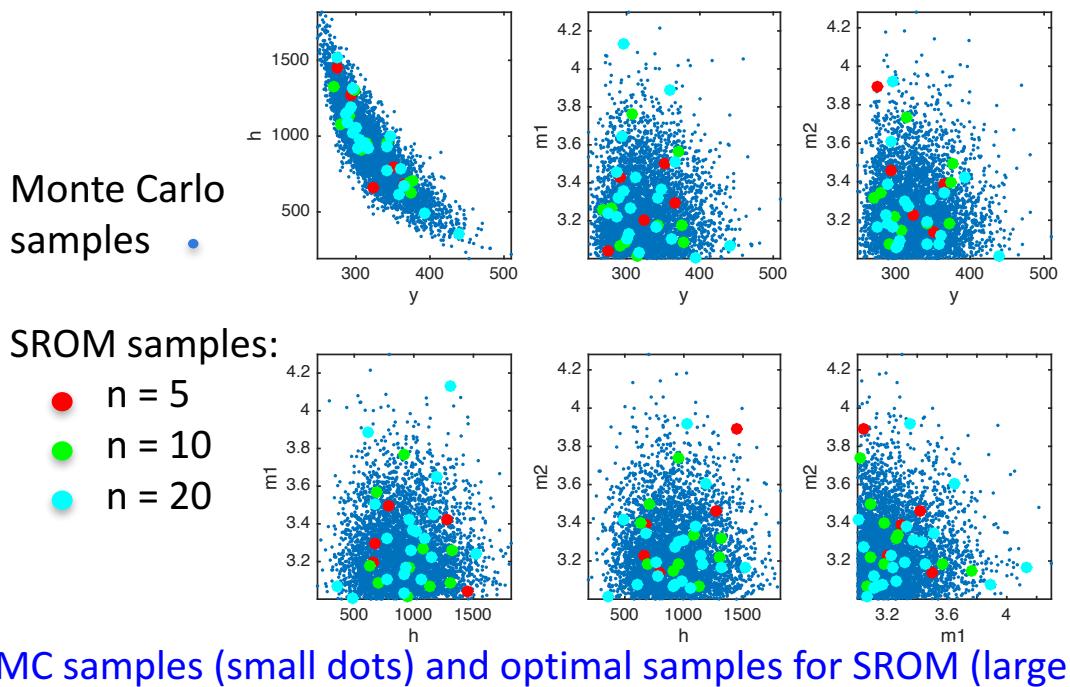


$$\Theta = \begin{bmatrix} Y \\ H \\ M_1 \\ M_2 \\ M_3 \end{bmatrix} \in R^d$$



SROM for Low-fidelity probability of failure

- Examples of 3 SROMs for the uncertain parameters.
- Force-displacement curves from Monte Carlo simulation two ways: (blue) with the SROM-based surrogate and (red) brute force finite-element simulation.
- We are developing tools to identify & prioritize hotspots based on surrogate results.



Another (well ironed) example: A304L laser weld failure

A little different problem... predict plastic instability, no damage

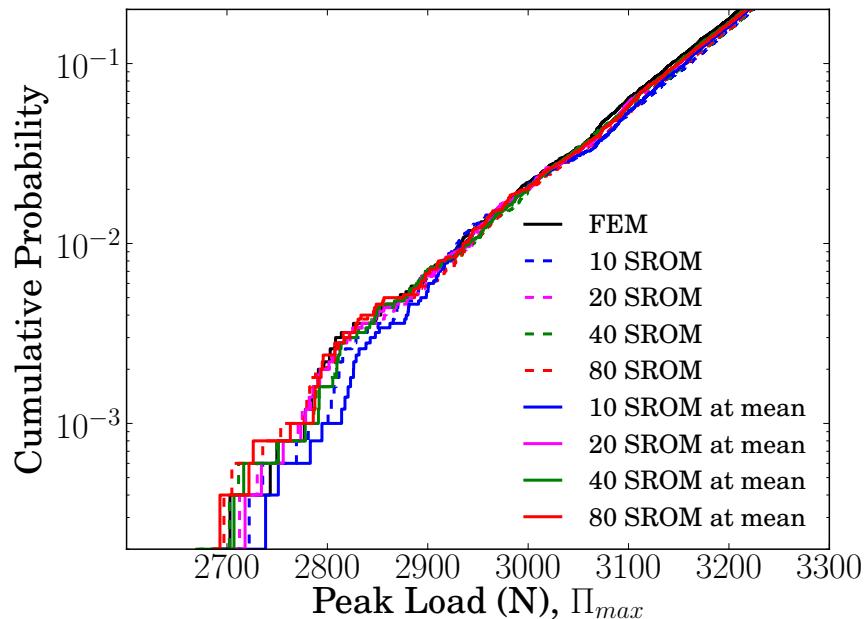
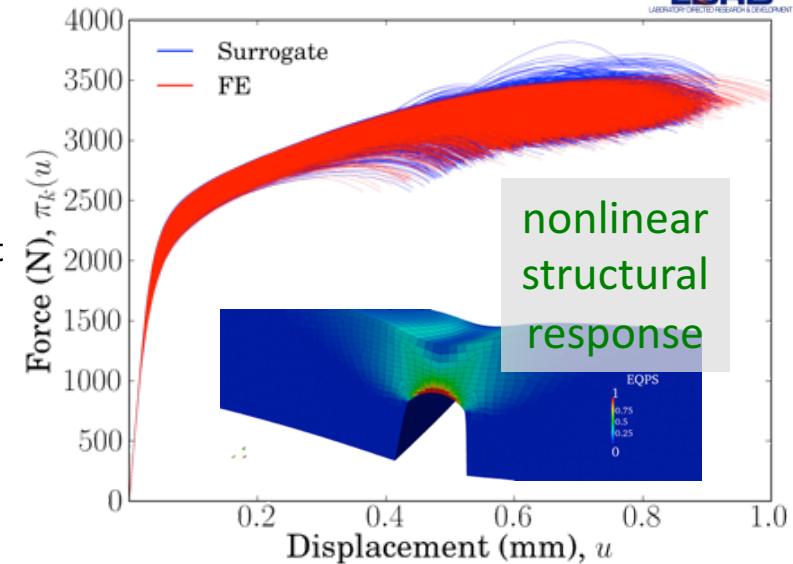
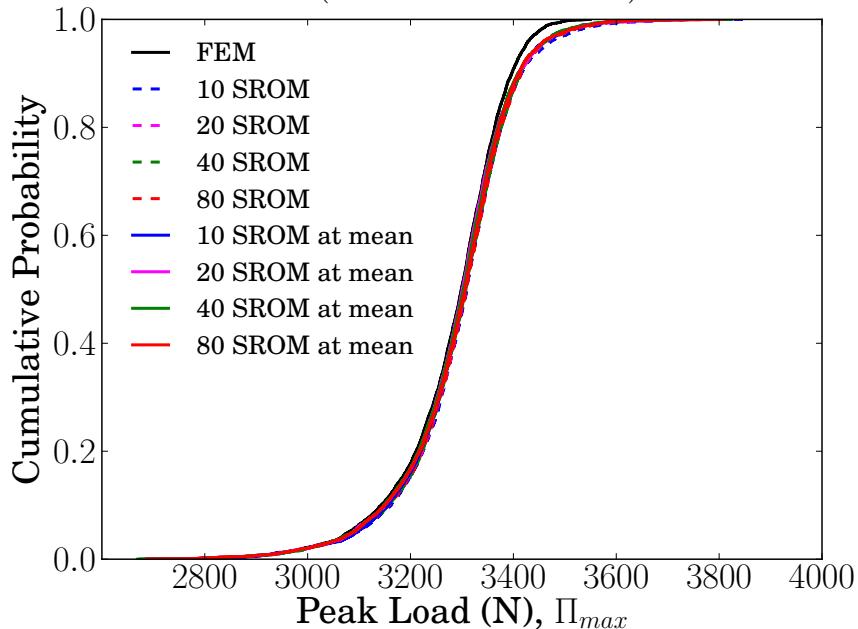
$$\begin{aligned} \sigma_y &= Y + \kappa & \dot{\kappa} &= [H - R\kappa] \dot{\epsilon}_p \\ \kappa(\epsilon_p) &= \frac{H}{R} [1 - \exp(-R\epsilon_p)] \end{aligned} \quad \left. \right\} \Theta = \begin{bmatrix} Y \\ H \\ R \end{bmatrix} \begin{array}{l} \text{initial yield stress} \\ \text{hardening (linear)} \\ \text{recovery coefficient} \end{array}$$

