

Exceptional service in the national interest



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

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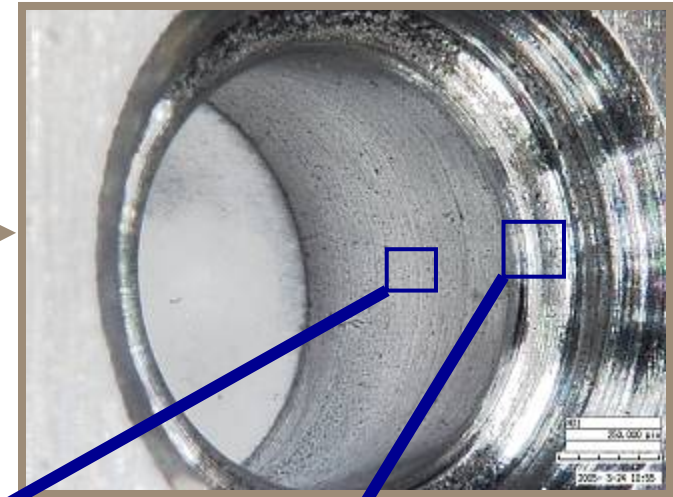
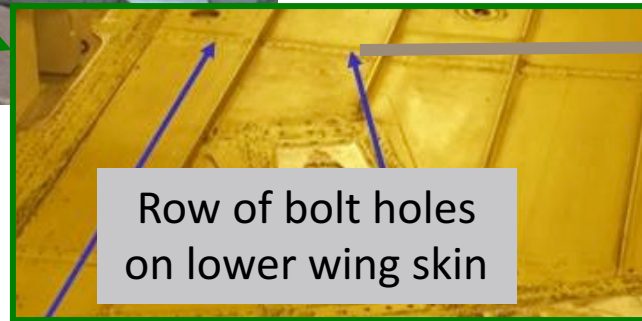
Outline

- Motivation & challenge
- Proposed algorithm for multiscale UQ
- Summary of engineering-scale UQ
- Mesosstructural 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

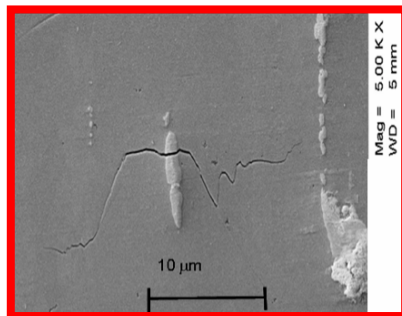
Why do multiscale? Because structural reliability is dependent on **random** microstructure (among other sources of randomness)



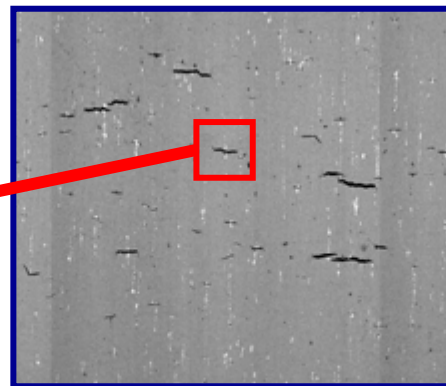
Engineering length scale (meters)



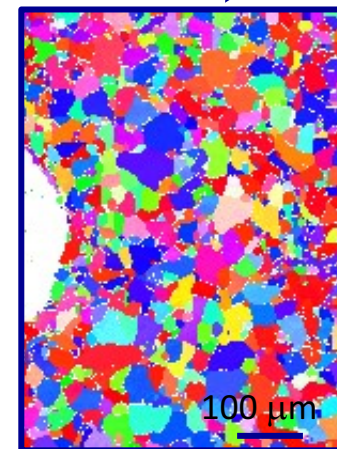
Structural feature (mm) – stress concentration or “hot-spot”



brittle particle



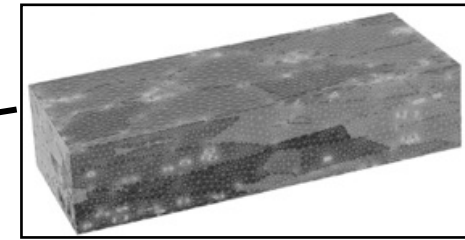
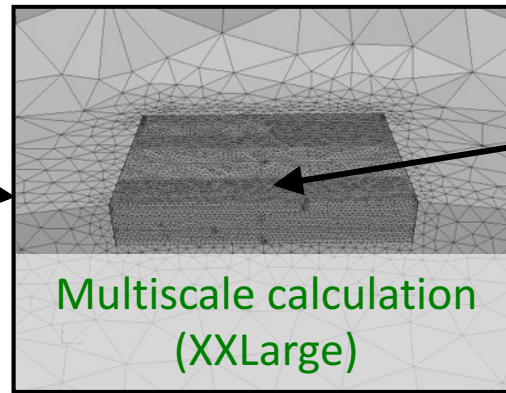
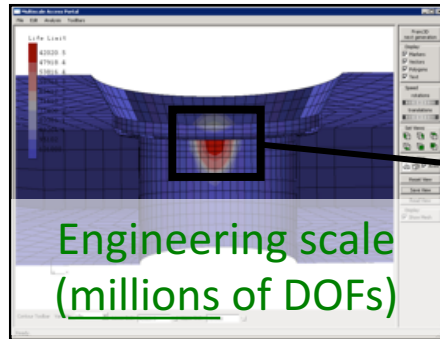
Microstructural length scale (μm)



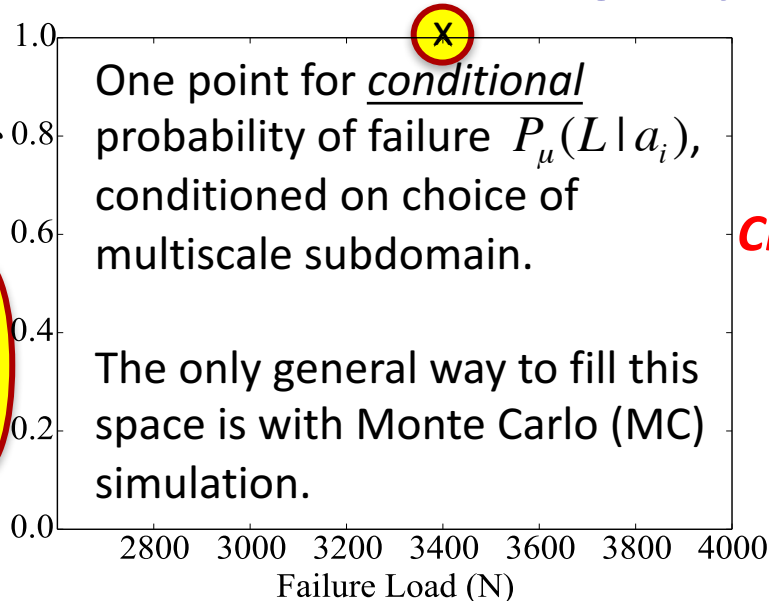
EBSD data shows randomly oriented grains

randomly distributed brittle particles embedded in randomly oriented, anisotropic matrix

One multiscale calculation is necessary but not sufficient

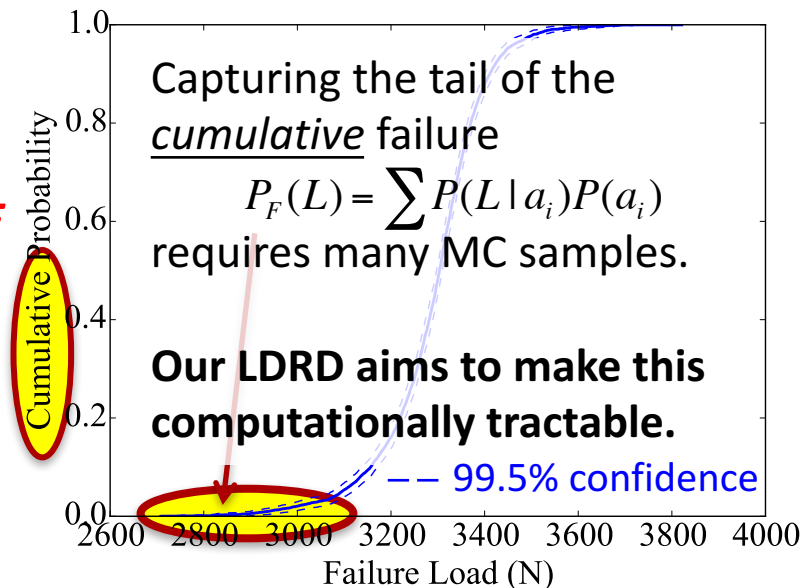


One multiscale calculation gives you this:



**OUR
CHALLENGE**

But you set out to compute this:

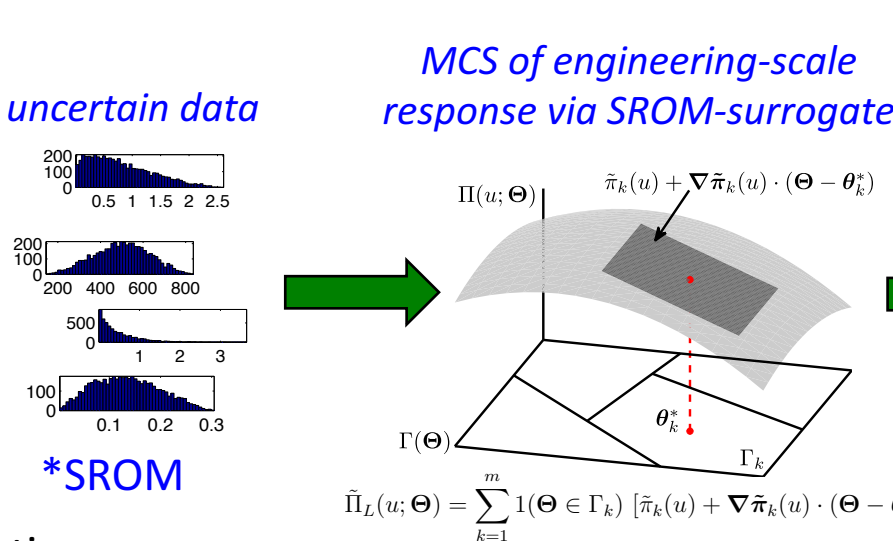


High level goal: tractably propagate fine-scale uncertainty through multiscale calculations

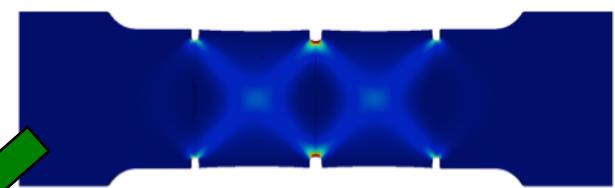
Why does Sandia care? Fracture is local and random, e.g., microstructure, and system/component reliability depends on phenomena occurring a various length scales.

Schematic of our novel hierarchical approach

Low fidelity



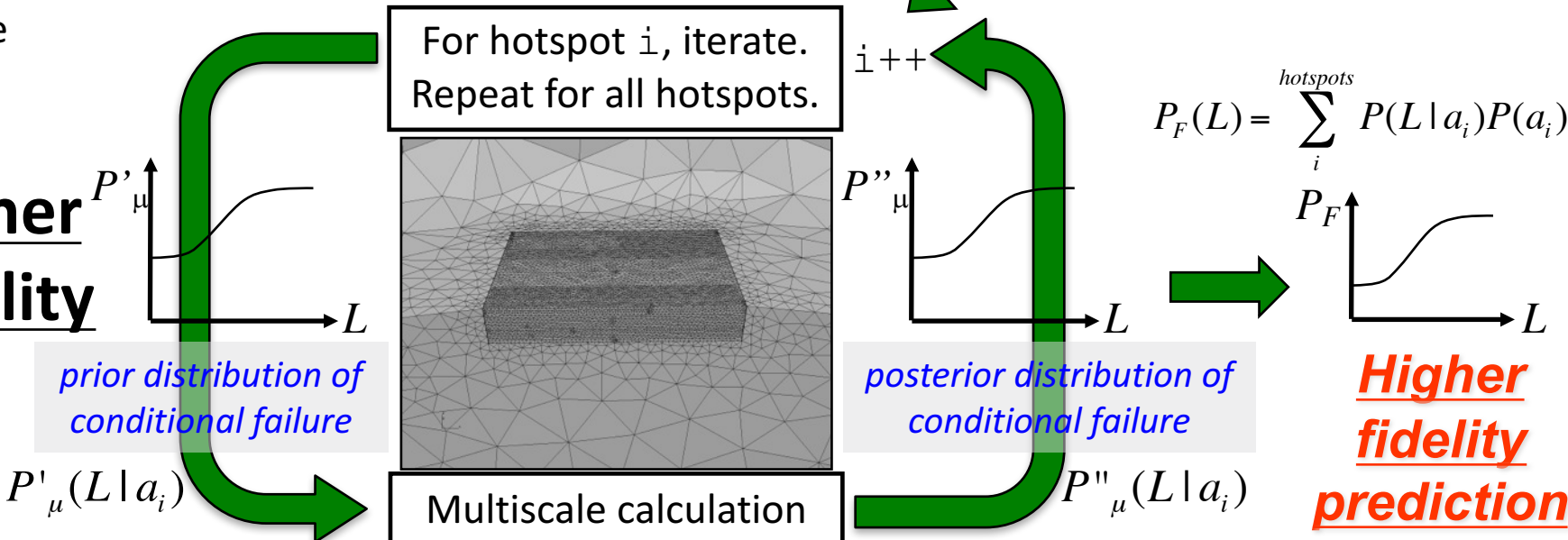
Hot-spot selection & prioritization



prior distribution

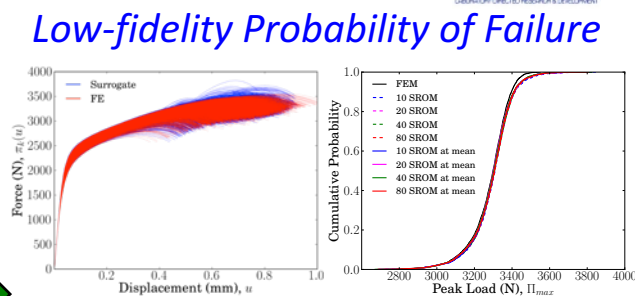
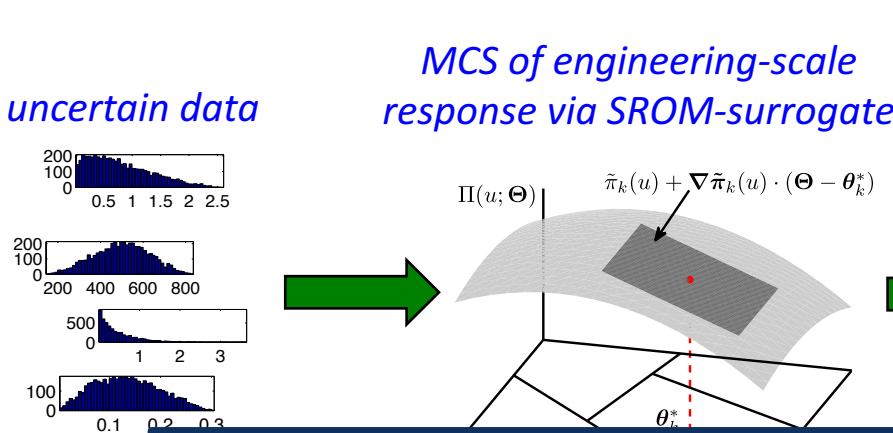
update

Higher fidelity



Schematic of our novel hierarchical approach

Low fidelity

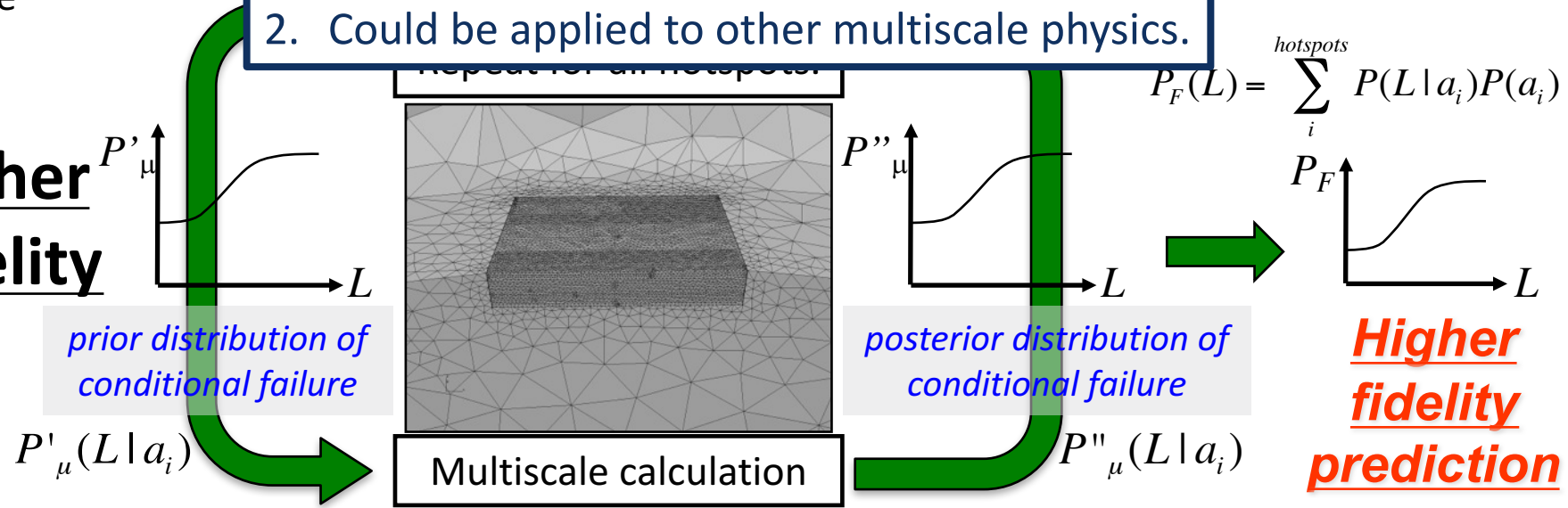


prior distribution
 update

Higher fidelity

***SRO Comments:**

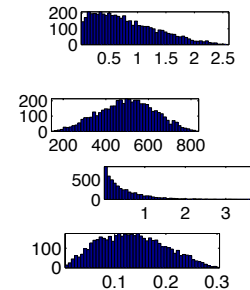
1. Independent of the multiscale numerical method, *e.g.*, use outcome from Foulk *et al.*
2. Could be applied to other multiscale physics.



