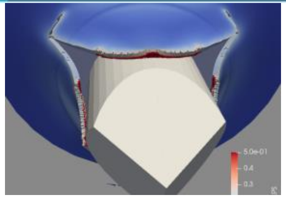
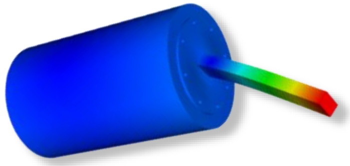
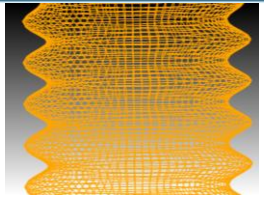
# Investigating the Microstructure and Properties Relationship of a Ta-alloy



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08/05/2025

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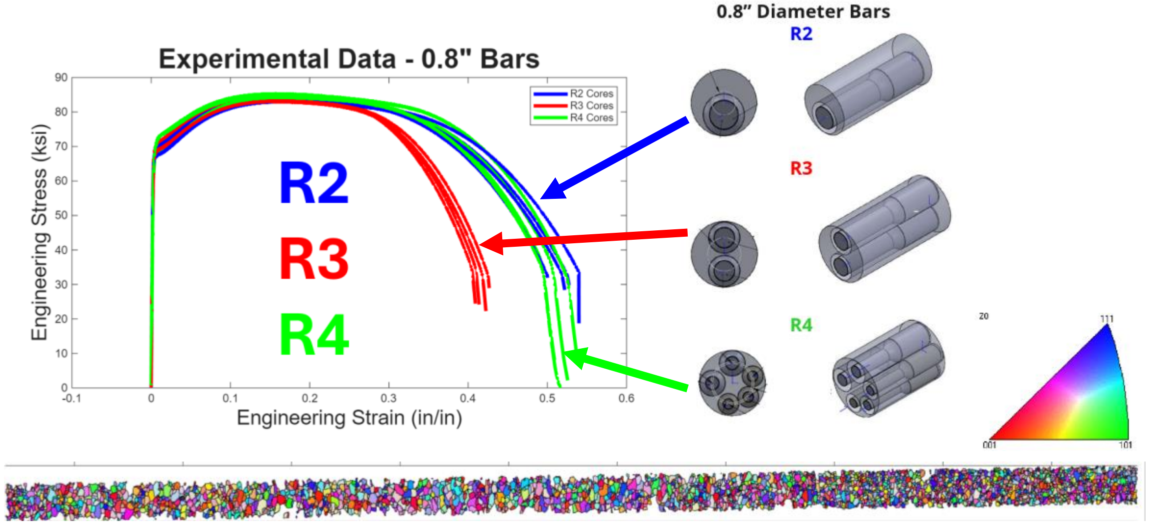
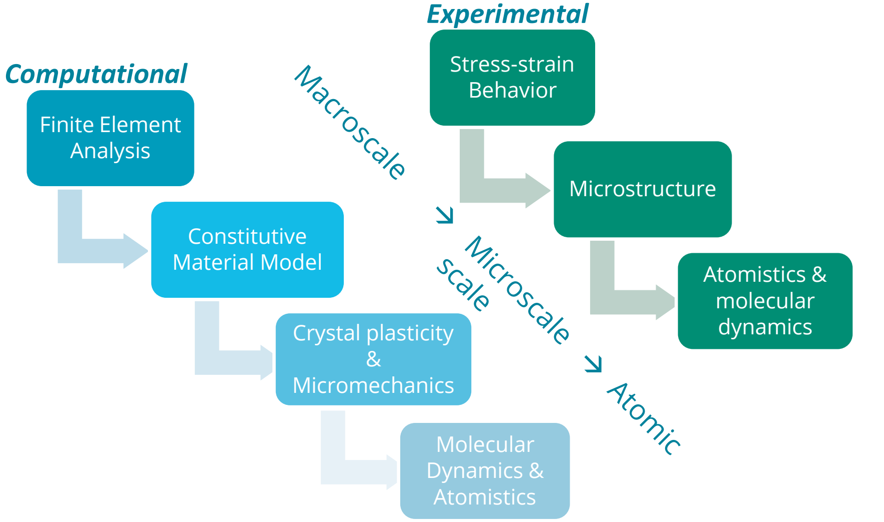
**SAND2025-09714PE**

# Project Overview




***Bar Center*** ← ***Differing Texture and Microstructure*** → ***Bar Surface***




## Technical Background

- Material: Tantalum – 10 wt% Tungsten
- Unexpected ductility response from set of tensile bars (R3) in comparison to their counterparts (R2&R4) across different bars that each differed in manufacturing process.
- Electron backscattered Diffraction (EBSD) from as-received bar highlighted microstructural and textural differences within radius of each bar.