uncertain parameters

CPU seconds

Brute force MCS	33,400,000
	(5,000 FE calculations)
10 SROM at mean	511,000
	(40 FE calculations)

~65x faster



Random Field Model – Definition

- Let $\mathbf{R}(\mathbf{x}) = (\psi_1(\mathbf{x}), \phi(\mathbf{x}), \psi_2(\mathbf{x}))'$, $\mathbf{x} \in D$, be a vector-valued random field model for the 3 Euler angles
- Model form

$$\mathbf{R}(\mathbf{x}) = \boldsymbol{\mu}(\mathbf{x}) + \mathbf{a}(\mathbf{x}) \mathbf{Y}(\mathbf{x}) = \begin{pmatrix} \mu_1(\mathbf{x}) \\ \mu_2(\mathbf{x}) \\ \mu_3(\mathbf{x}) \end{pmatrix} + \begin{pmatrix} \sigma_1(\mathbf{x}) & 0 & 0 \\ 0 & \sigma_2(\mathbf{x}) & 0 \\ 0 & 0 & \sigma_3(\mathbf{x}) \end{pmatrix} \begin{pmatrix} Y_1(\mathbf{x}) \\ Y_2(\mathbf{x}) \\ Y_3(\mathbf{x}) \end{pmatrix}$$

$$Y_k(\mathbf{x}) = h_k(G_k(\mathbf{x})) = F_k^{-1} \circ \Phi(G_k(\mathbf{x})), \quad k = 1, 2, 3$$

$$\mathbb{E}[G_k(\mathbf{u}) G_l(\mathbf{v})] = \rho_{kl}(\mathbf{u}, \mathbf{v})$$

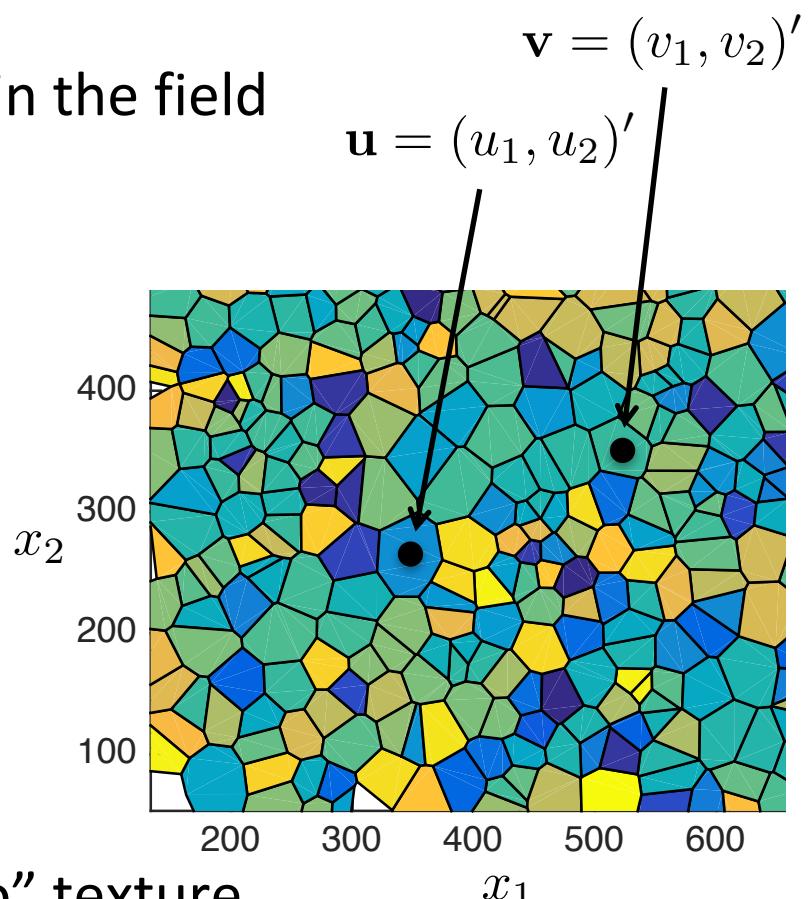
- μ_k and σ_k are the mean and standard deviations of R_k
- F_k is related to the marginal CDF of R_k
- $\mathbf{G} = (G_1, G_2, G_3)'$ is a vector-valued Gaussian random field with zero mean, unit variance, and correlation functions $\{ \rho_{kl} \}$