Example objectives & uncertainties considered

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

uncertain data



Low fidelity

Engineering scale constitutive model

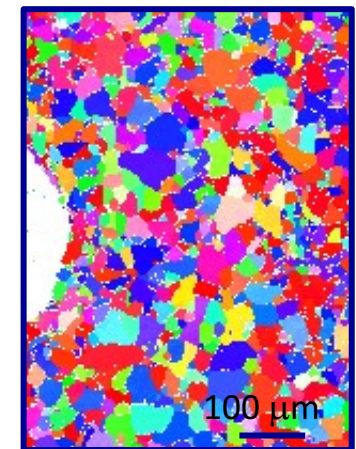
- plasticity parameters
- damage parameters

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



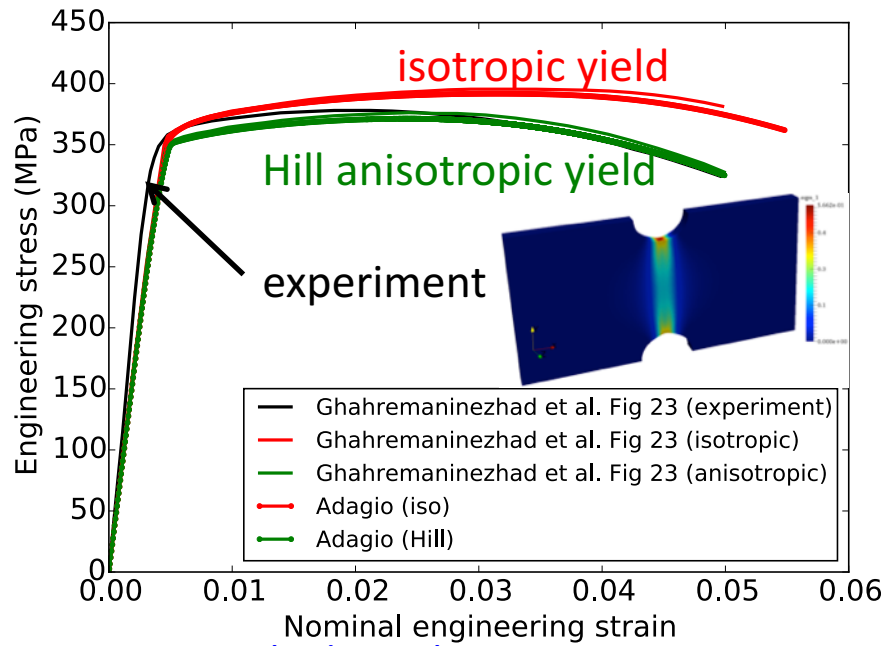
Engineering-scale model

- 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:

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

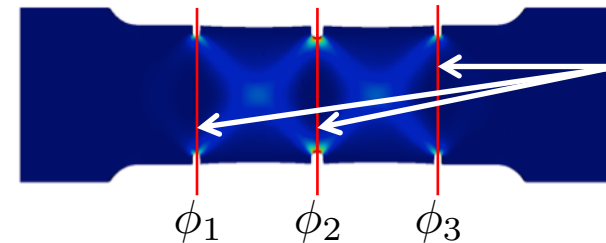
$$\dot{\eta} = \eta \dot{\epsilon}_p \left[N \left\| \frac{I_1}{\sqrt{J_2}} \right\| \right]$$



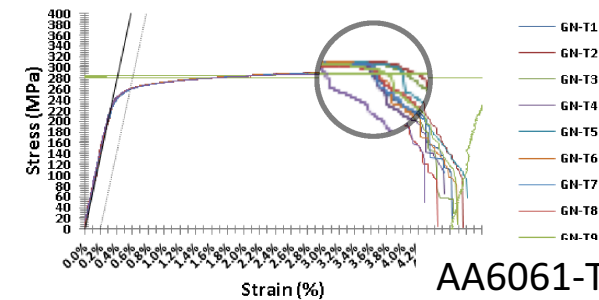
Notched Tensile Data – AA6061

(Ghahremaninezhad and Ravi-Chandar IJF 2012)

FE model (strain contour plot)

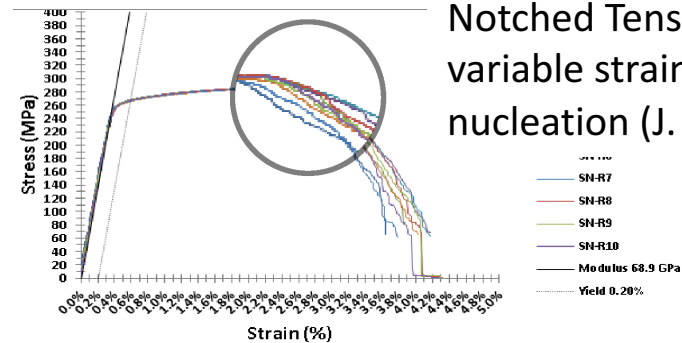


localization planes



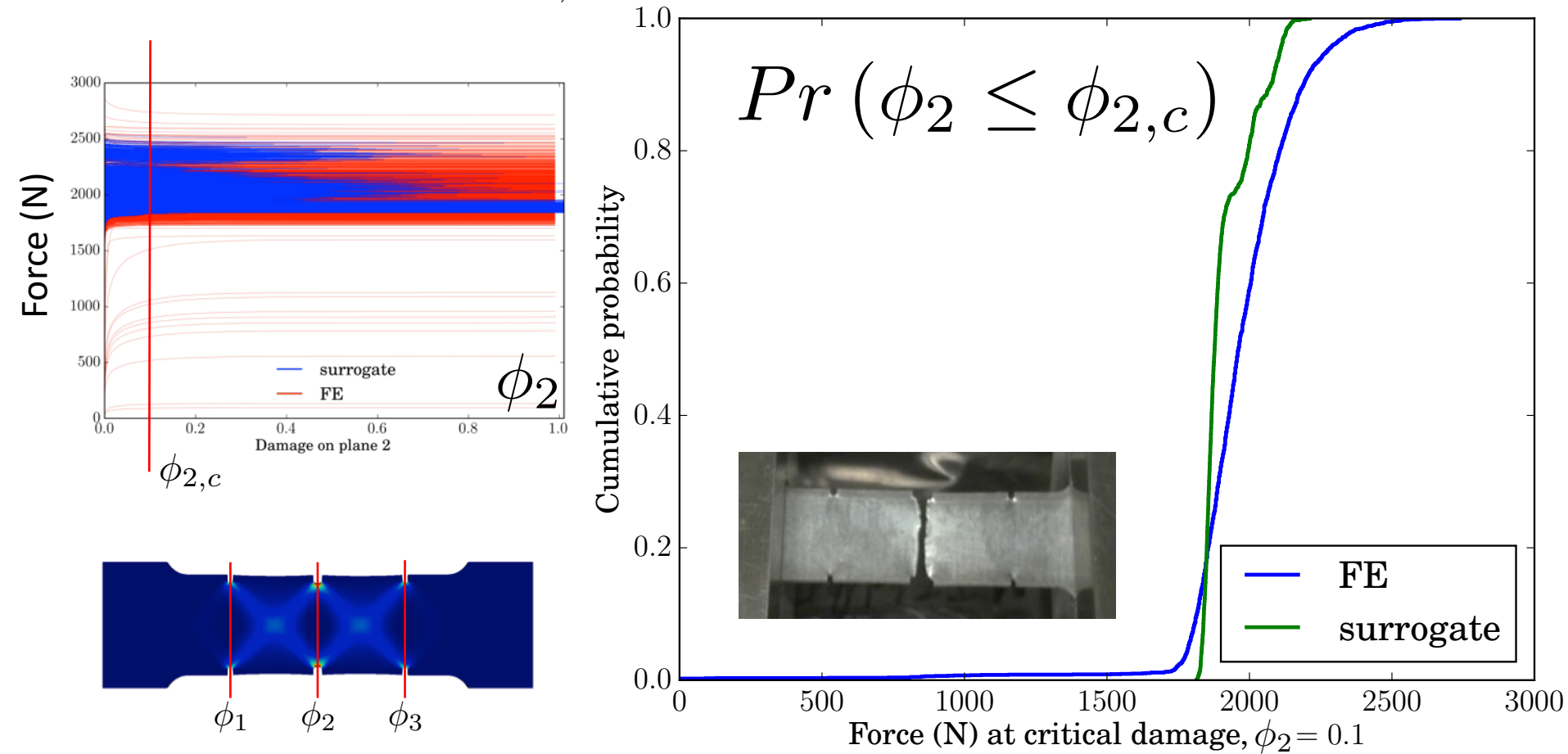
AA6061-T6

Notched Tension –
variable strain-to-
nucleation (J. Carroll)



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.*, $\phi_{2,c} = 10\%$.

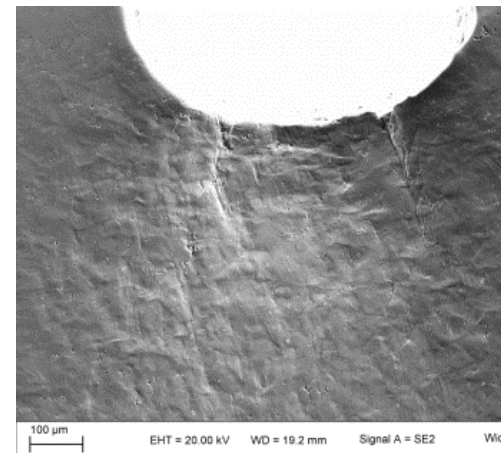
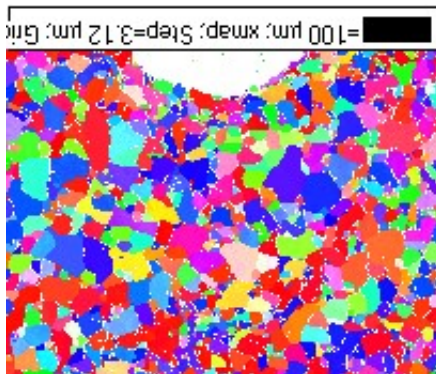
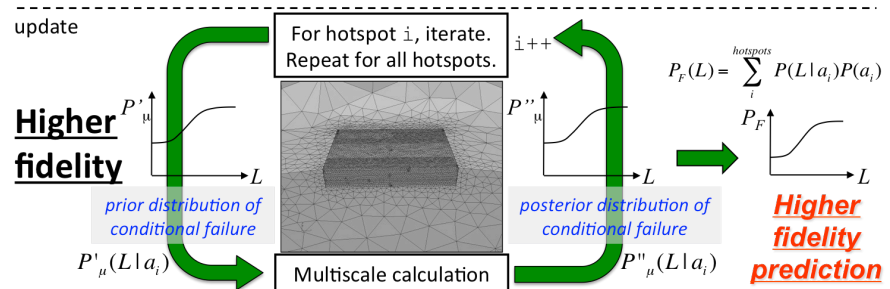


Higher fidelity – focused on texture

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

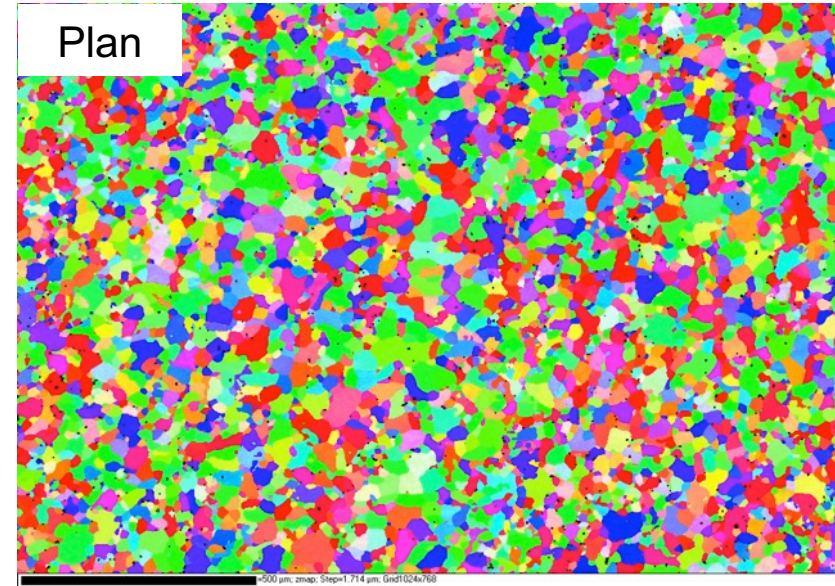
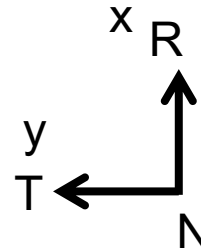
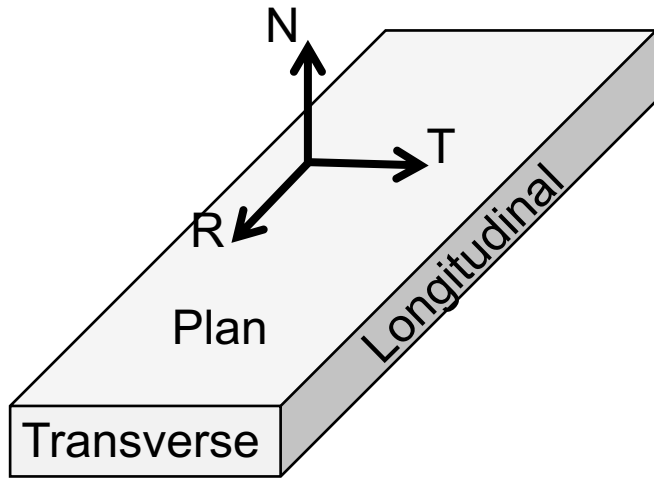
Things we need:

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



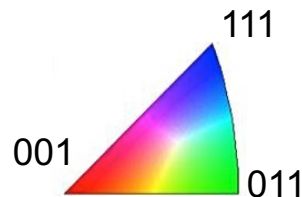
AA 6061-T6 – EBSD measurements/images at a notch tip

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

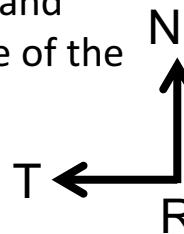


From Ghahremaninezhad & Ravi-Chandar, and confirmed for our material, mean grain size of the rolled 6061 microstructure:

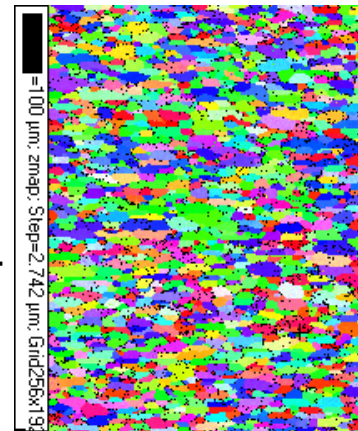
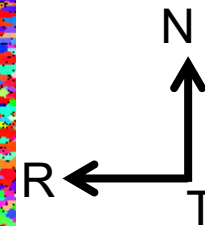
y-z mean 15 μm
x-z mean 14 μm
x-y mean 39 μm



Transverse

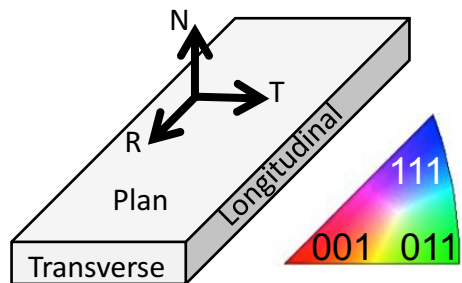
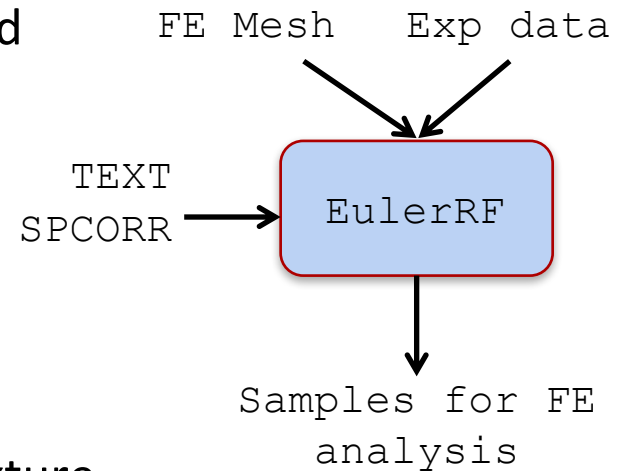


Longitudinal

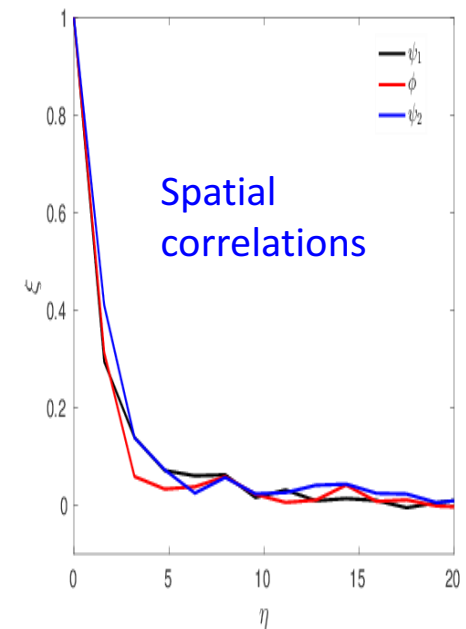
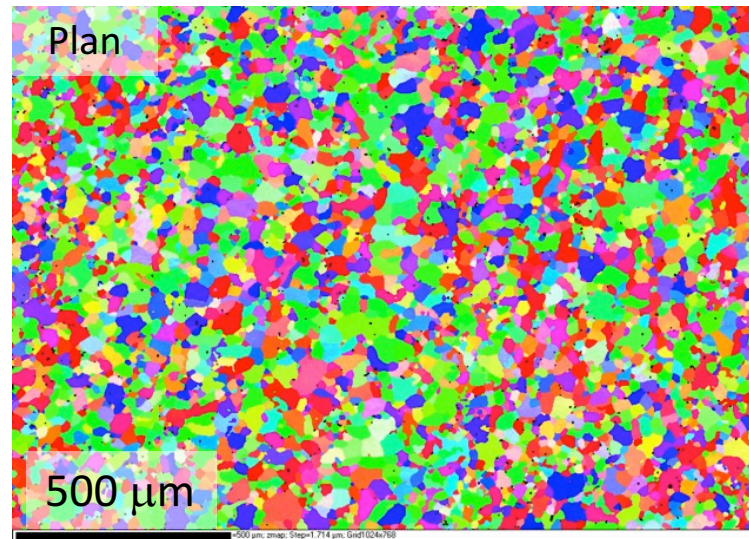