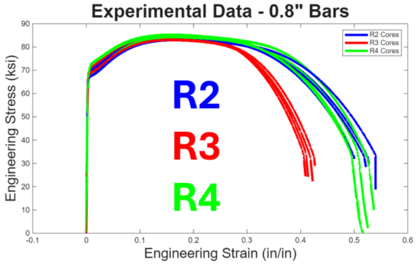
## Research Tasks

1. Analyze macro-scale fracture surfaces to identify property changes potentially linked to microstructural and texture variation using EBSD scan data.
2. Generate and analyze 3D microstructures from experimental data using statistical tools to quantify differences across samples.
3. Run and post-process Sierra simulations, comparing simulated stress-strain curves with prior test data to asses the influence of microstructure on mechanical response.

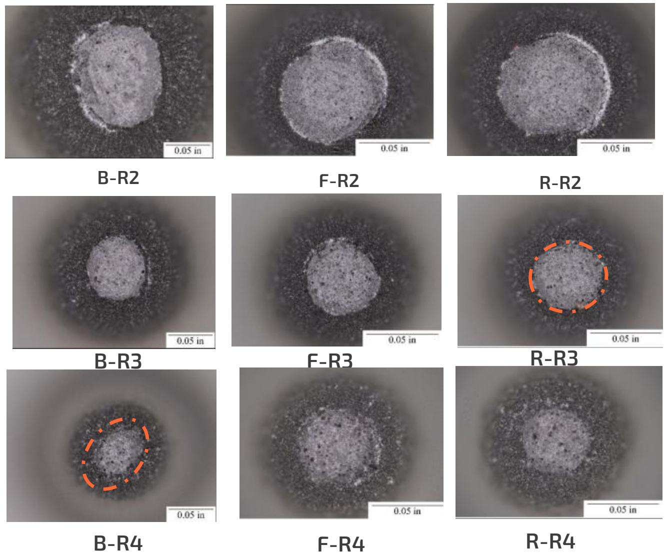
**Goal:** Improve understanding of whether local (radial) microstructure/texture transition results in mechanical property differences in intermediate sized specimens.