Random Field Model – Calibration

1. Estimate mean and standard deviation functions, μ and σ
2. Define spatial correlation functions
 - Can map correlation of \mathbf{G} to correlation of \mathbf{R}
 - Functional form: exponential or linear decay
 - Homogeneous, isotropic
 - Parameter estimates using least-squares, or user-specified
3. Select marginal distribution functions
 - Choose a functional form
 - Consistent with physics
 - Beta distribution is a good choice
 - Parameter estimates using Method of Maximum Likelihood
 - Empirically-based
 - Requires a medium sized data set

Capturing spatial correlation

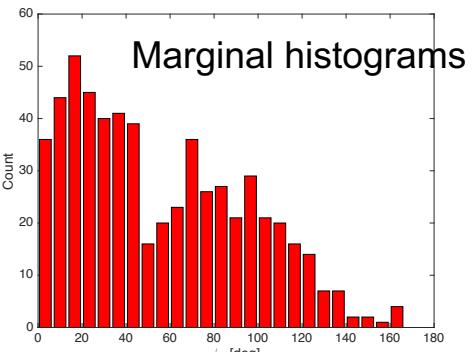
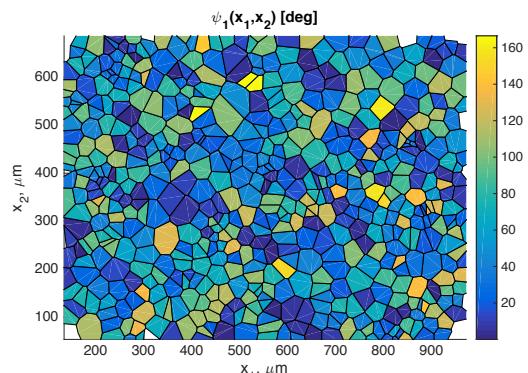
- A measure of the (average) linear dependence between two points in the field
 - Auto correlation function of ψ_1
 $E[\psi_1(\mathbf{u}) \psi_1(\mathbf{v})]$
 - Cross correlation between ψ_1 and ϕ
 $E[\psi_1(\mathbf{u}) \phi(\mathbf{v})]$
- Special cases
 - Statistically homogeneous
 Depends on $(\mathbf{u} - \mathbf{v})$
 - Statistically isotropic
 Depends on $\|\mathbf{u} - \mathbf{v}\|$
- Provides one way to model “micro” texture



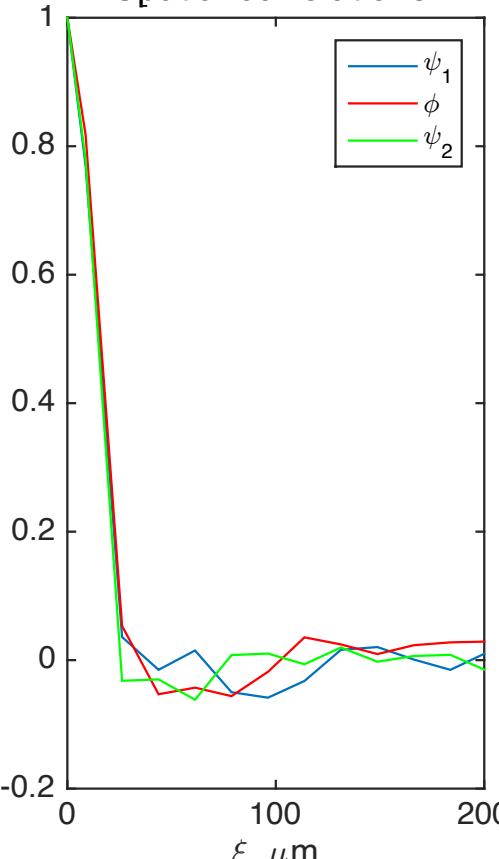
Experimental Data

EBSD data from Ta
wire **Not AA6061

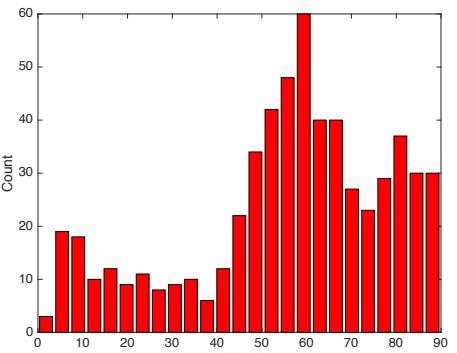
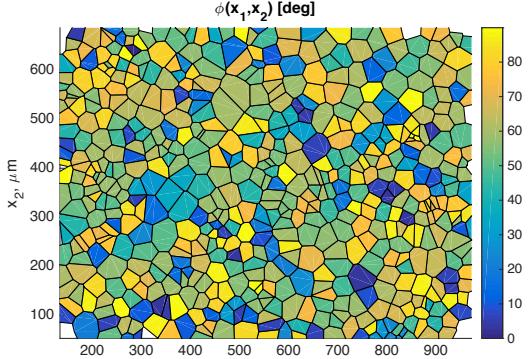
Angle 1: ψ_1



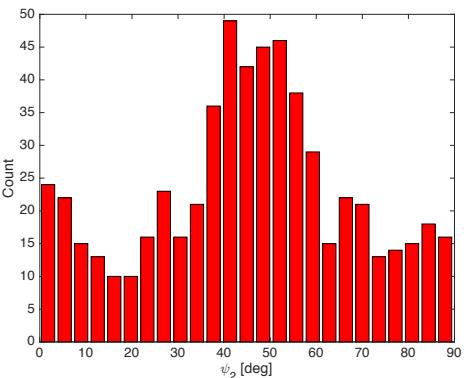
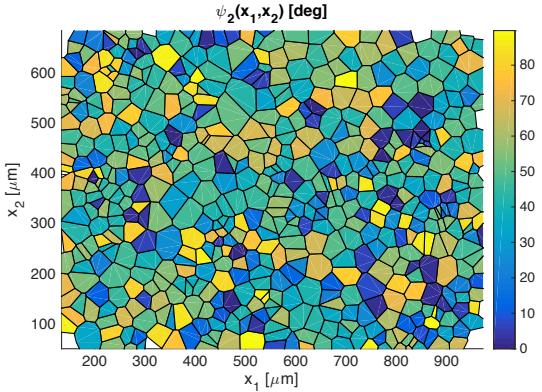
Spatial correlations