“EulerRF” Code

- 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



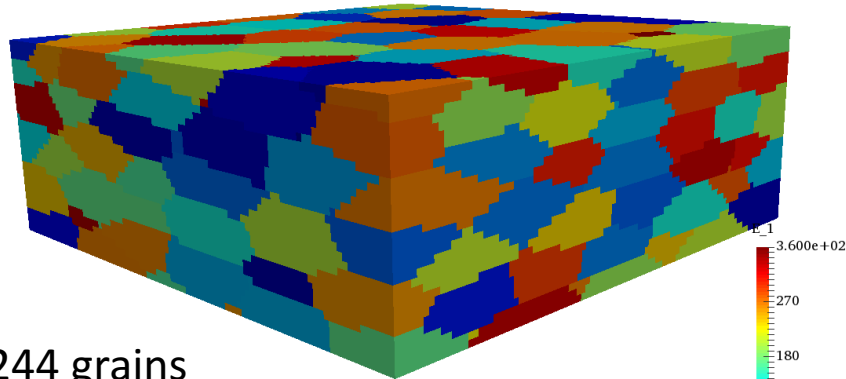
Ghahremaninezhad *et al.*,
mean grain size:
y-z mean 15 μm
x-z mean 14 μm
x-y mean 39 μm



3D Samples for AA 6061 T6 rolled sheet

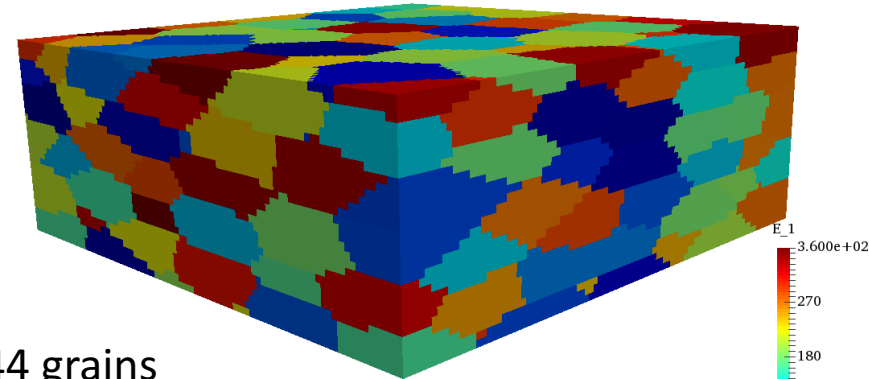
- 2 samples each macro-texture (left) & micro-texture (right)

“Macro” texture

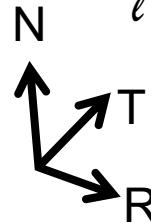
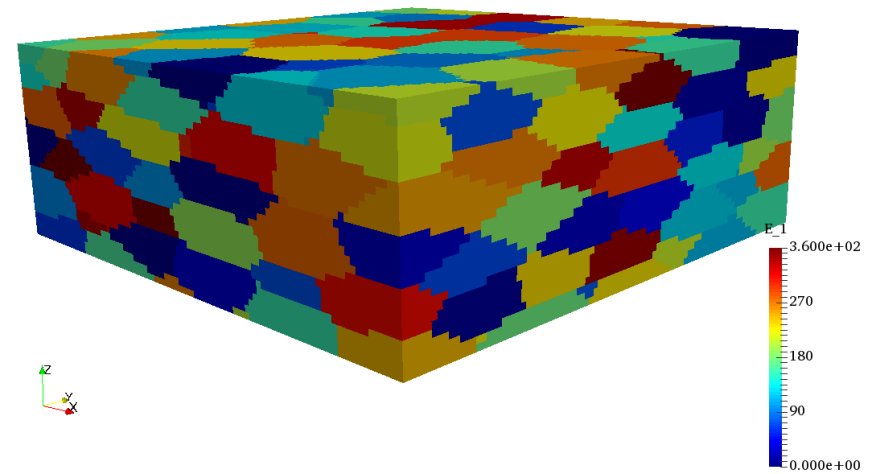
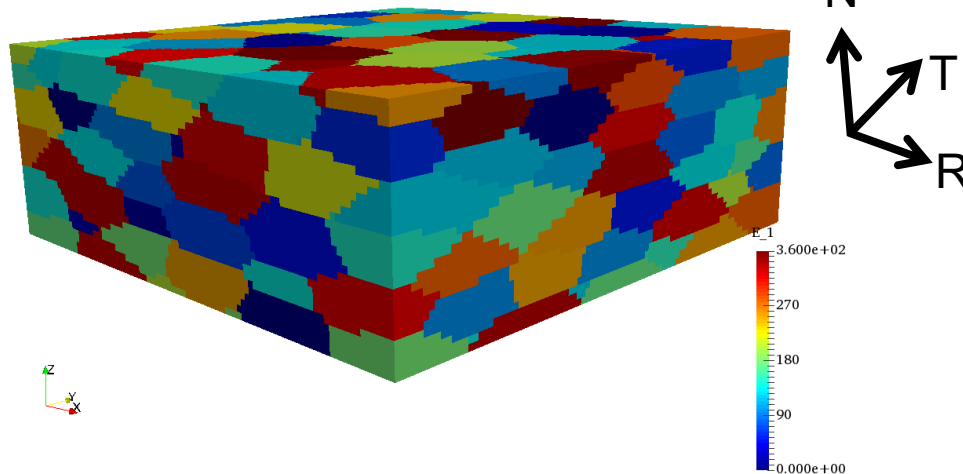


244 grains
294,912 elements
no correlation

“Micro” texture

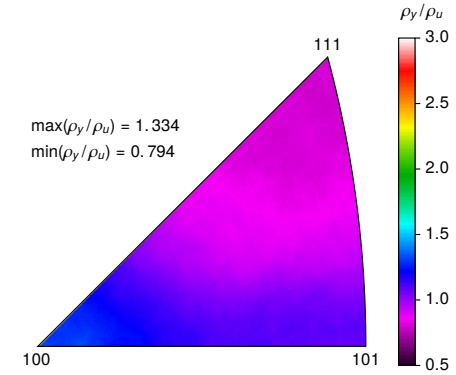
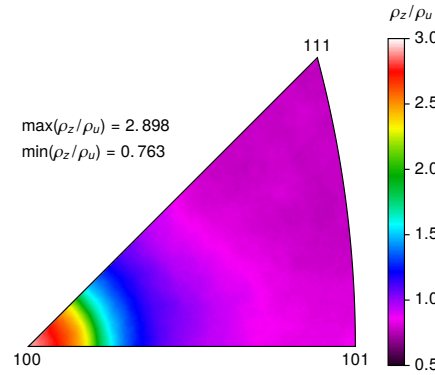
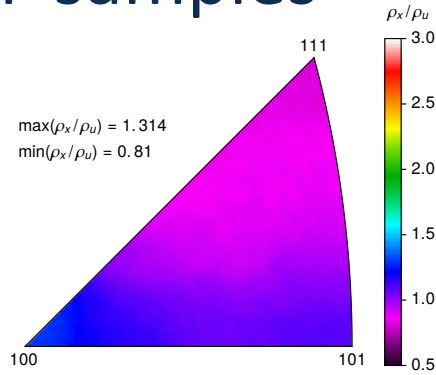


244 grains
294,912 elements
 $\ell = 16 \mu\text{m}$ (grains $39 \times 39 \times 14 \mu\text{m}$)

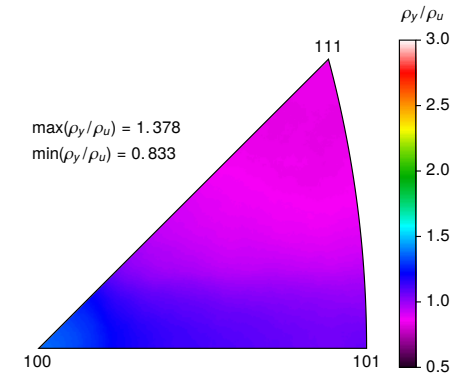
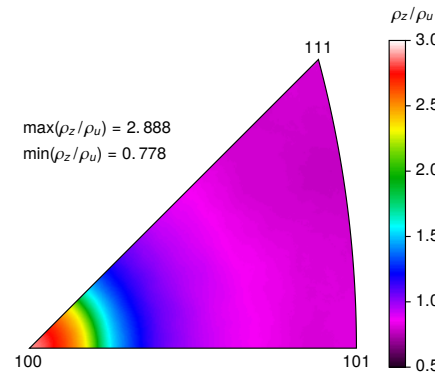
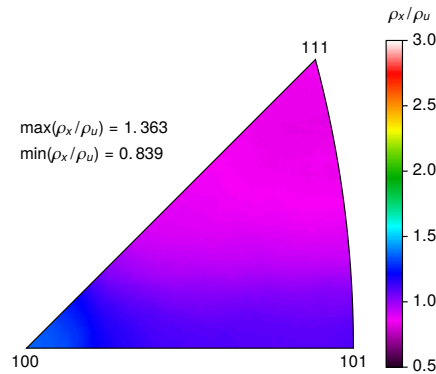


Inverse pole figure (IPF) comparing EBSD to eulerRF samples

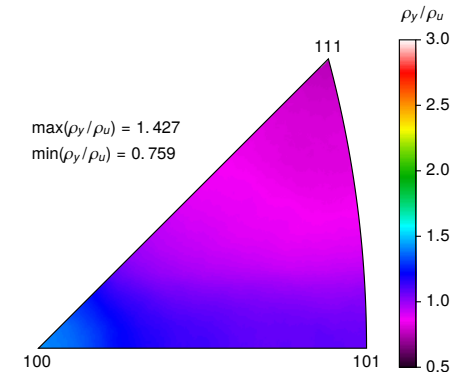
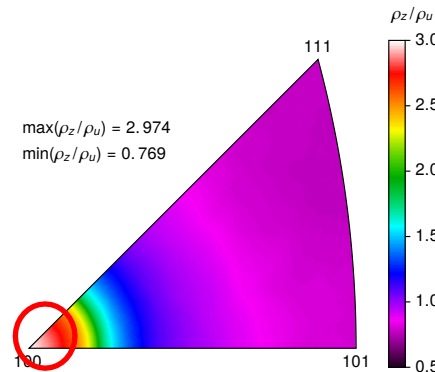
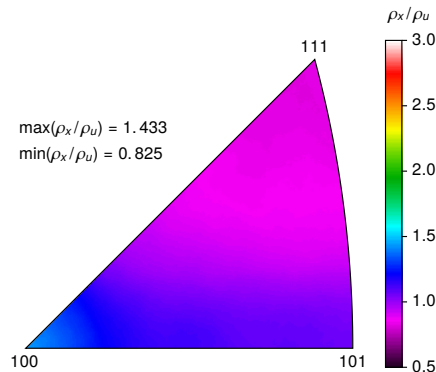
measured
EBSD data



macro-
texture



micro-
texture



Crystal plasticity formulation

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

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

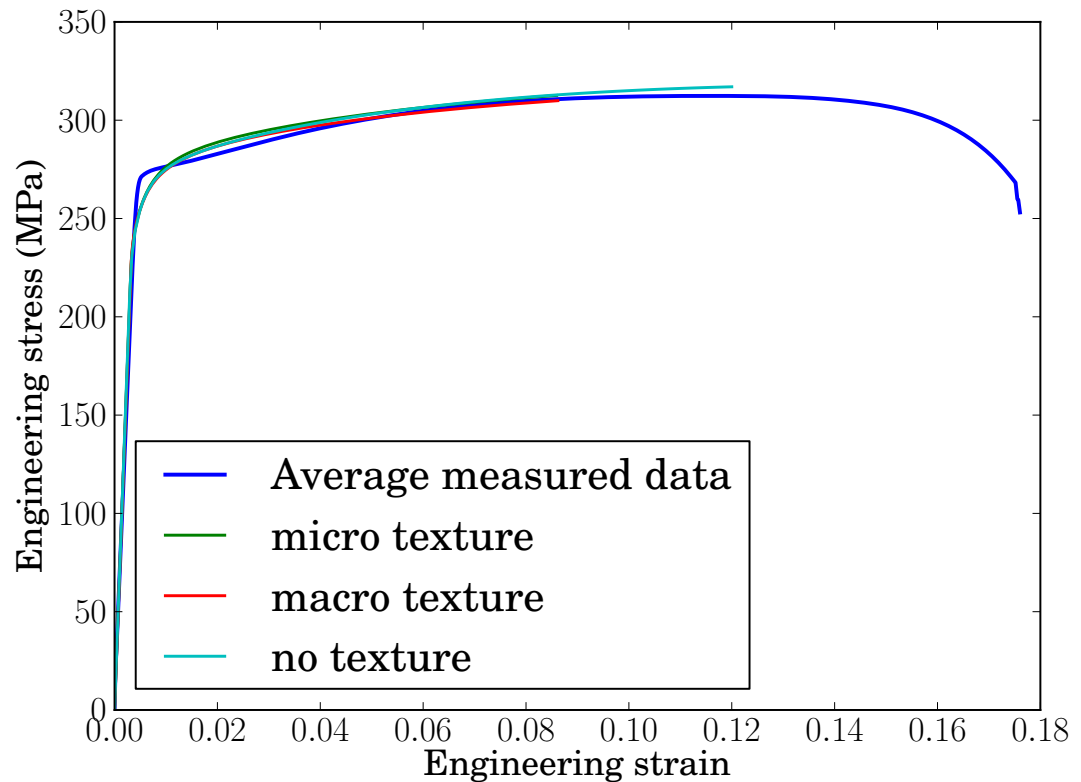
$$\mathbf{P}^{\alpha} = \mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha}$$

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

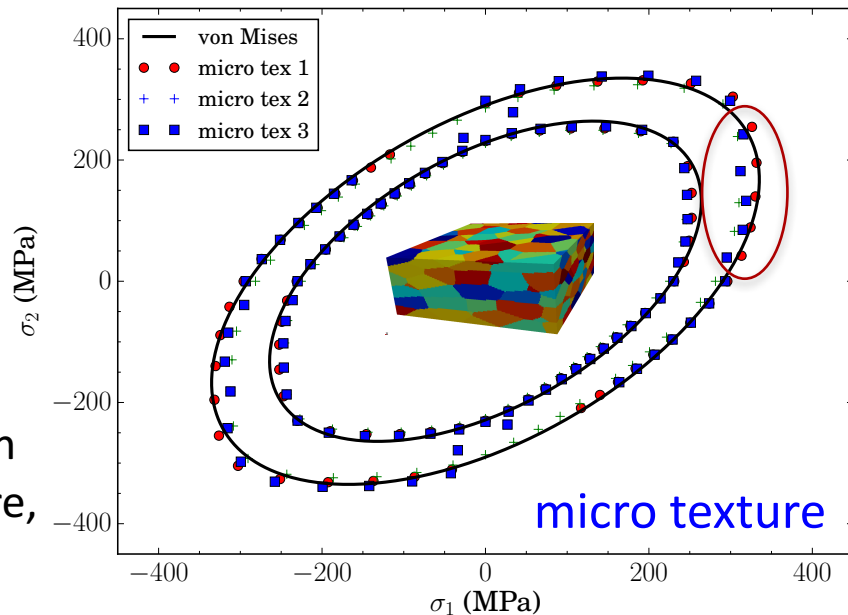
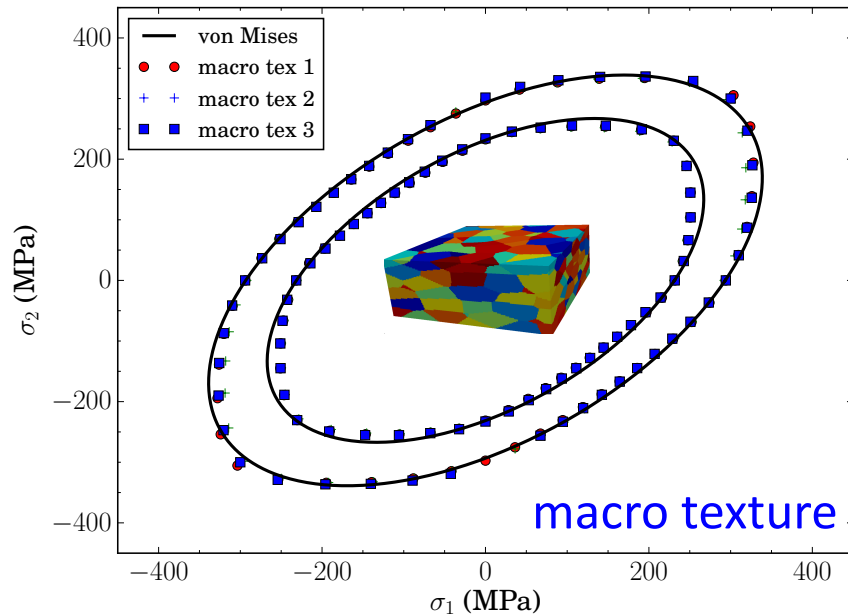
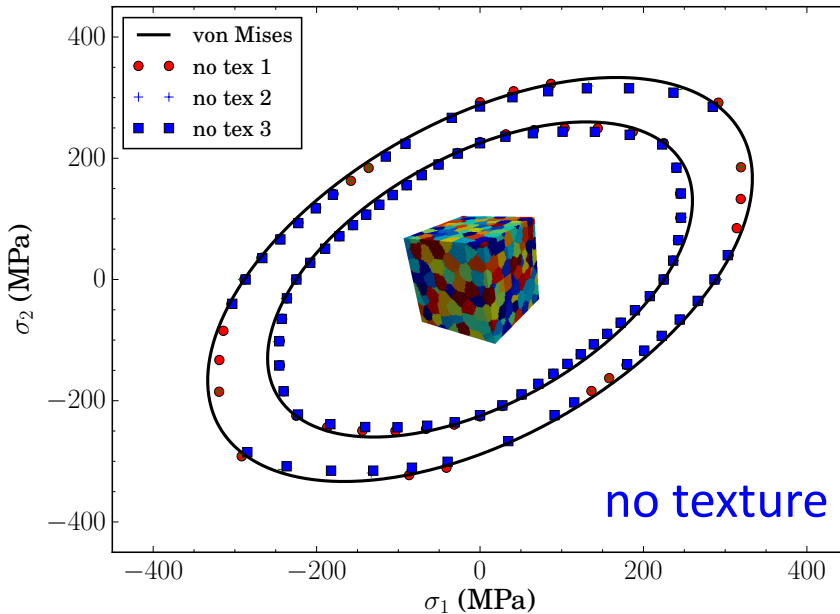
$$\dot{g} = G_0 \left(\frac{g_{s_0} - g}{g_{s_0} - g_0} \right) \dot{\gamma}$$