# Microstructure Experimental Characterization

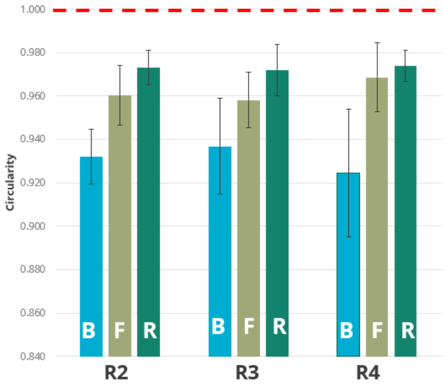
## Fracture Surface Evaluation




### Fracture Surfaces



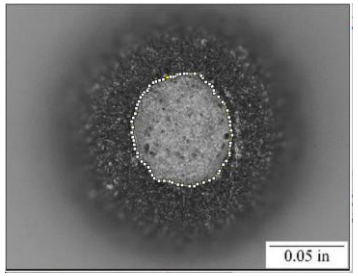

### Circularity




### Aspect Ratio


B - 1.125" Rotary Forged
F - 0.8" Rotary Forged
R - 0.8" Rolled

### IMAGE J Measurements




**Circularity**

$$Circularity = \frac{4\pi \times Area}{Perimeter^2}$$

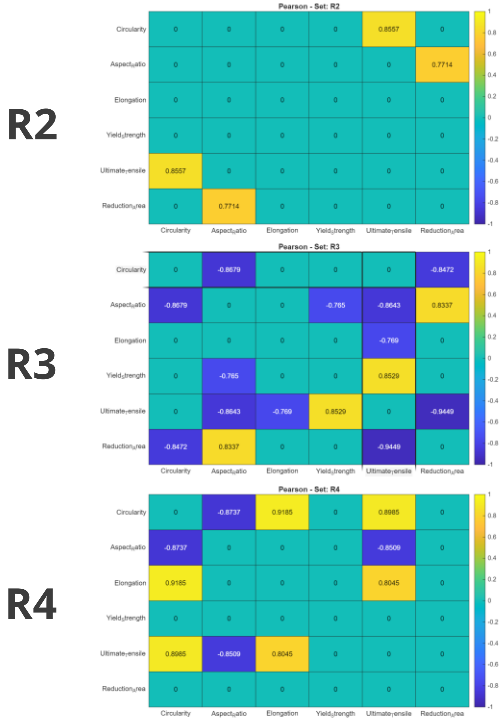
**Aspect Ratio**

$$Aspect\ Ratio = \frac{Major\ Axis}{Minor\ Axis}$$

**Fracture Surface Circularity and Aspect Ratio**

- 1.125" Rotary Forged Bar had lowest circularity (0.925-0.937) and highest aspect ratio (1.13-1.27)
- 0.8" bars-rotary and rolled-both exhibited similar higher circularities and similar lower aspect ratios
- **R3 samples also followed a similar trend as the parent bar**.

### Pearson Correlation



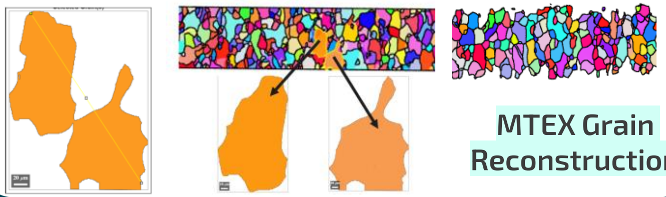

**Pearson Correlation Analysis**

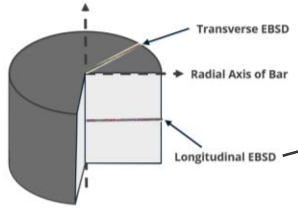
- R3 illustrates more extremes of positive and negative correlations in comparison to its counterparts (R2&R4)

**No definitive correlation was found from the macro-fracture features to their mechanical behavior**

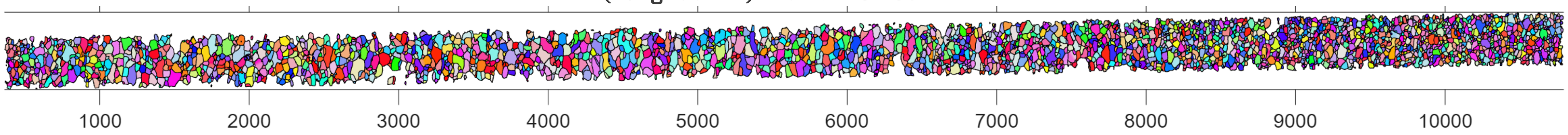
# Microstructure Computational Characterization