Angle 2: ϕ

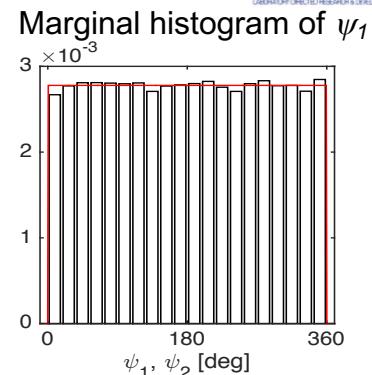
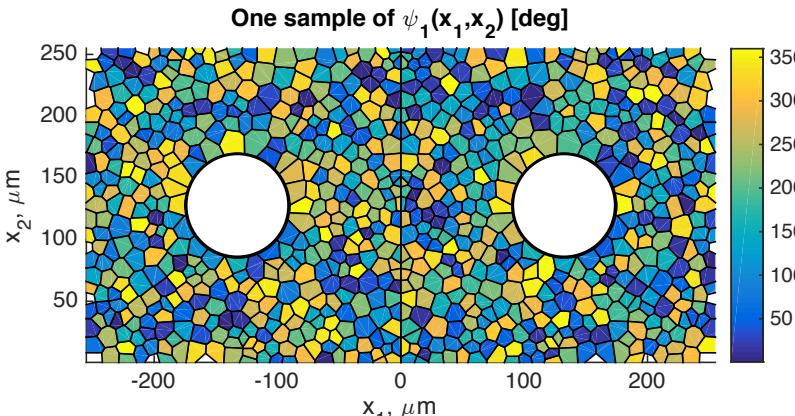


Angle 3: ψ_2

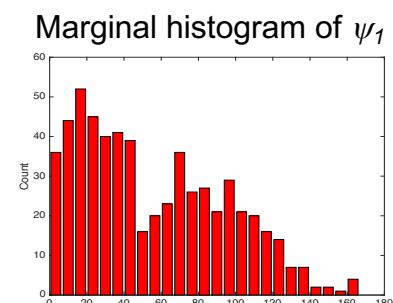
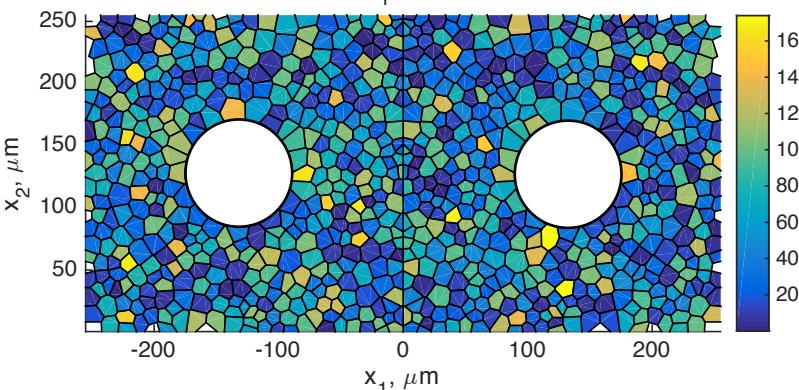


2D example from EulerRF

Zero texture, zero spatial correlation

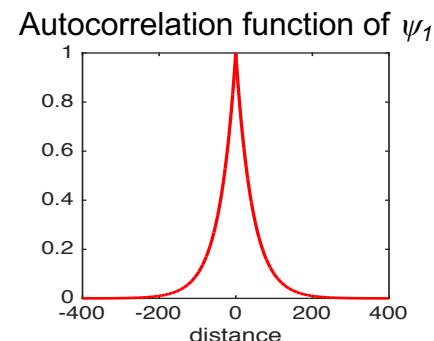
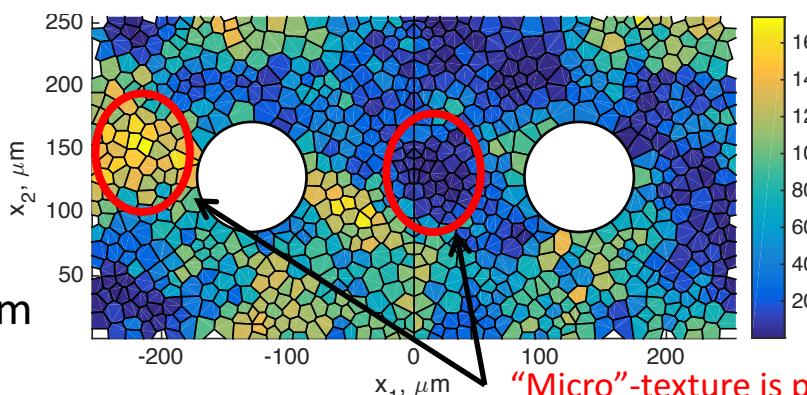