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

| | 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 |



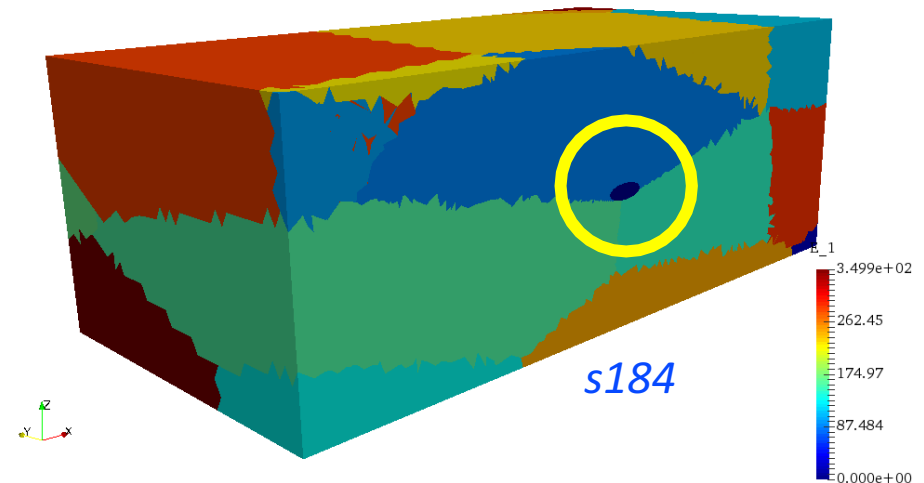
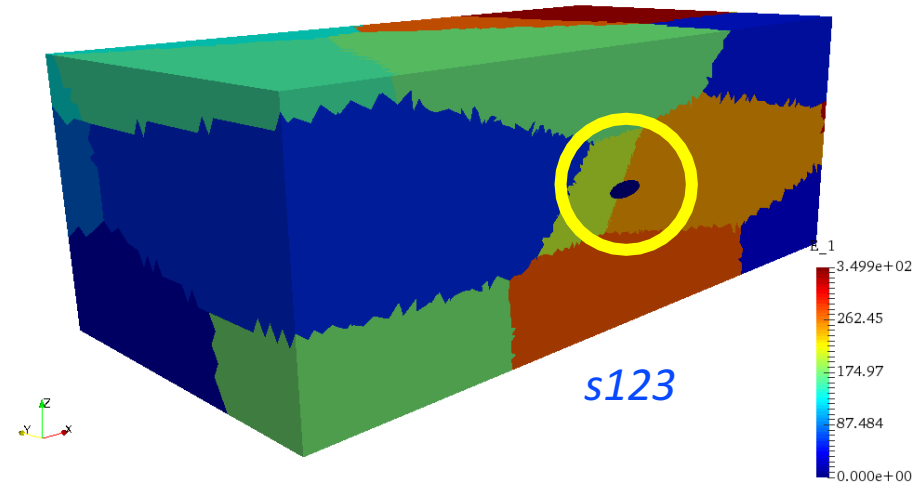
Yield surfaces recovered from simulations w/ various textures



- 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/ ~ 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.

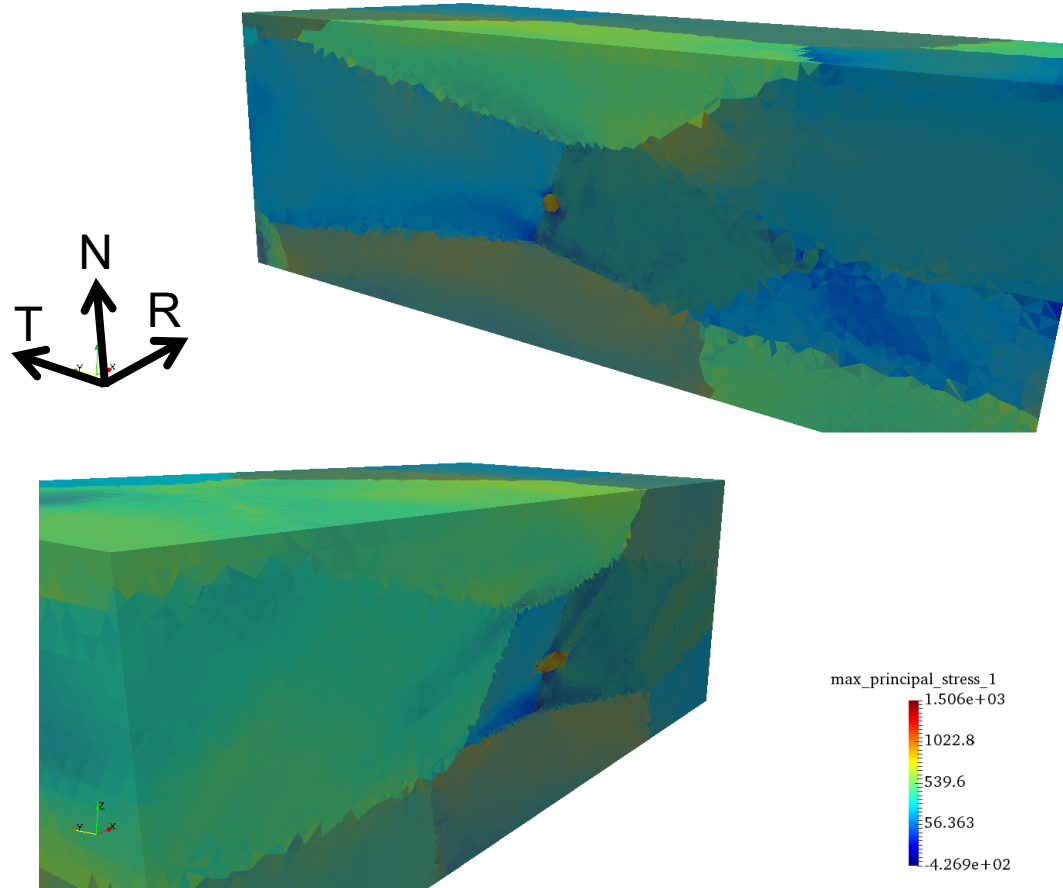
$$Pr(\bar{\epsilon}_{RVE} \in S)$$

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

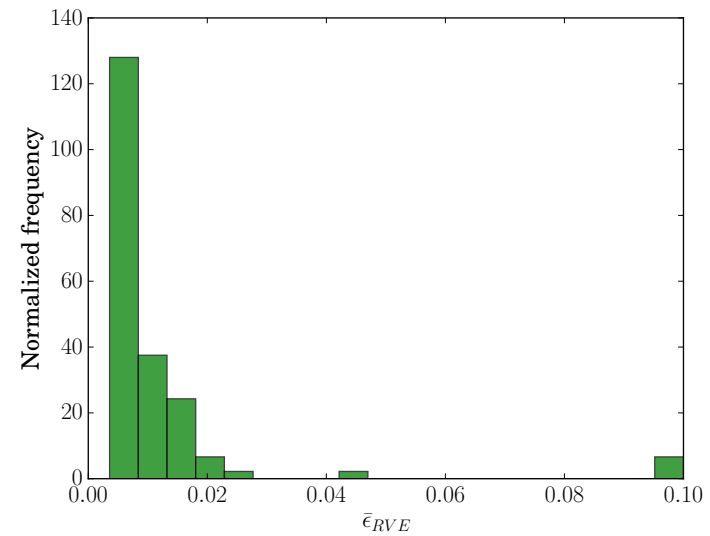
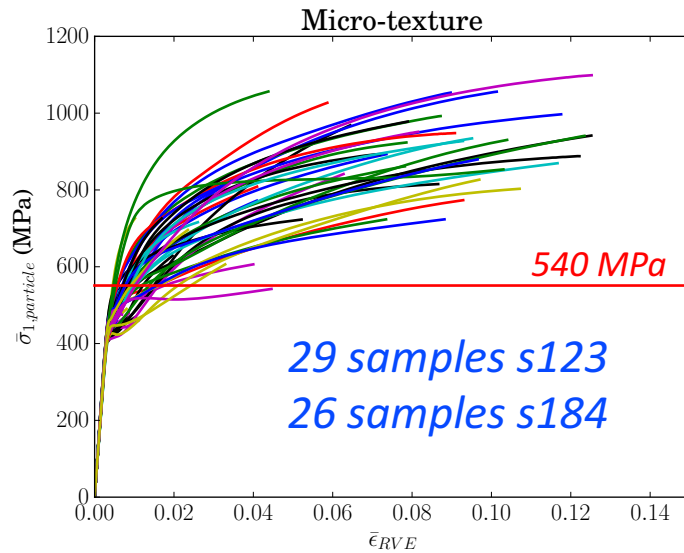
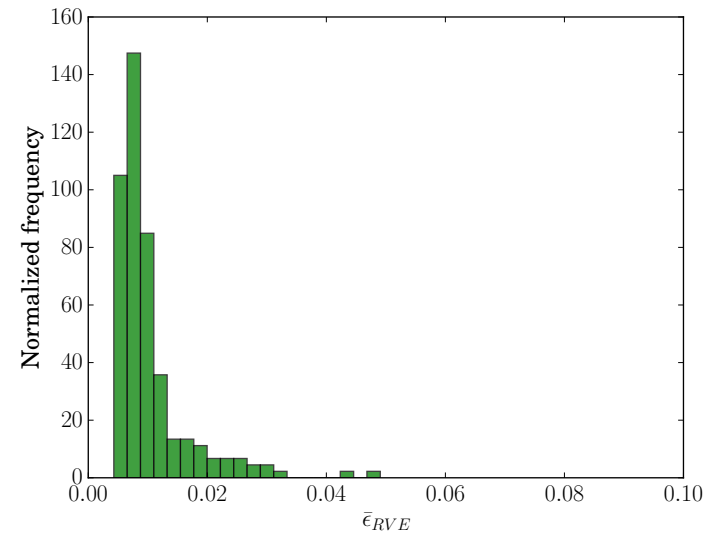
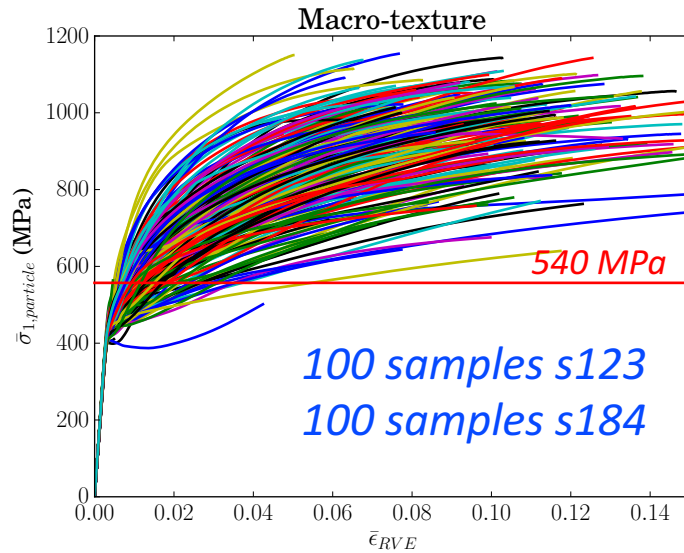
$$g(\bar{\epsilon}_{RVE}) = \bar{\sigma}_{p,cr} - \bar{\sigma}_p(\bar{\epsilon}_{RVE})$$

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

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



Mean max principal stress in particle

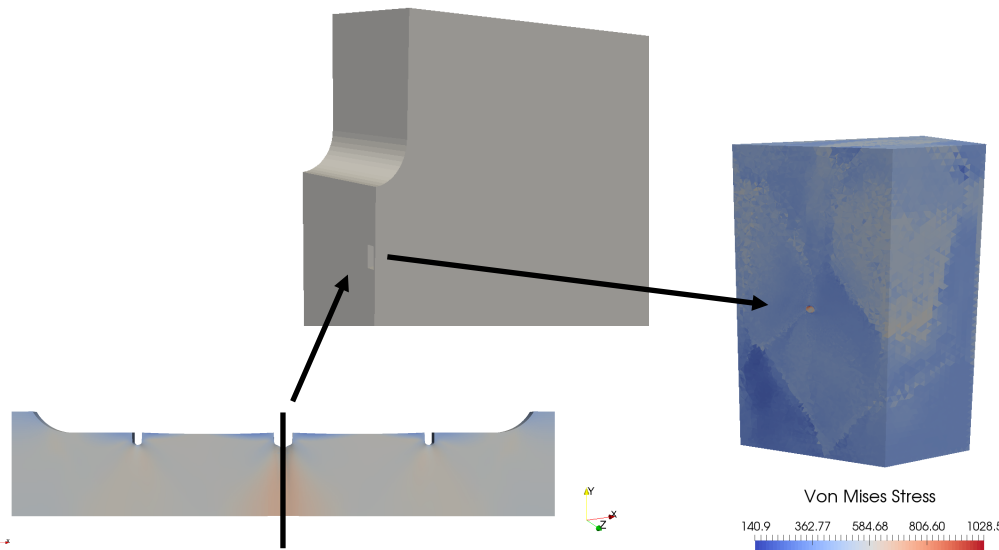


Bridging length scales

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

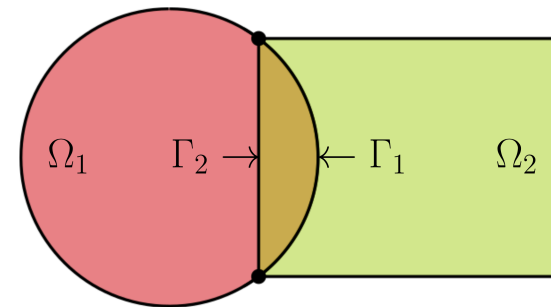
Submodeling:

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

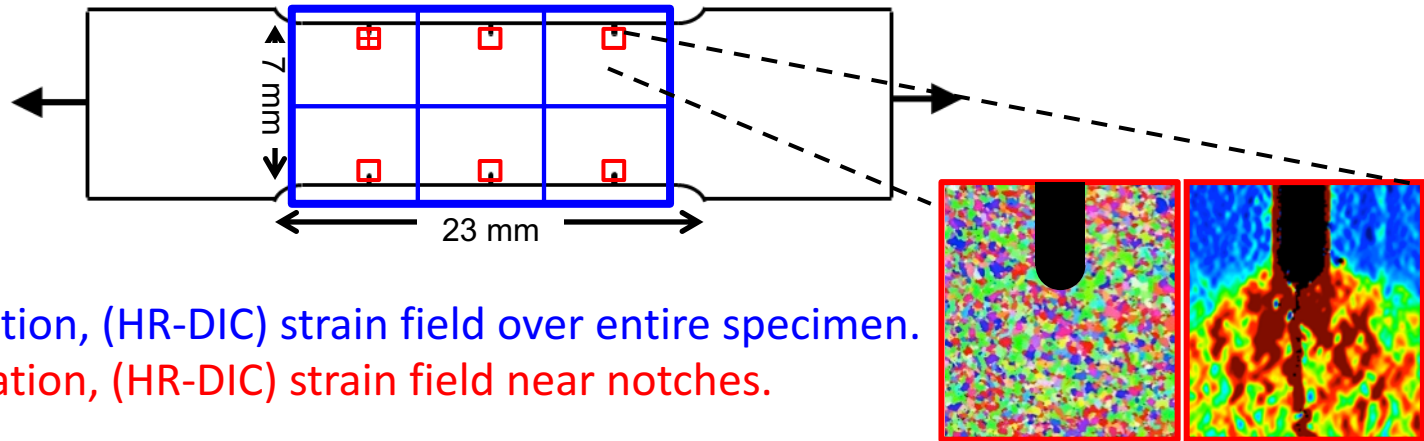


Schwarz-based solution scheme:

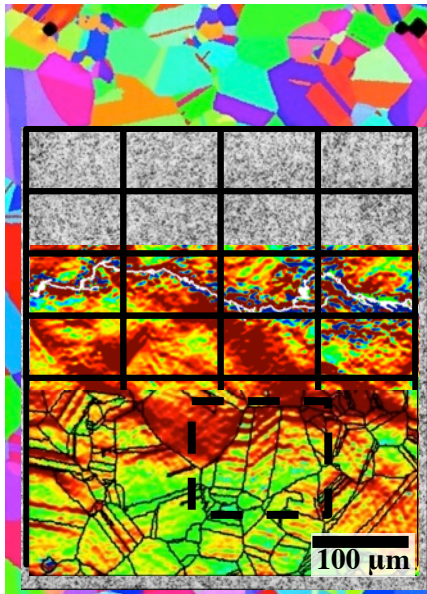
- Solve PDE by any method on Ω_1 using an initial guess for Dirichlet BCs on Γ_1 .
- Solve PDE by any method (can be different than for Ω_1) on Ω_2 using Dirichlet BCs on Γ_2 that are the values just obtained for Ω_1 .
- Solve PDE using Dirichlet BCs on Ω_1 that are the values just obtained for Ω_2 .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



Multiscale DIC for experimental validation



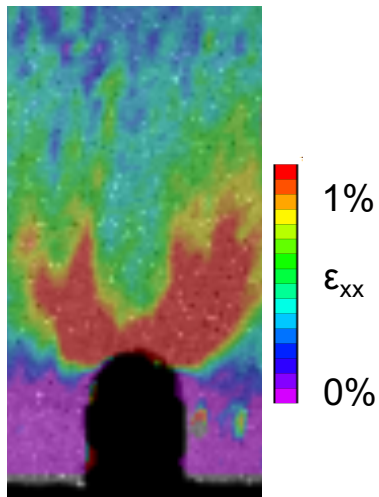
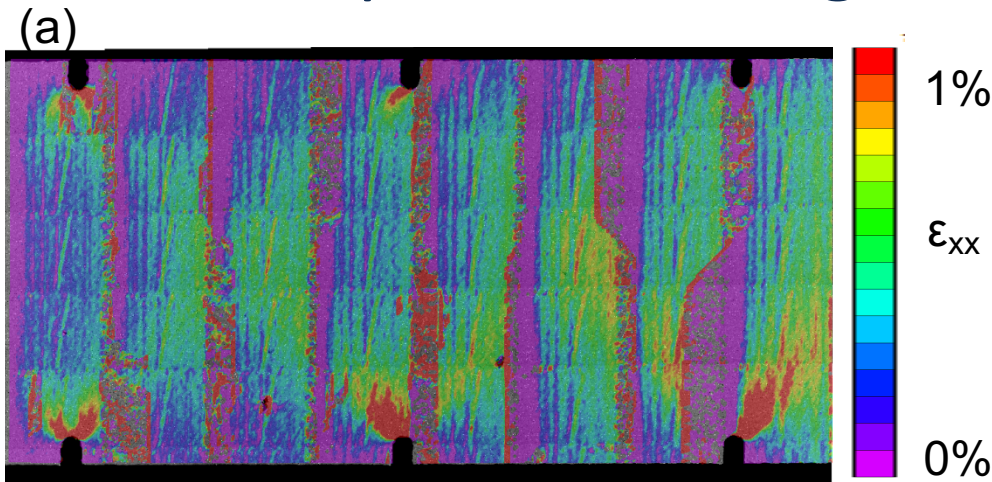
- Low magnification, (HR-DIC) strain field over entire specimen.
- High magnification, (HR-DIC) strain field near notches.