With macro-texture based on data file, zero spatial correlation

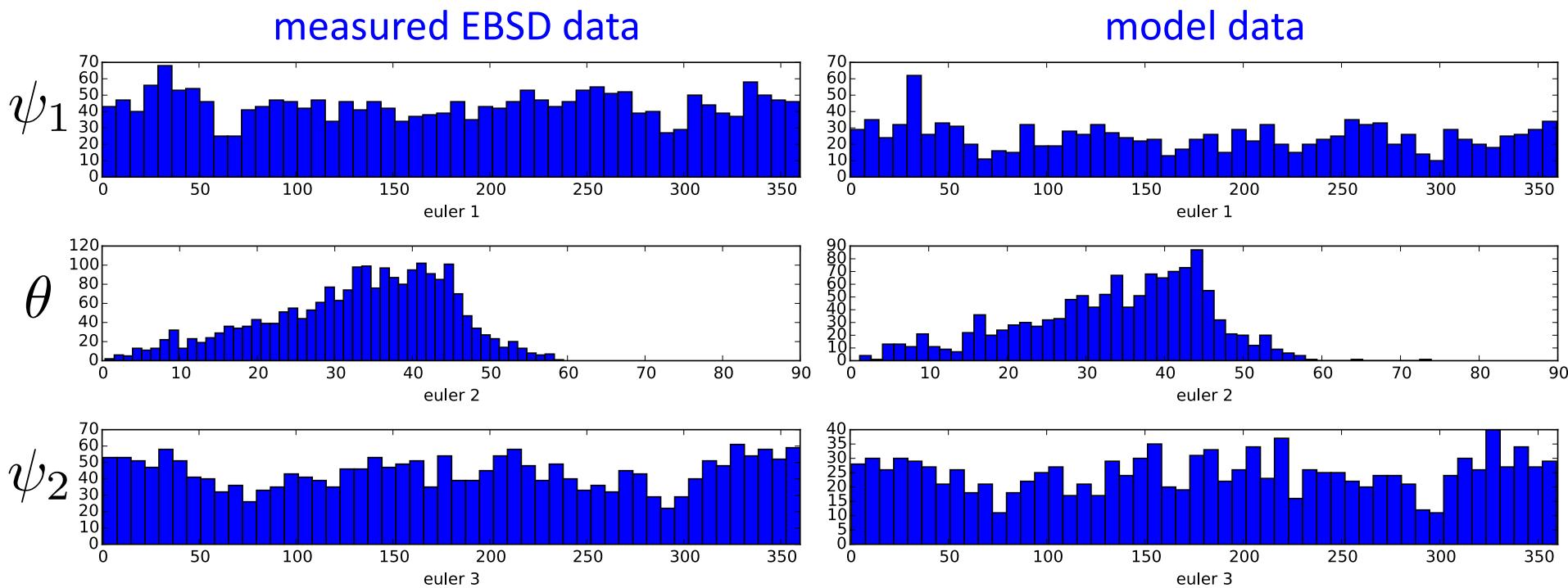


With micro-texture, *i.e.*, including spatial correlation

- Texture based on data file
- Isotropic (exponential) spatial correlation with correlation length = 200 μm

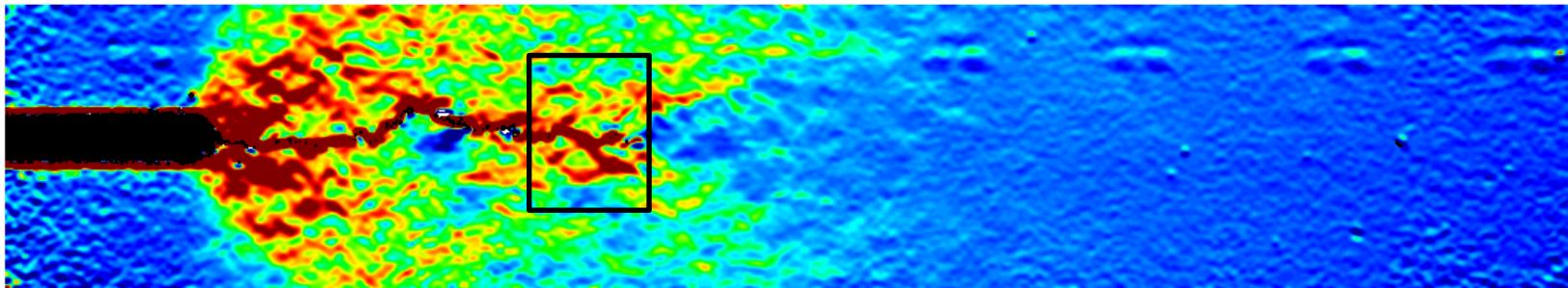


Comparing histograms – data vs. texture samples



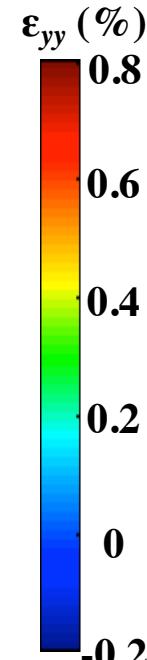
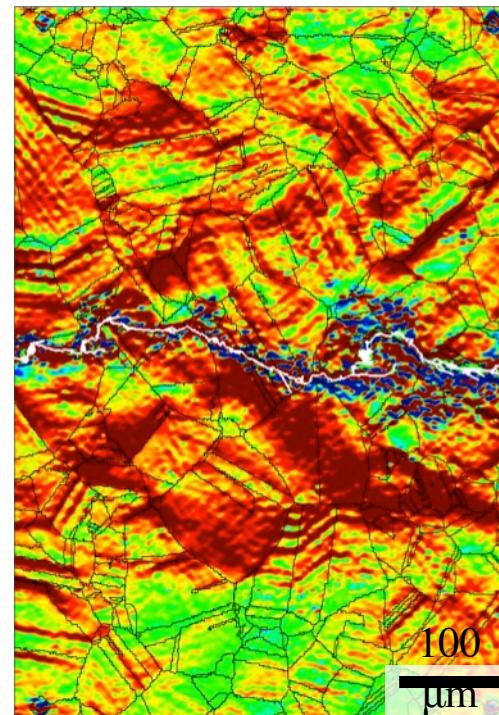
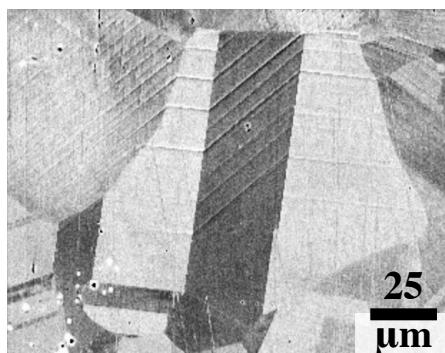
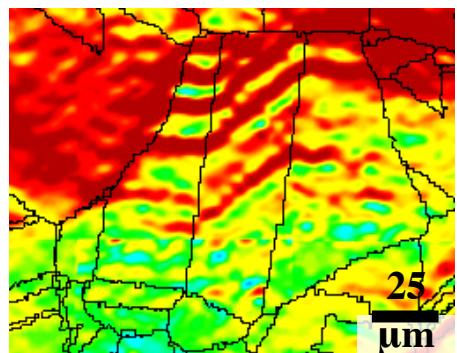
- Histograms drawn for the individual Euler angles

Multiscale DIC overlays low and high resolution



Entire width of specimen

- Low magnification, HR-DIC gives good mesoscale resolution over large regions (centimeters).
- High magnification, HR-DIC gives sub-grain level resolution over hundreds of microns.



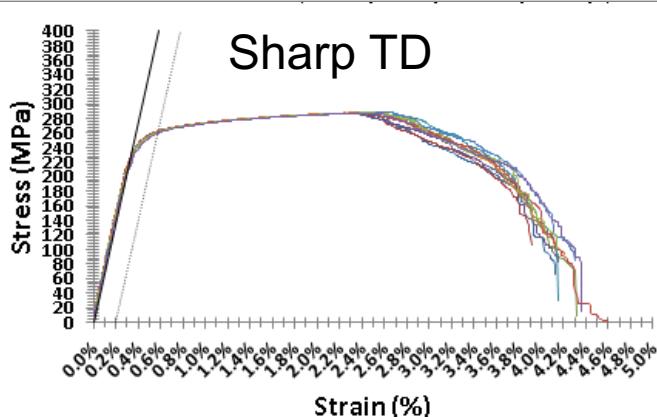
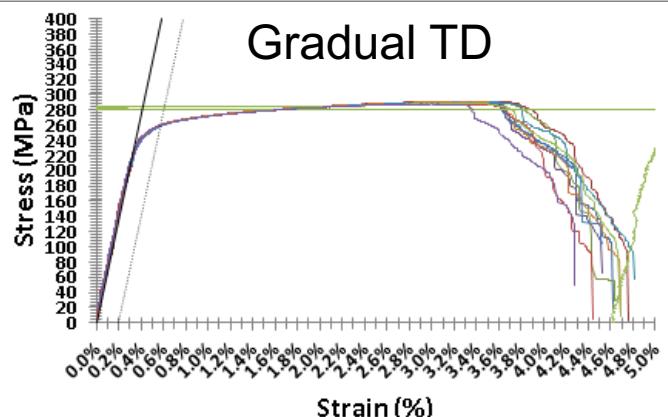
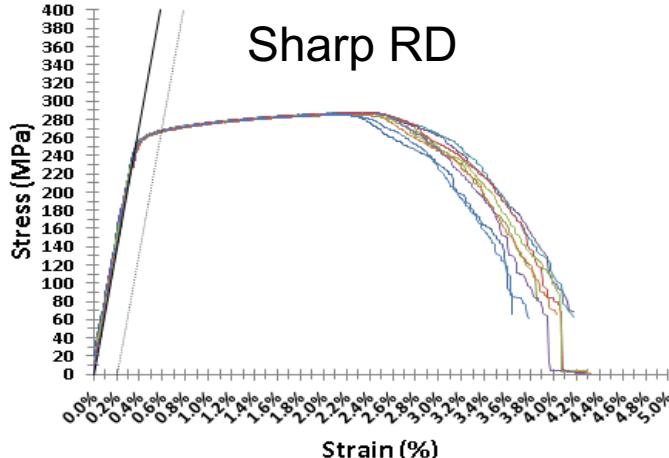
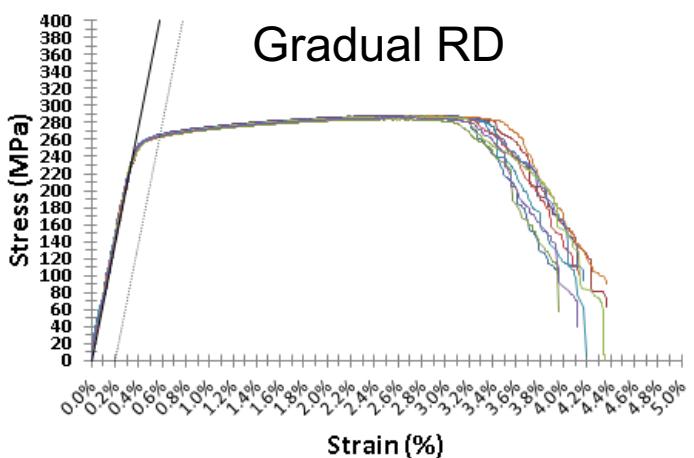
Carroll *et al.*, *Rev. Sci Inst.*, v. 81 (2010)

Carroll *et al.*, *Int J. Fracture*, v. 180 (2012)

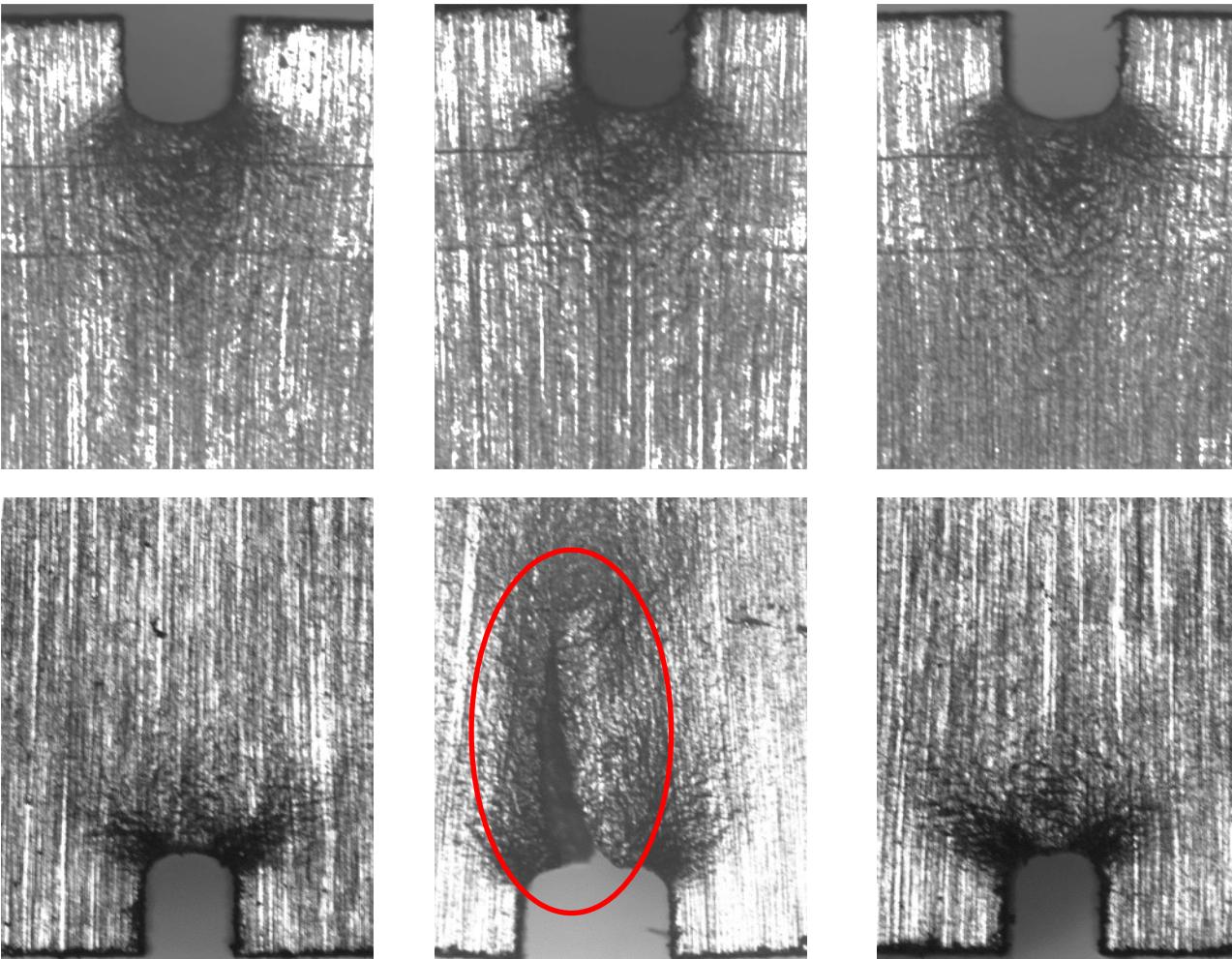
Carroll *et al.*, *Int. J. Fatigue*, (2013)