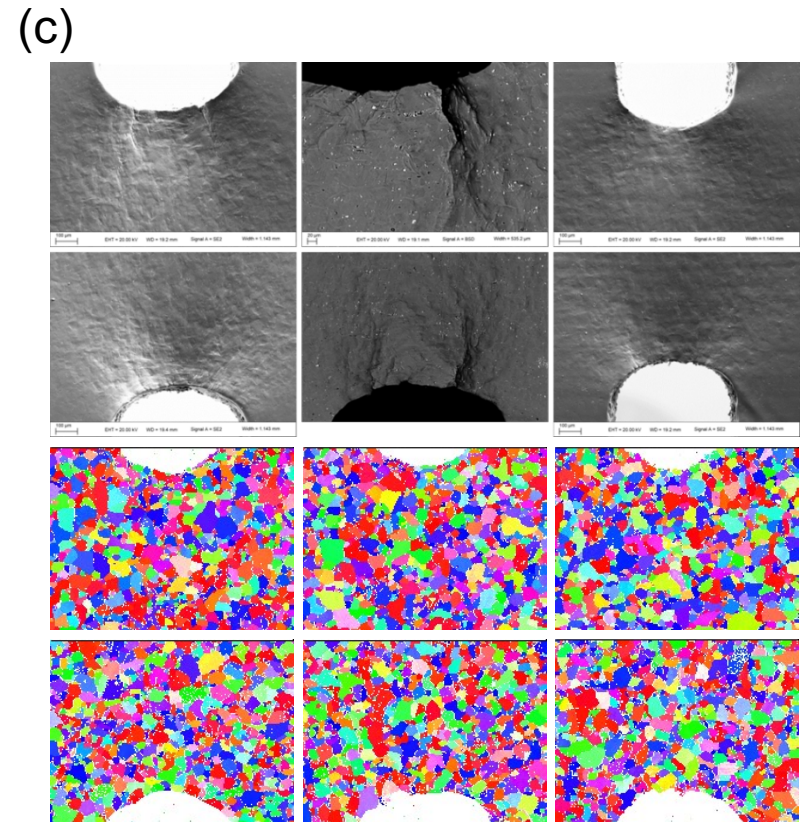
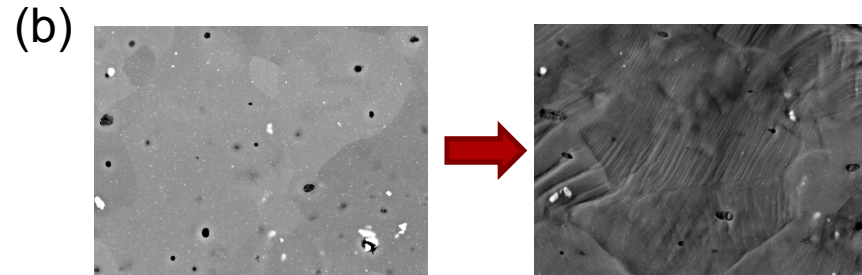
1. EBSD: microstructure
2. Capture reference images
3. Load specimen
4. Capture deformed images
5. DIC on each image location.
6. Stitch DIC results into large field of view
7. Overlay Microstructure

Requires a multi-resolution speckle pattern

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

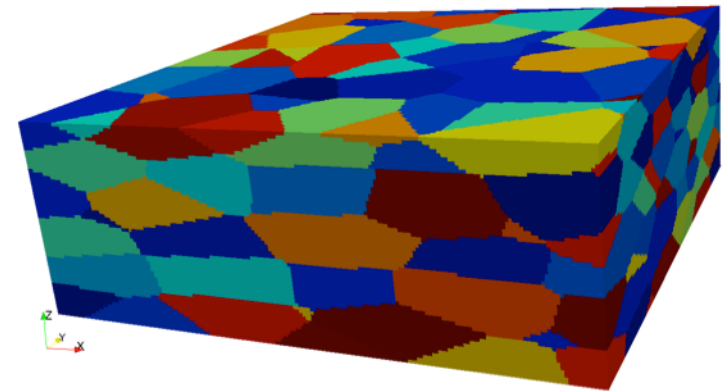
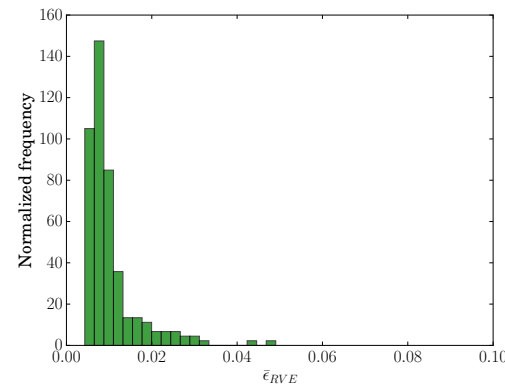
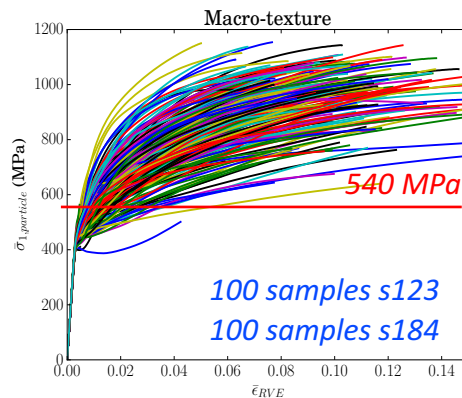


- (a) Learning to correct or eliminate lens distortion for low magnification SEM images.
- (b) Need to capture more images throughout loading because the material looks so different near failure.
- (c) Natural speckles lose contrast at high load levels we are interested in.



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?

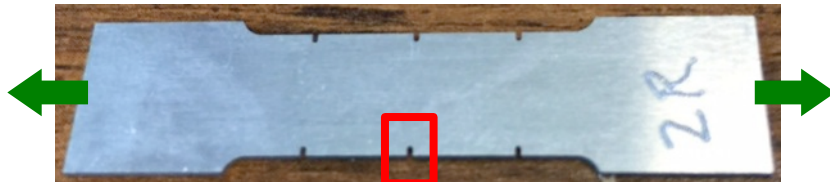
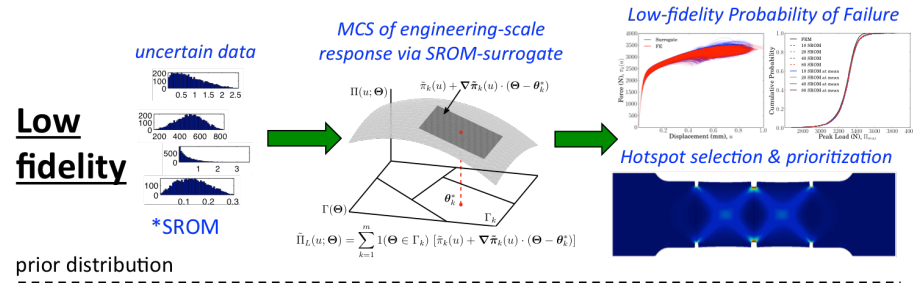
- Intentionally blank

Details needed for low fidelity simulation

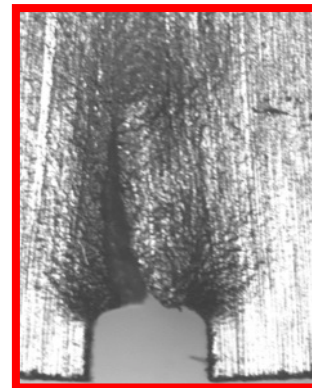
Example: low fidelity prediction of the probability of crack nucleation in an aluminum 6061-T6, engineering “component”

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 hotspot selection

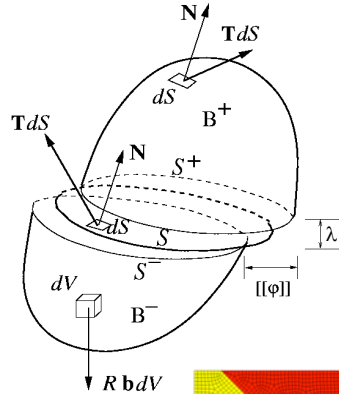


predict nucleation for AA6061-T6
“component” in monotonic loading



Localization elements to regularize

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

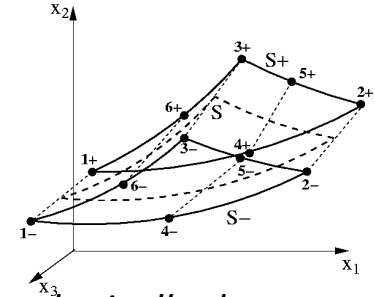


$$F = F^{\parallel} F^{\perp}$$

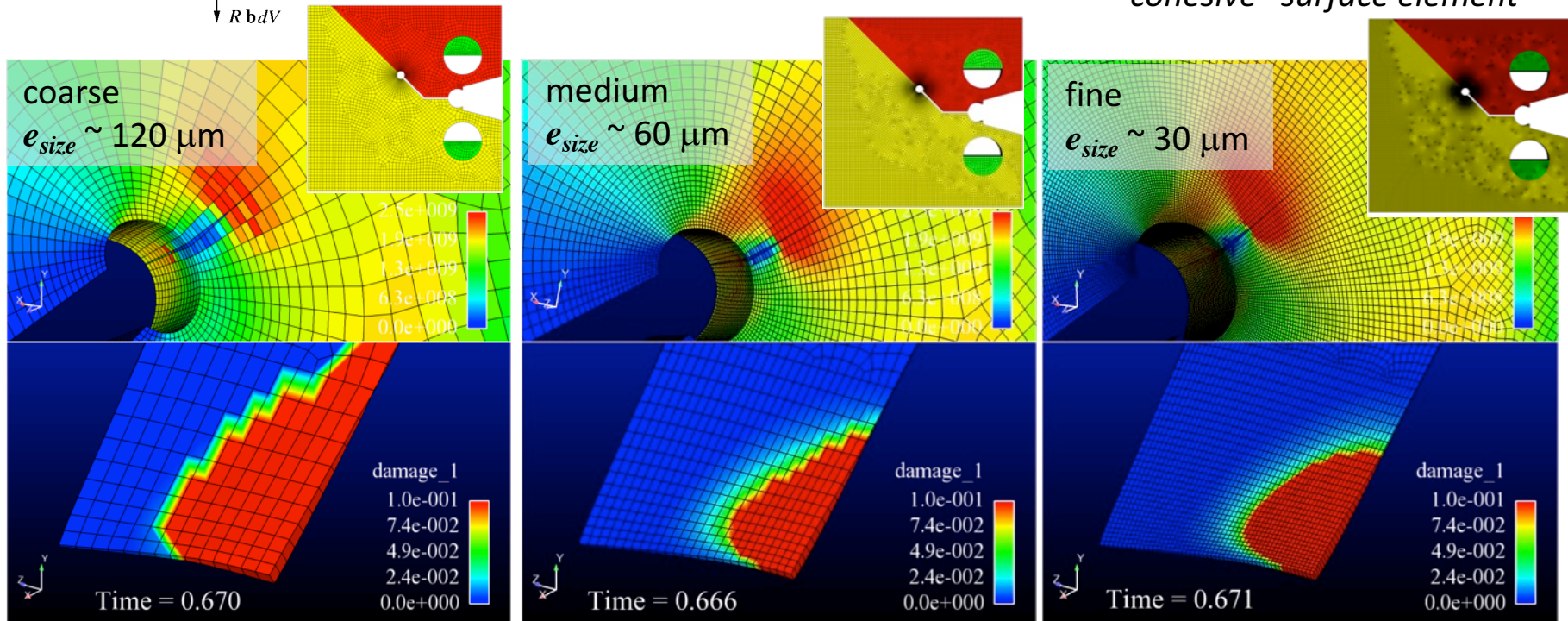
$$F^{\parallel} = g_i \otimes G^i \quad F^{\perp} = I + \frac{[\lambda]}{l} \otimes N$$

$$F = F^{\parallel} + \frac{[\lambda]}{l} \otimes N$$

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:

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

Estimates of SROM statistics given
SROM sample size n

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

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

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

Estimates of sample statistics
given q samples of Θ

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

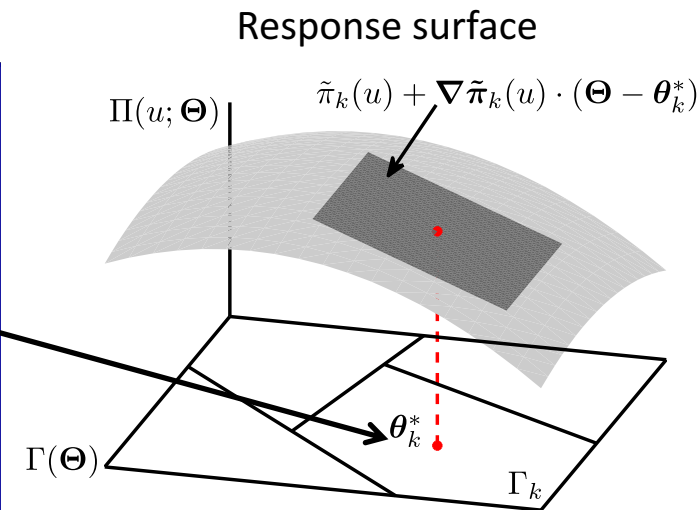
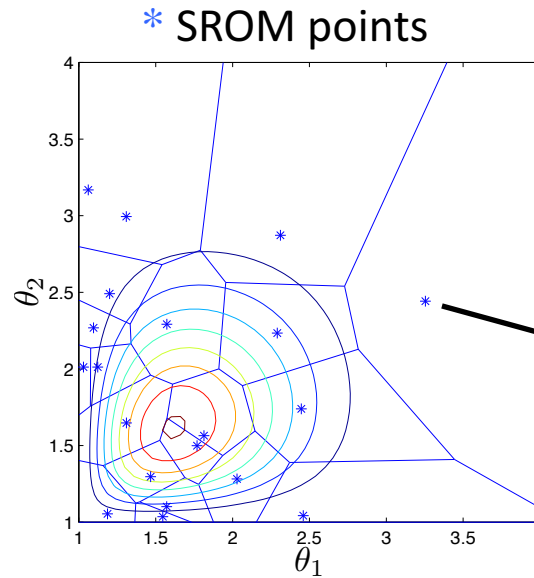
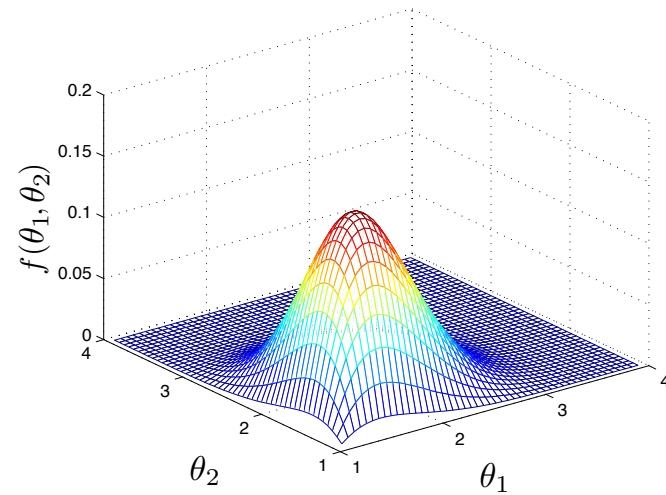
$$\hat{F}_s(x) = \sum_{i=1}^q (1/q) 1(\theta_{i,s} \leq x)$$

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

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

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

- 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.

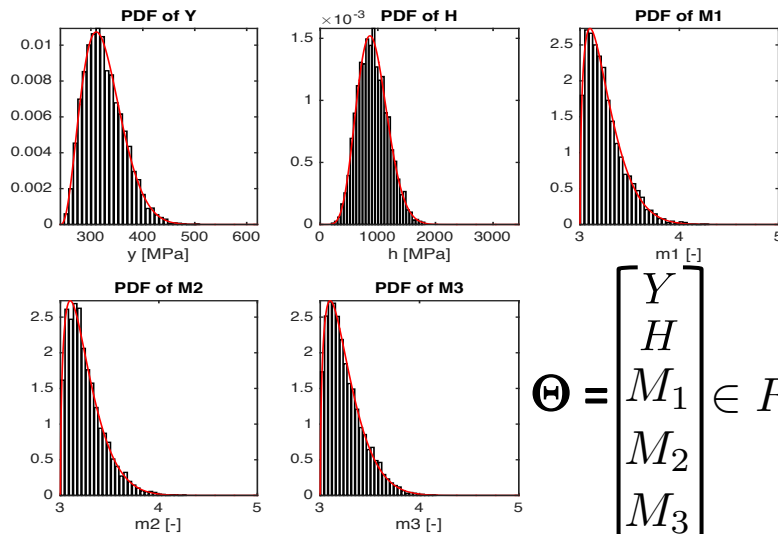
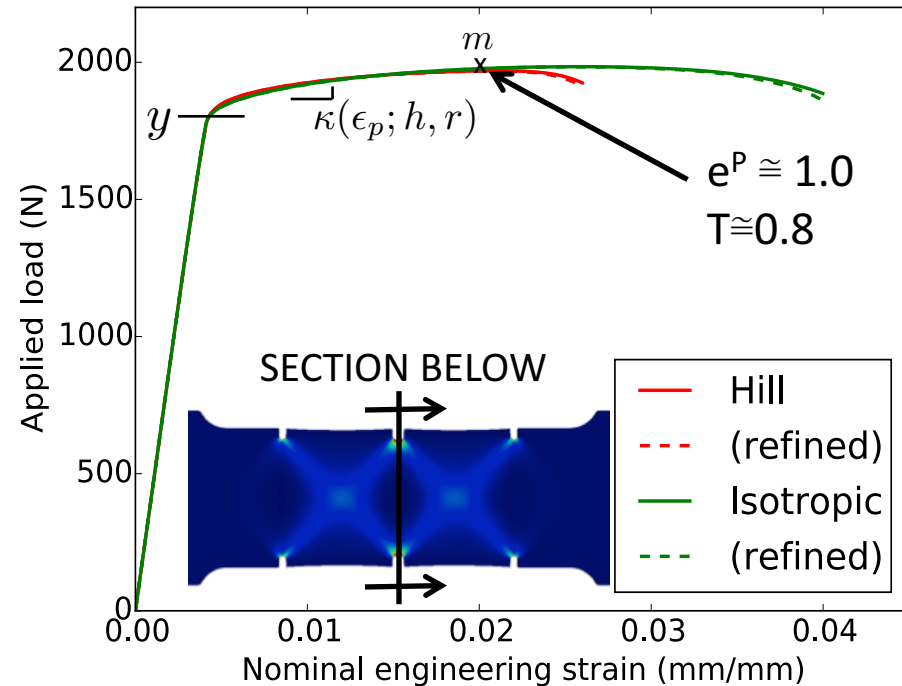
Calculations demonstrating progress toward the goal

- 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

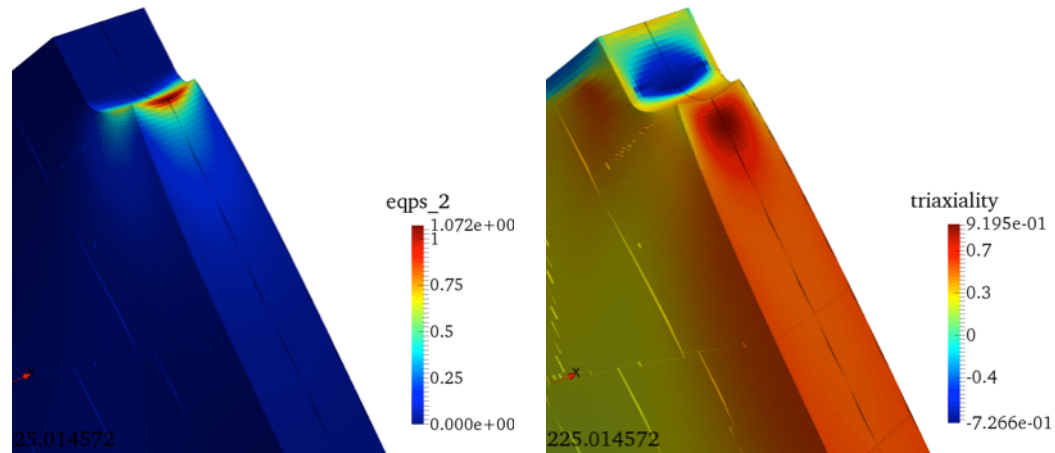
$$\dot{\phi} = \sqrt{\frac{3}{2}} \dot{\epsilon}_p \frac{1 - (1 - \phi)^{m+1}}{(1 - \phi)^m} \sinh \left[\frac{2(2m - 1)}{2m + 1} \frac{p}{\sigma_{vm}} \right]$$

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

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



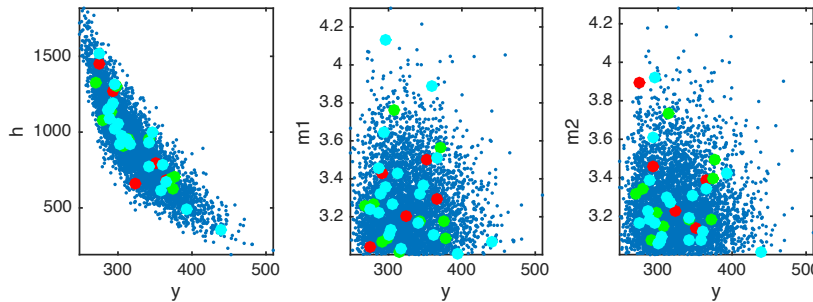
$$\Theta = \begin{bmatrix} Y \\ H \\ M_1 \\ M_2 \\ M_3 \end{bmatrix} \in R^d$$



SROM for Low-fidelity probability of failure

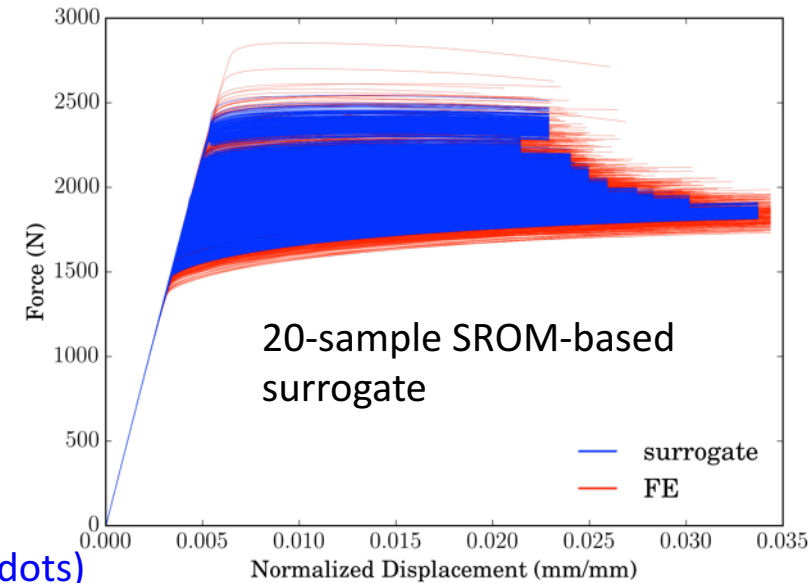
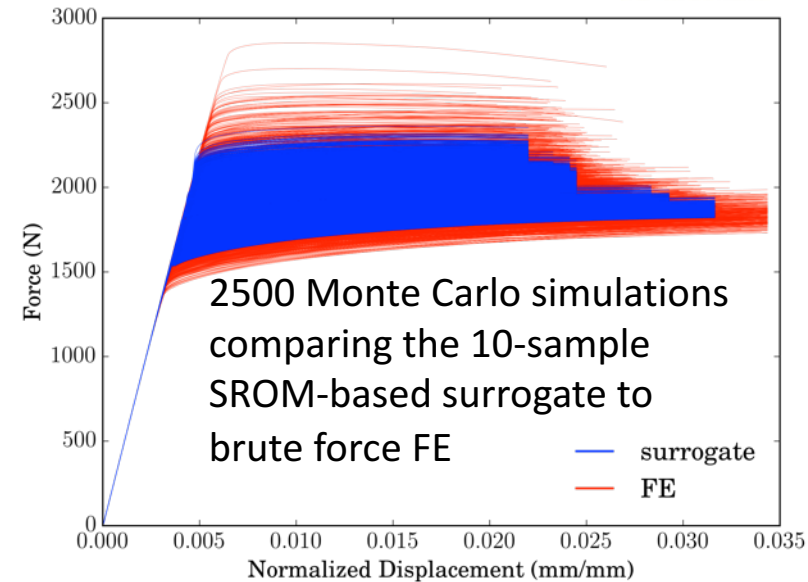
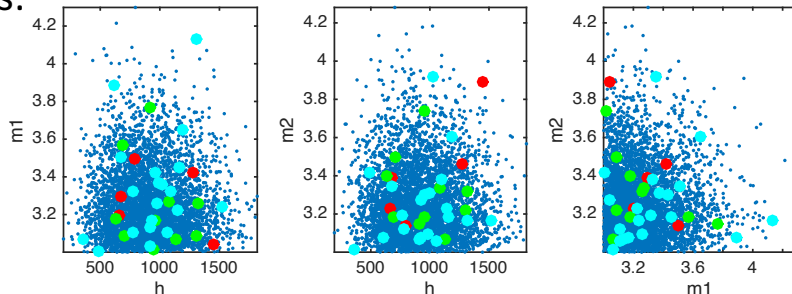
- Examples of 3 SROMs for the uncertain parameters.
- Force-displacement curves from Monte Carlo simulation two ways: (blue) with the SROM-based surrogate and (red) brute force finite-element simulation.
- We are developing tools to identify & prioritize hotspots based on surrogate results.

Monte Carlo samples



SROM samples:

- red dot: $n = 5$
- green dot: $n = 10$
- cyan dot: $n = 20$



MC samples (small dots) and optimal samples for SROM (large dots)

Another (well ironed) example: A304L laser weld failure

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

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

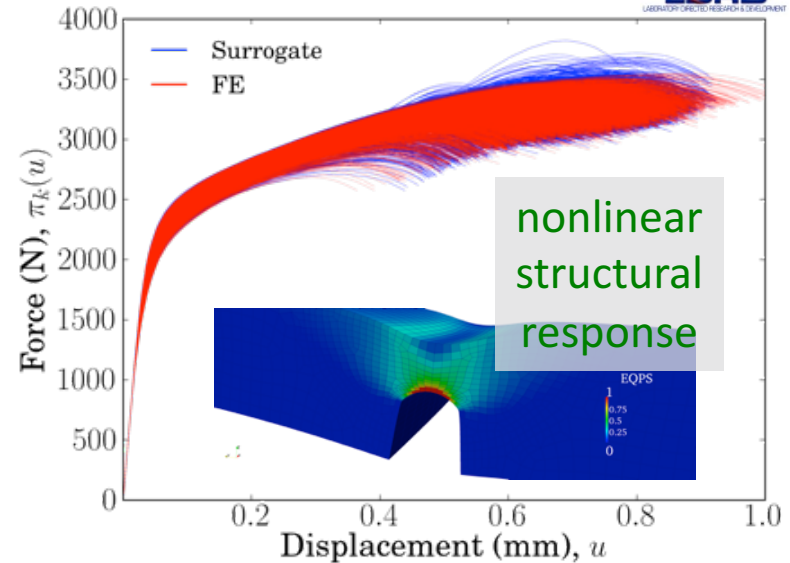
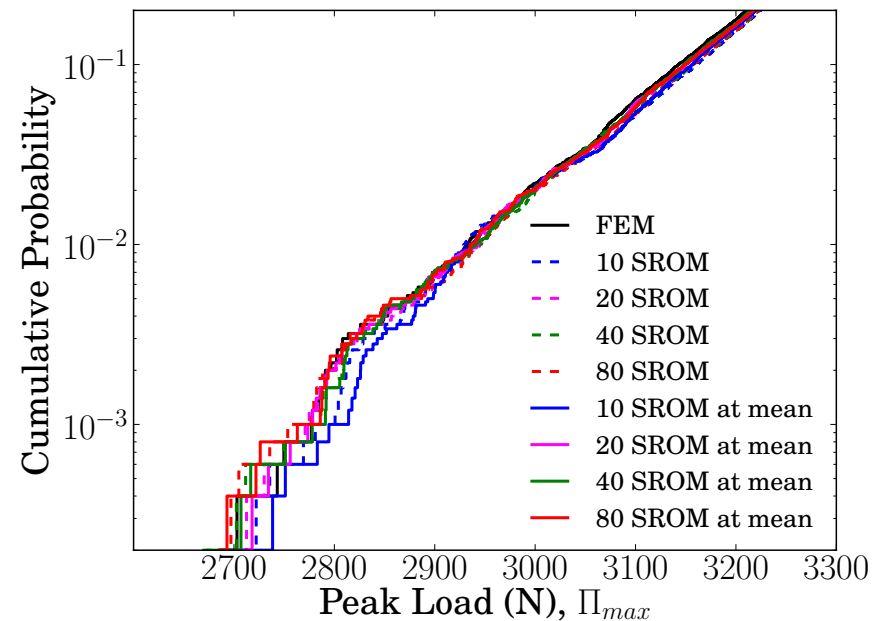
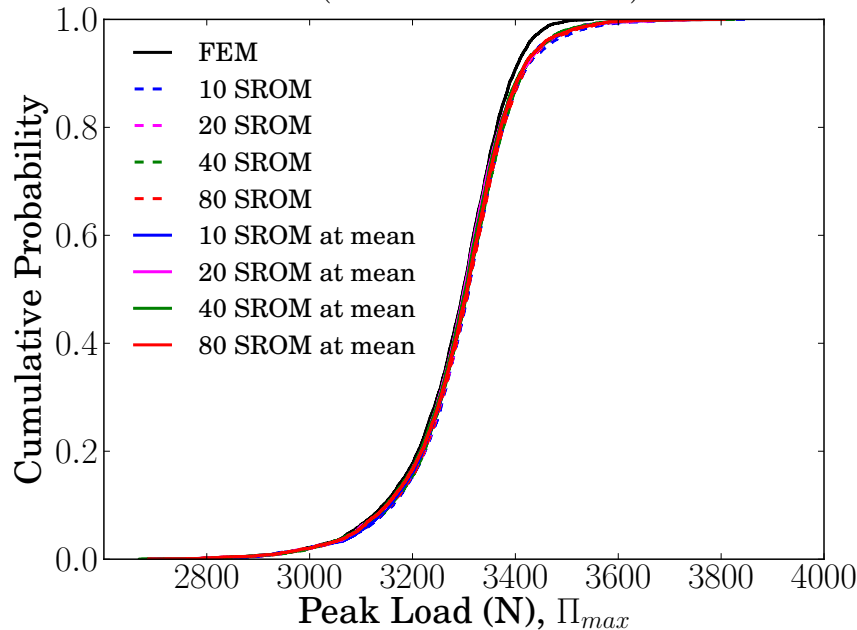
uncertain parameters

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

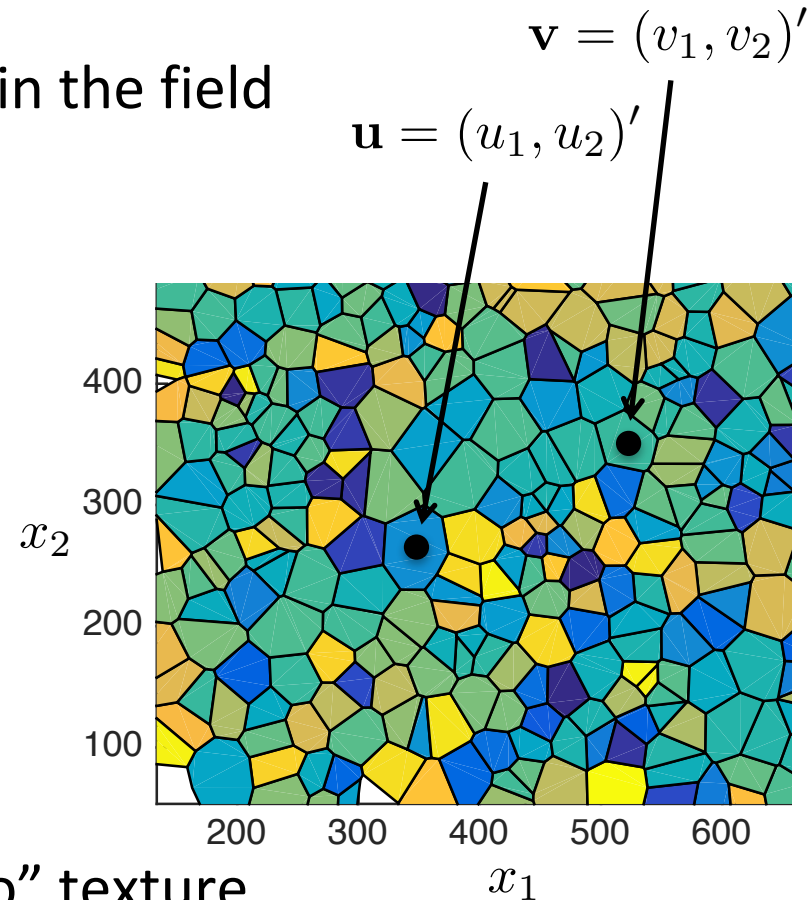
$$E[\psi_1(\mathbf{u}) \phi(\mathbf{v})]$$

- Special cases

- Statistically homogeneous
Depends on $(\mathbf{u} - \mathbf{v})$

- Statistically isotropic
Depends on $\|\mathbf{u} - \mathbf{v}\|$

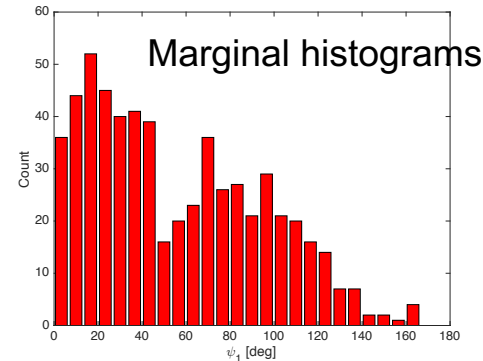
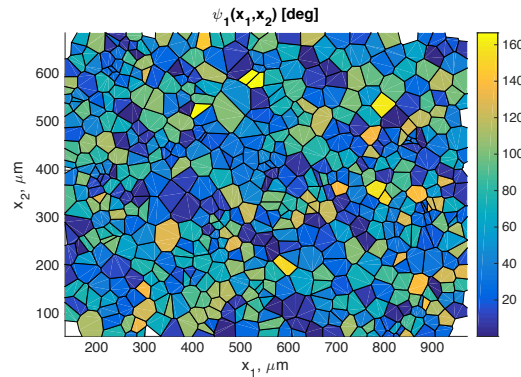
- Provides one way to model “micro” texture