Consider variability in material properties through uniaxial tension tests and 2-notch specimens

Notch Geometry Variability



Fracture of first specimen initiated at a center notch with significant plasticity in all notches.

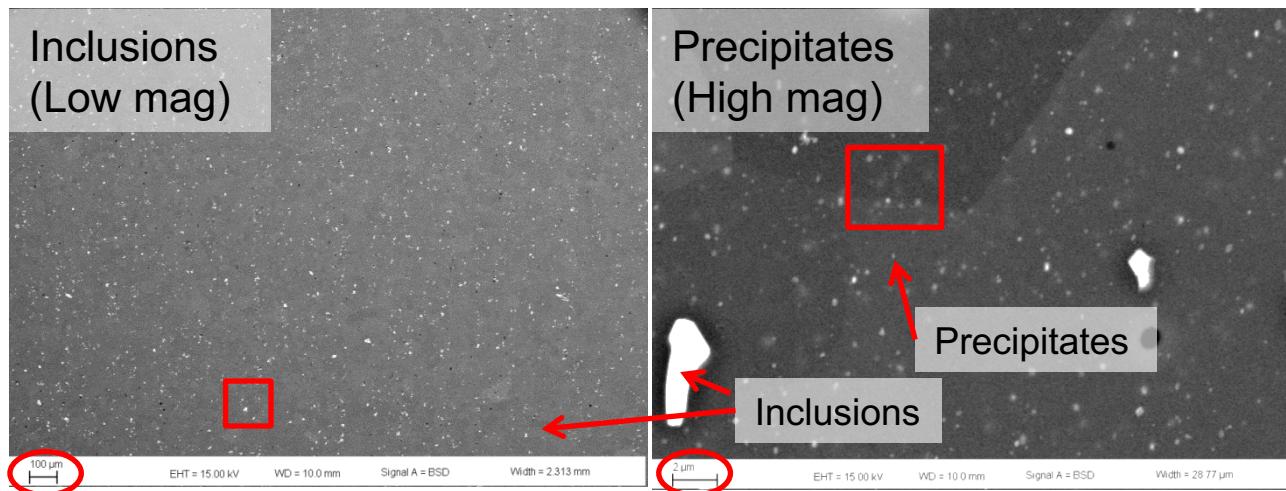
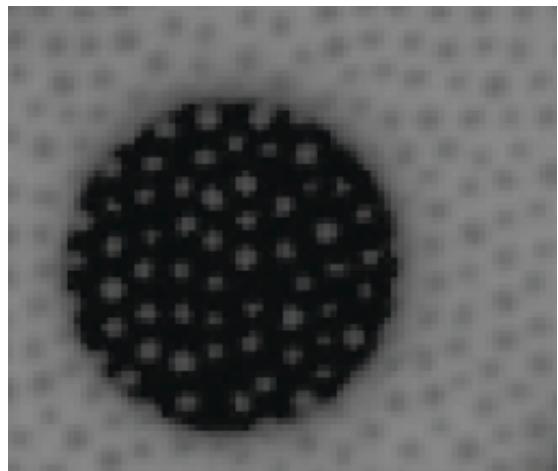


- Unstable crack growth occurred after this substantial crack was observed.

Multiscale digital image correlation

Currently pursuing 3 avenues for multiscale speckling:

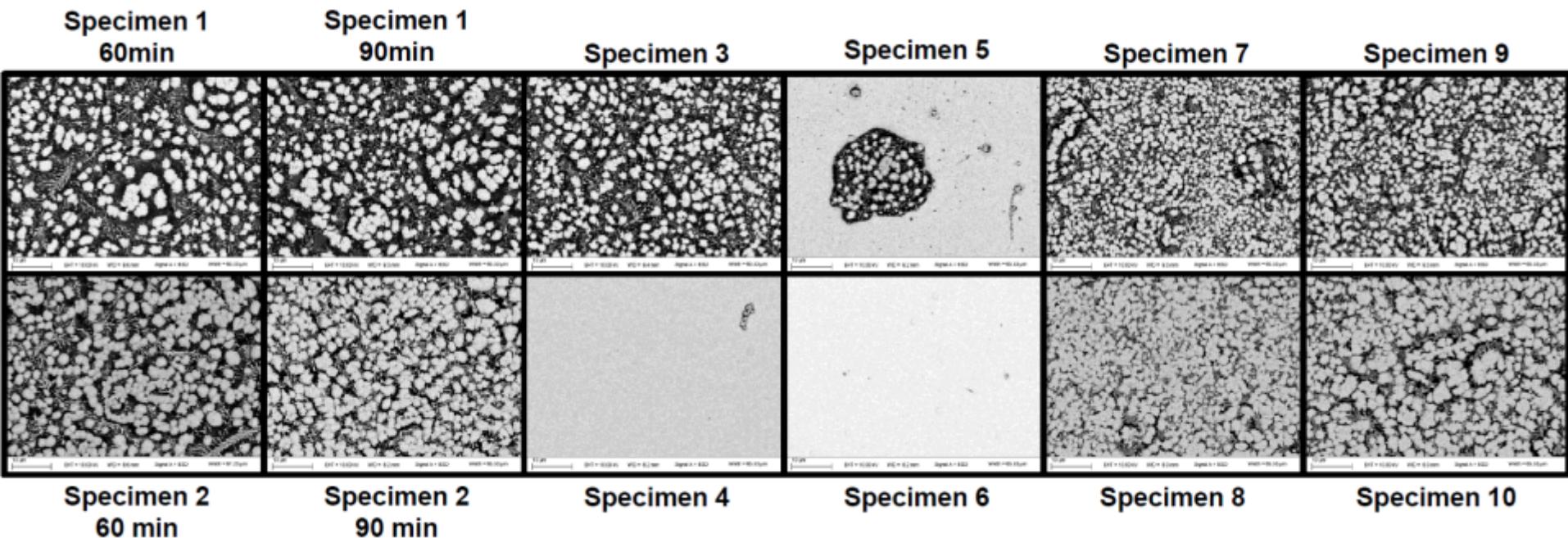
- Bi-color pattern with conductive paint for coarse and Cu powder for fine.
- Microstamping a fractal speckle pattern through external company.
- Inherent precipitates and inclusions will probably work, but only for small-scale plasticity (~1% strain).



Resolution down to ~150 μm

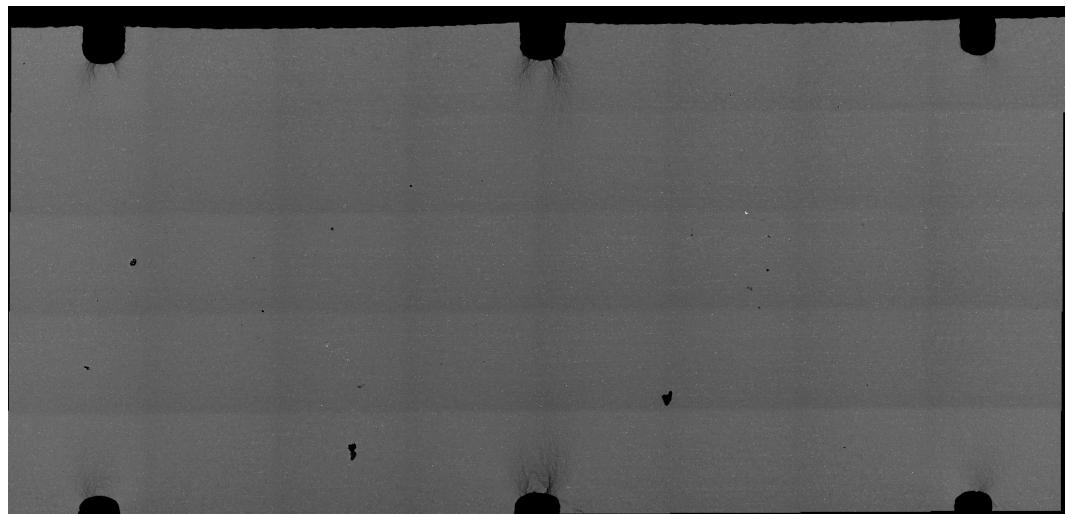
Resolution down to ~4 μm

Various instantiations of a multiscale speckle pattern by sputtering gold

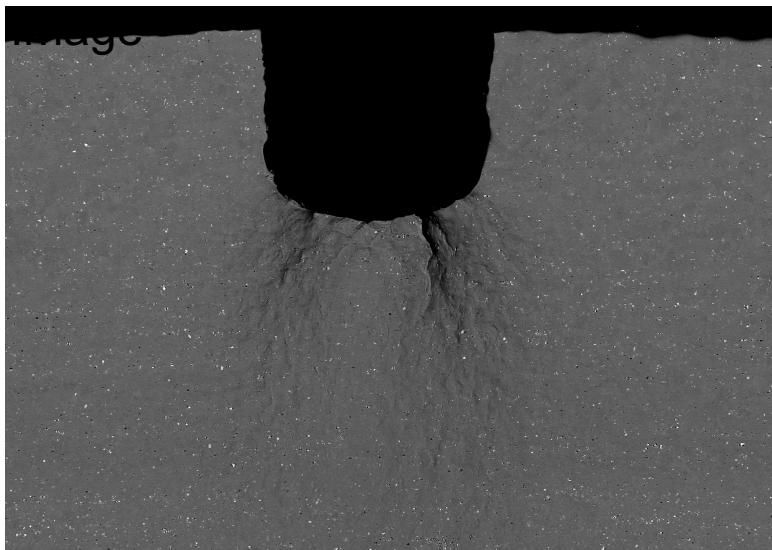


Multiscale imaging

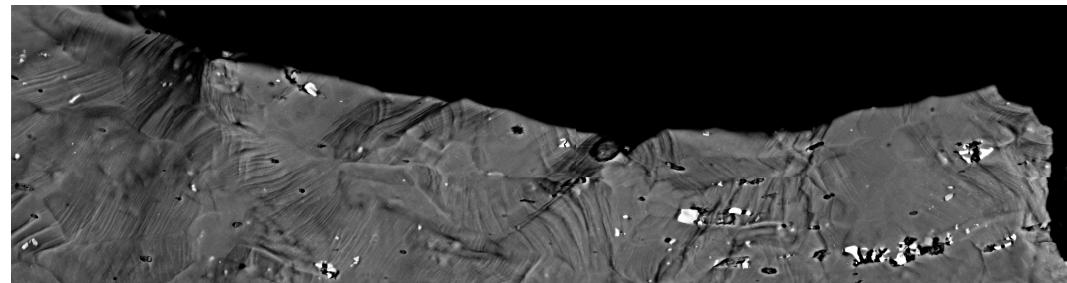
Low Resolution Montage



Low Resolution Single



High Resolution Montage



High Resolution Single Image