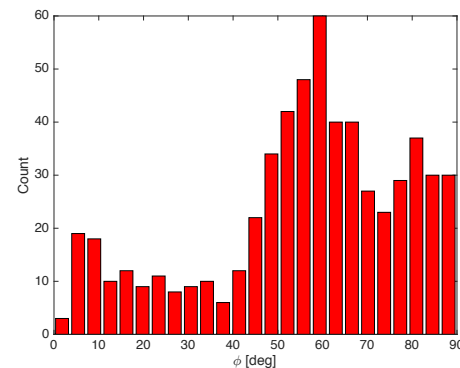
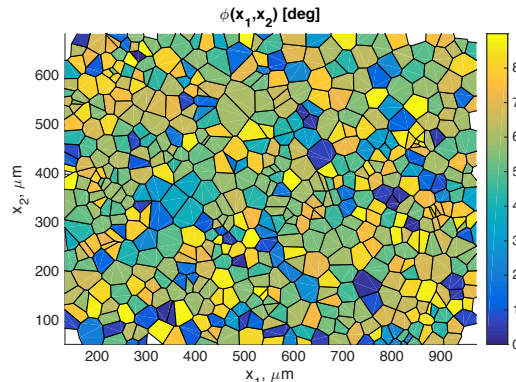
Experimental Data

EBSD data from Ta wire **Not AA6061

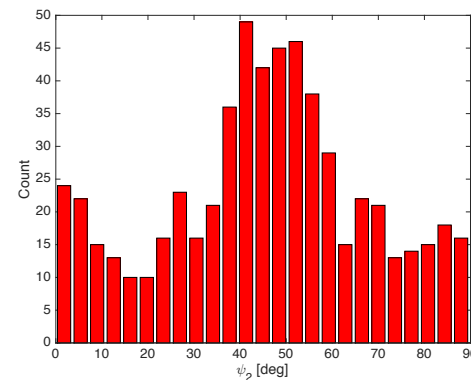
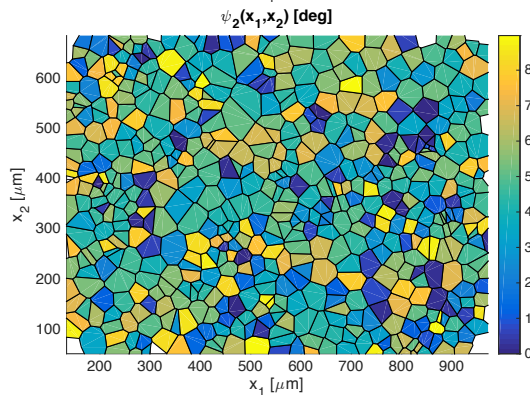
Angle 1: ψ_1



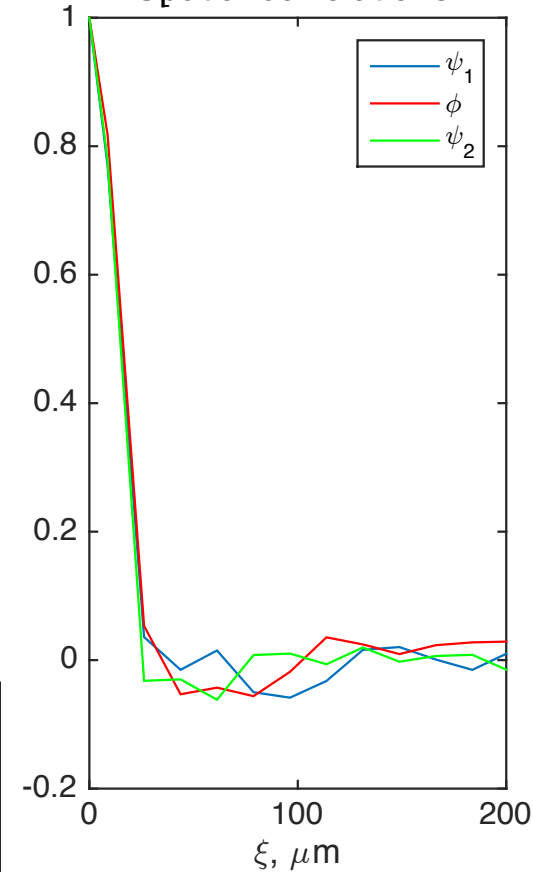
Angle 2: ϕ



Angle 3: ψ_2

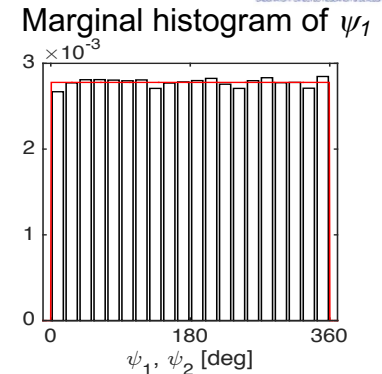
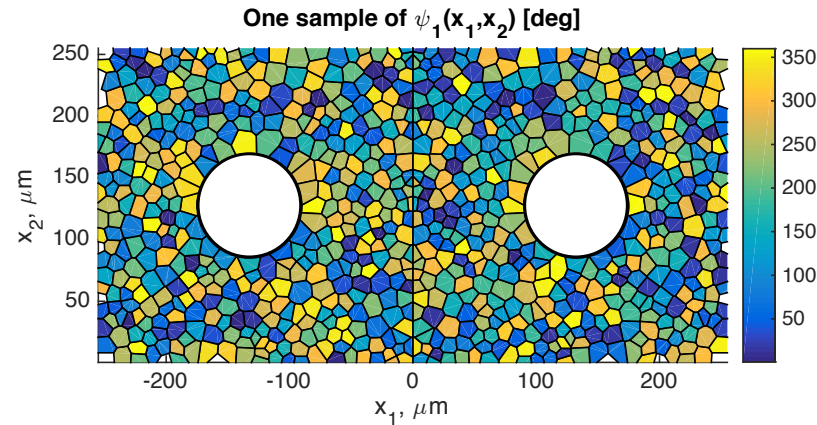


Spatial correlations

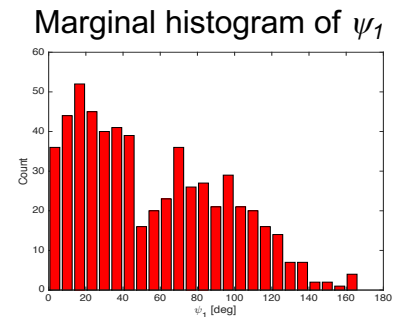
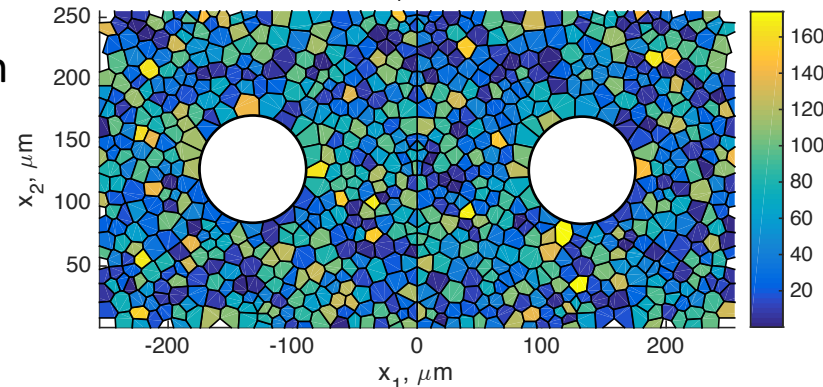


2D example from EulerRF

Zero texture, zero spatial correlation

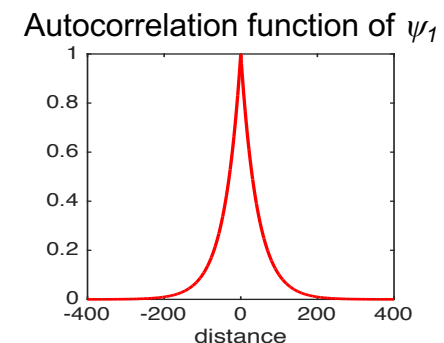
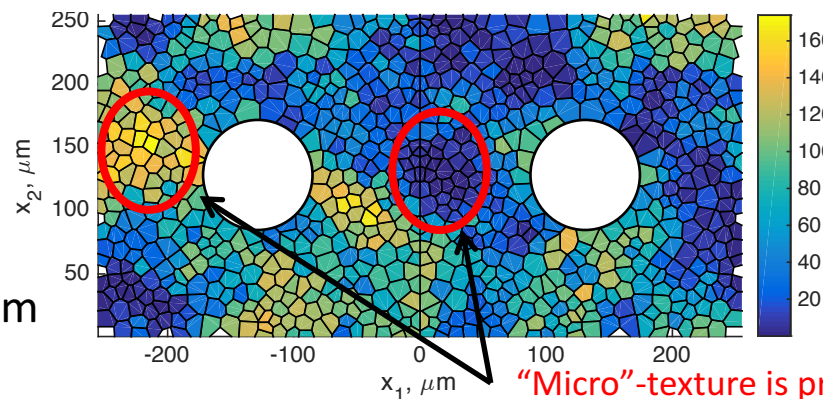


With macro-texture based on data file, zero spatial correlation



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

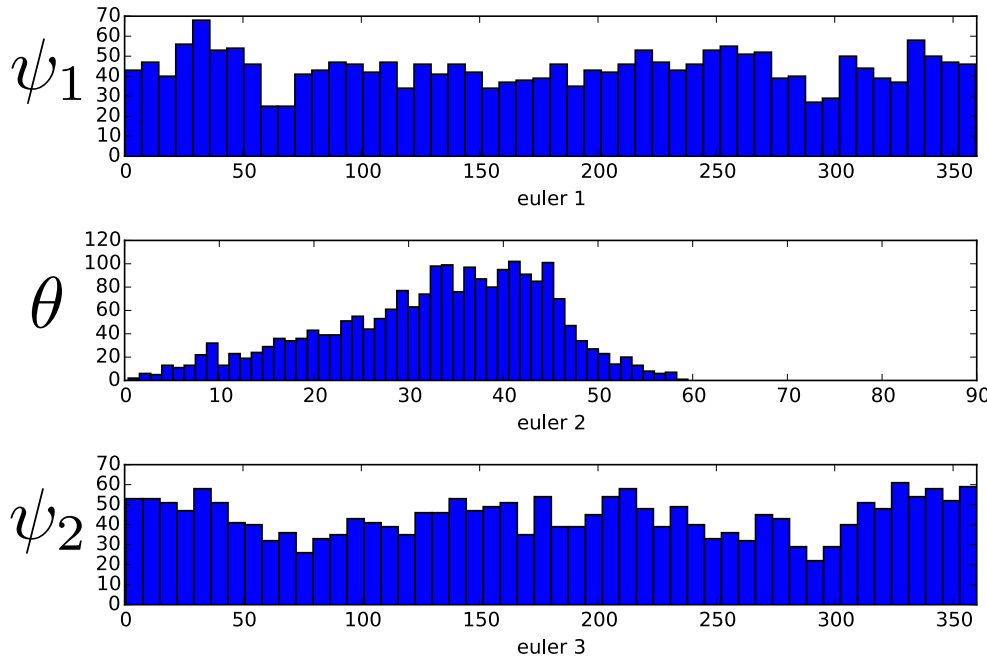
- Texture based on data file
- Isotropic (exponential) spatial correlation with correlation length = 200 μm



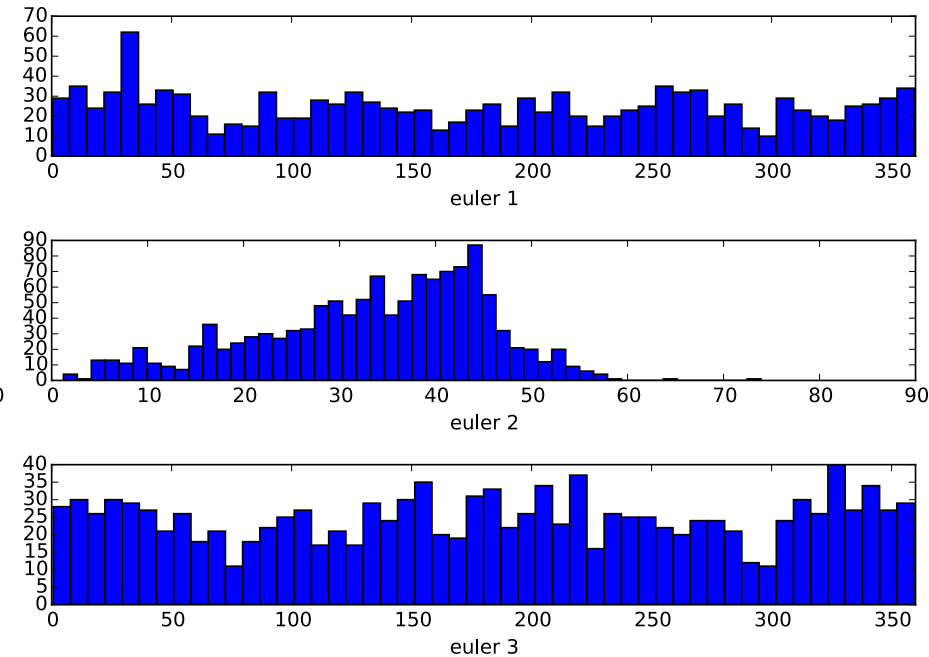
"Micro"-texture is present

Comparing histograms – data vs. texture samples

measured EBSD data

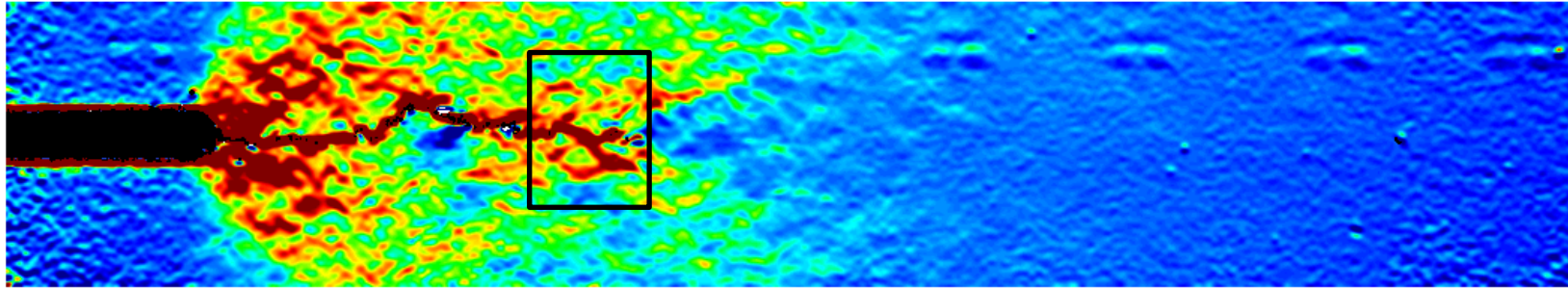


model data



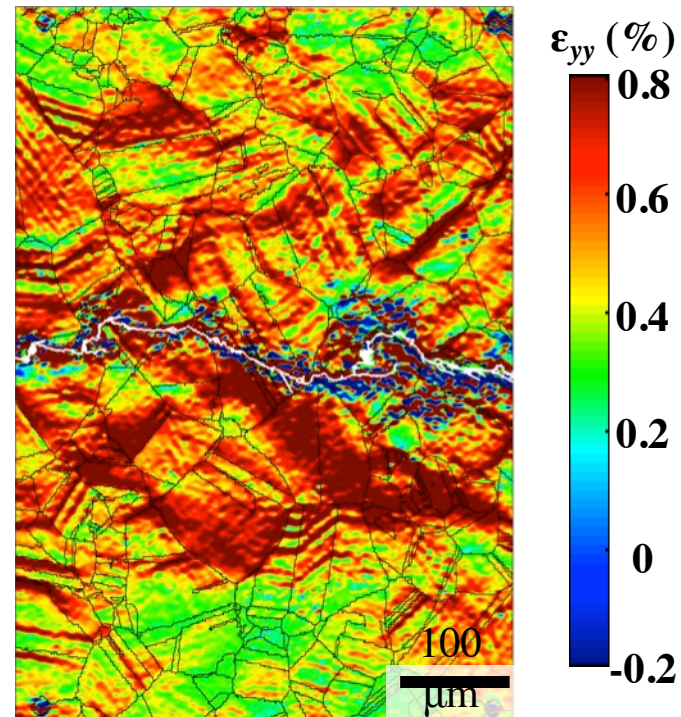
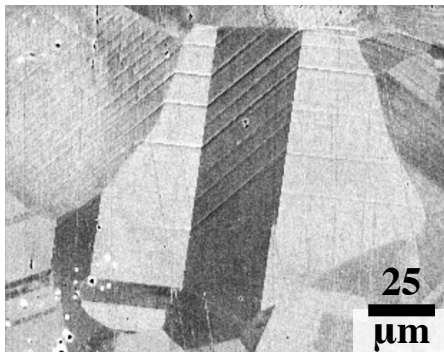
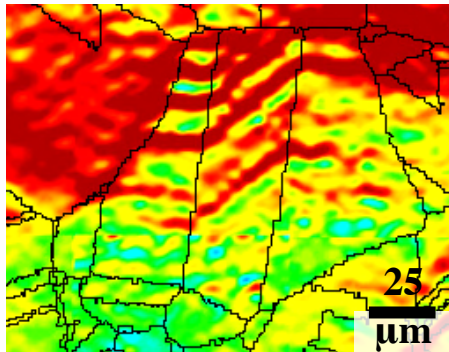
- Histograms drawn for the individual Euler angles

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.



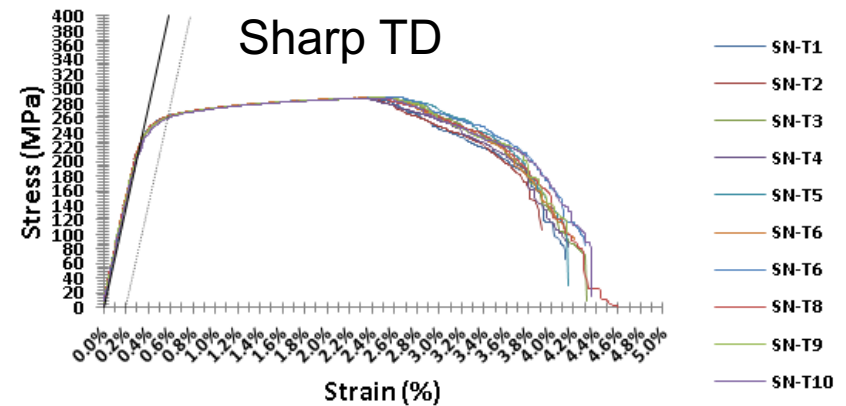
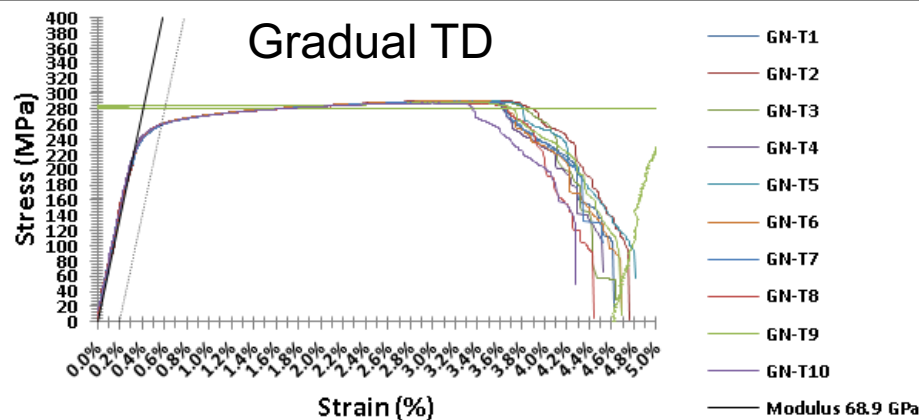
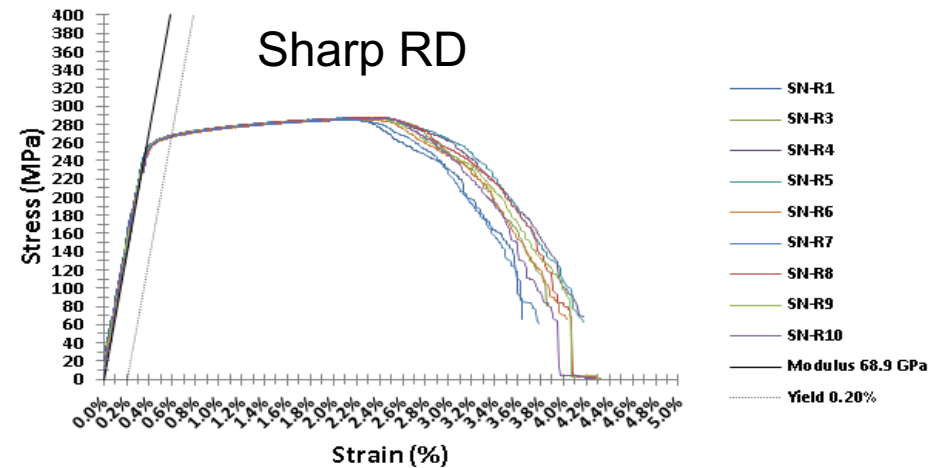
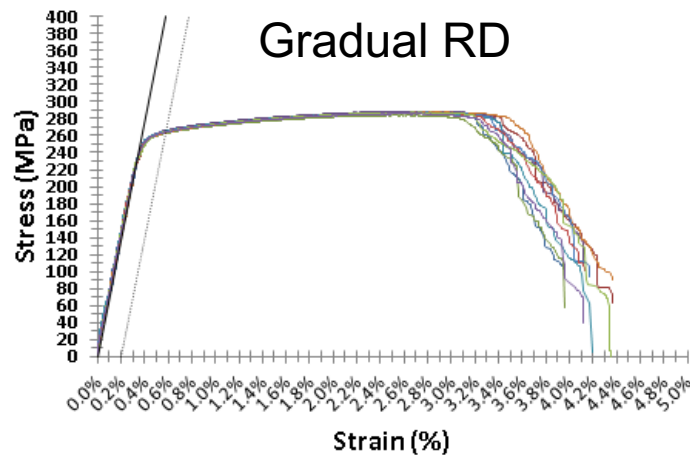
Carroll *et al.*, *Rev. Sci. Instr.*, v. 81 (2010)

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

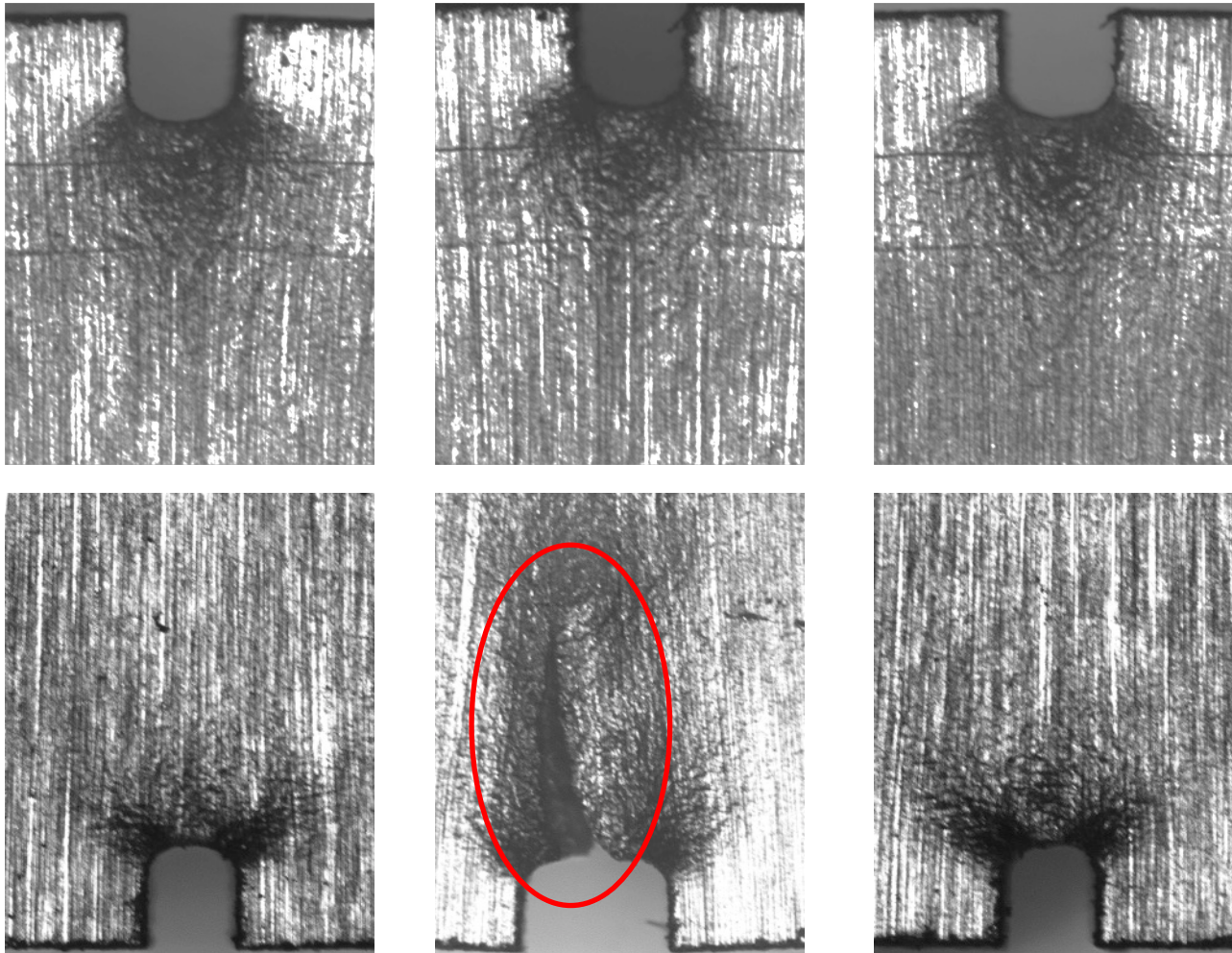
Carroll *et al.*, *Int. J. Fatigue*, (2013)

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.

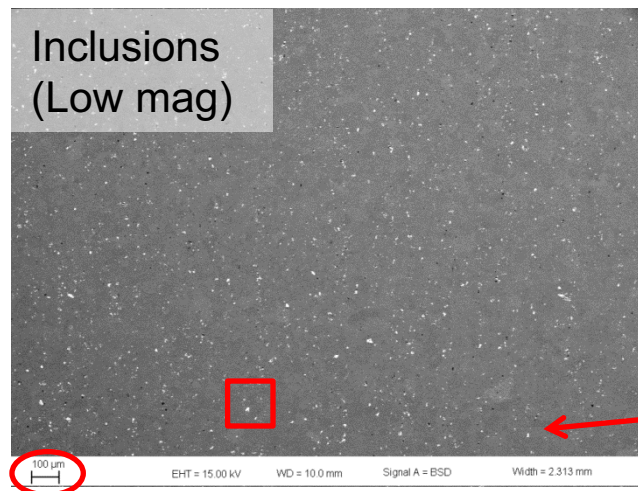
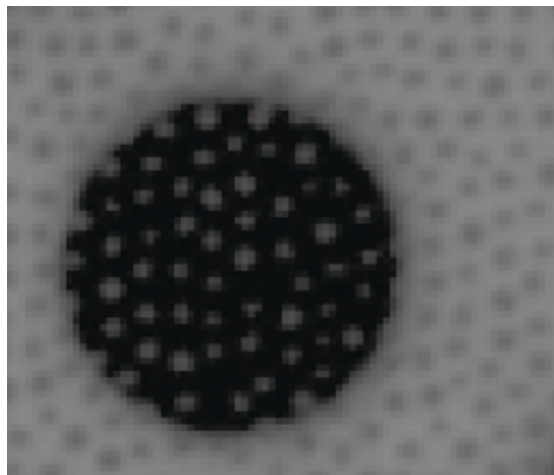


- Unstable crack growth occurred after this substantial crack was observed.

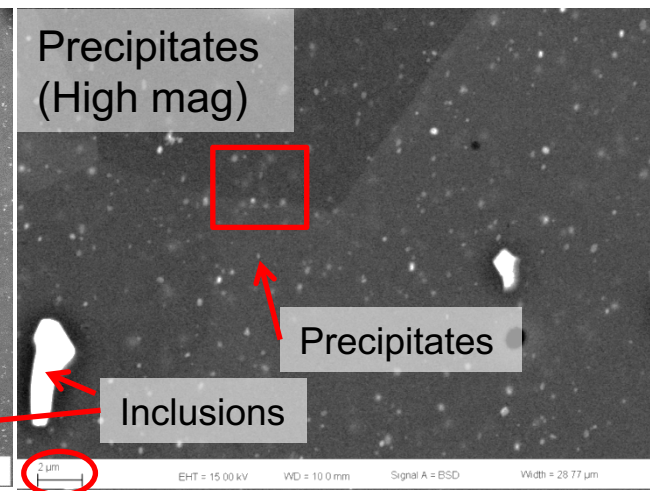
Multiscale digital image correlation

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 ($\sim 1\%$ strain).

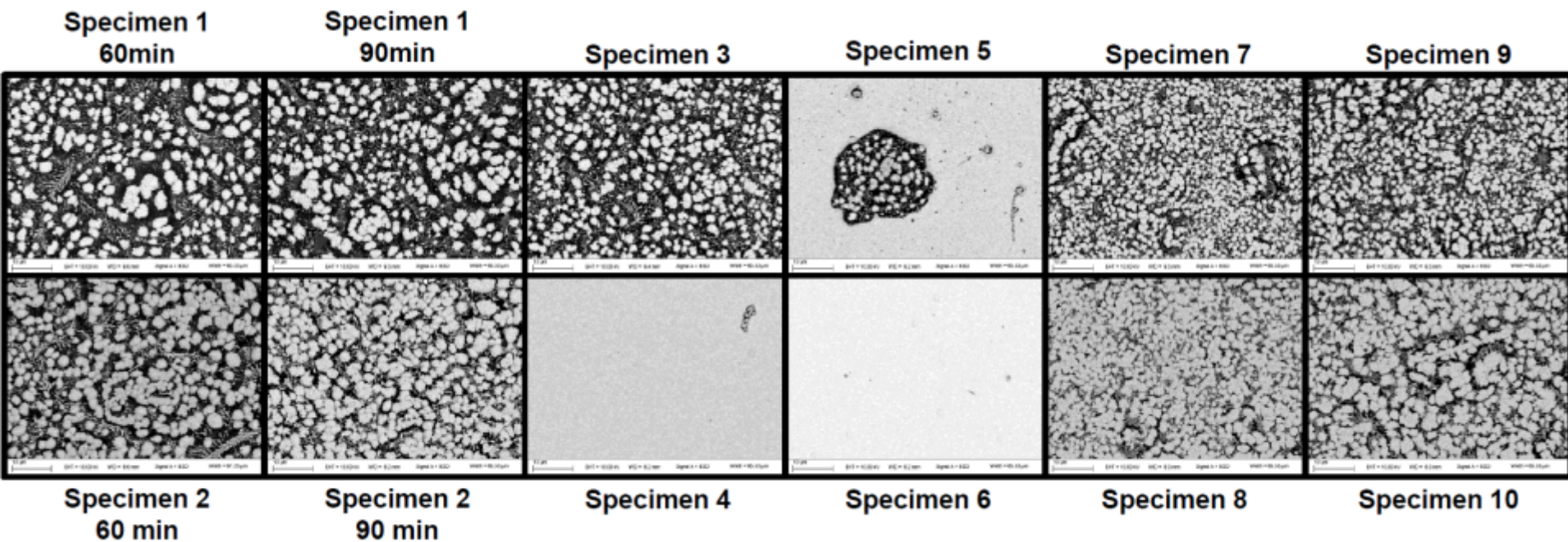


Resolution down to $\sim 150 \mu\text{m}$



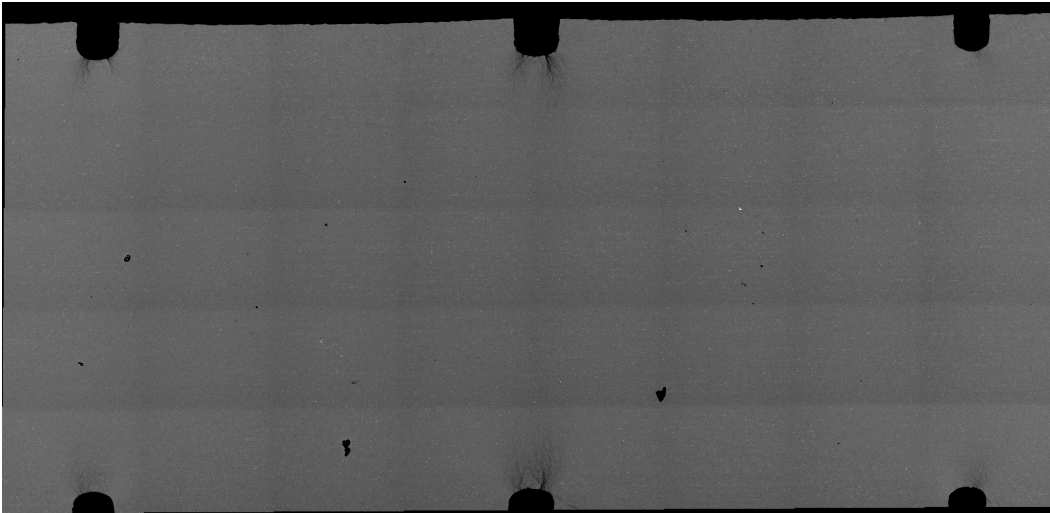
Resolution down to $\sim 4 \mu\text{m}$

Various instantiations of a multiscale speckle pattern by sputtering gold

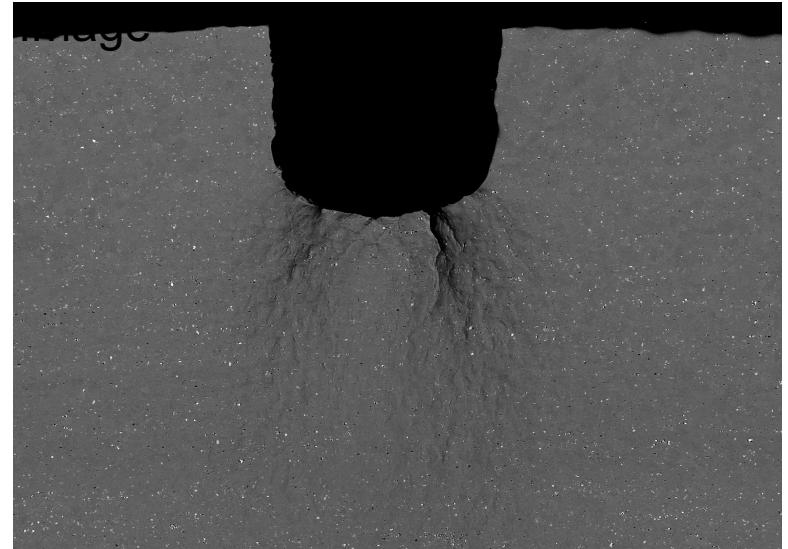


Multiscale imaging

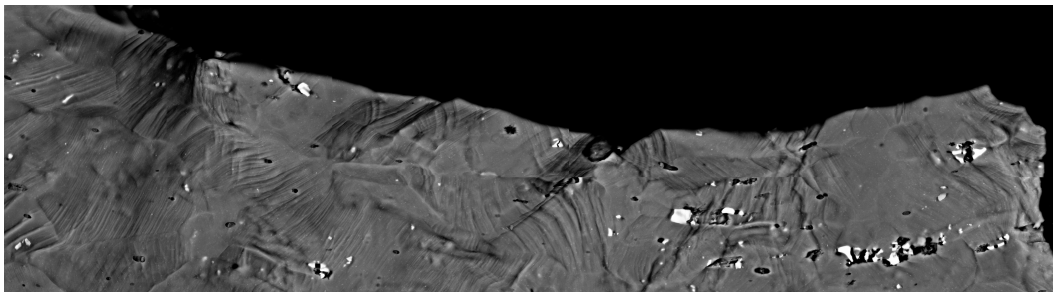
Low Resolution Montage



Low Resolution Single Image



High Resolution Montage



High Resolution Single Image