## Tensile Extraction Location and Microstructure
### Longitudinal EBSD scan of 0.8" rotary forged bar



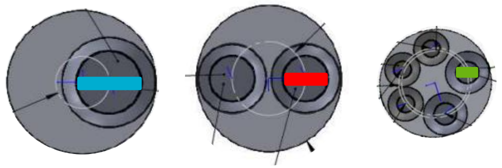




(Longitudinal) Radial EBSD Scan

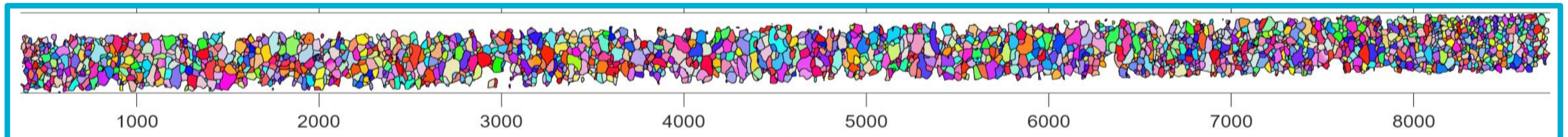



0.8" Rotary Forged Bar:
Tensile Specimen Cross-Section Extractions

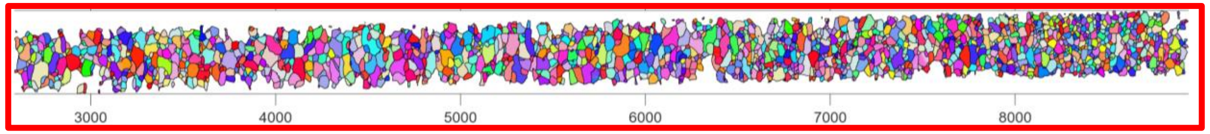
R2 R3 R4



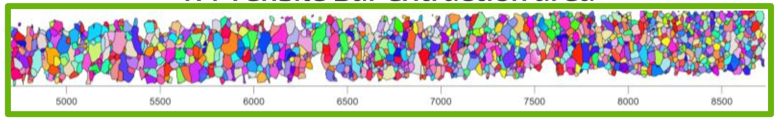
R2 Tensile Bar extraction area

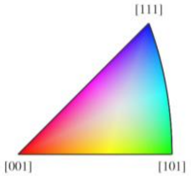



R3 Tensile Bar extraction area



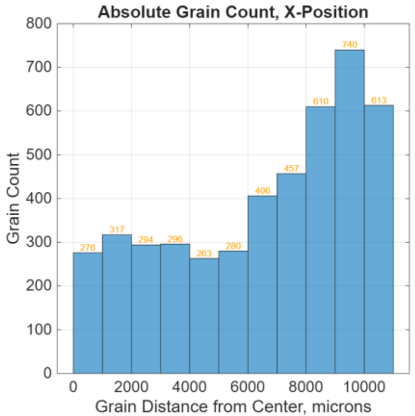

R4 Tensile Bar extraction area



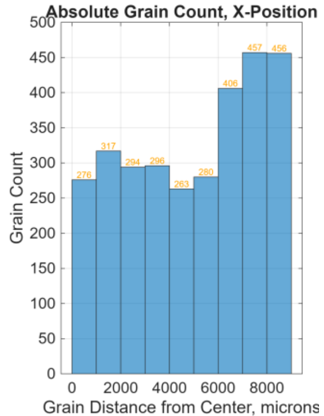




## Grain Count based on X-Axis Position

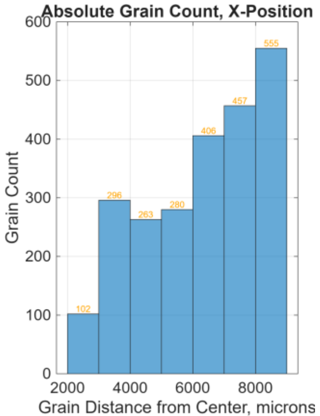
Radial Scan



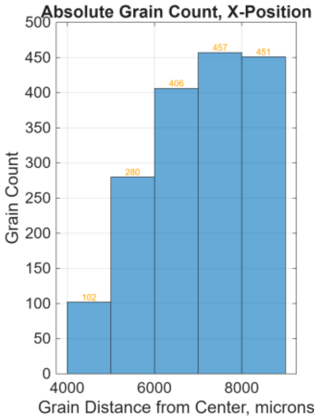

R2




R3



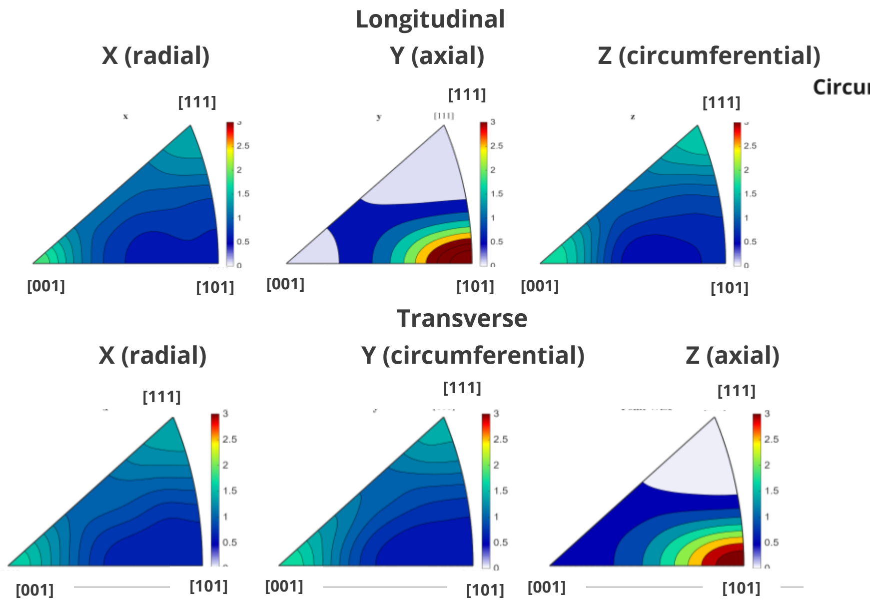

R4

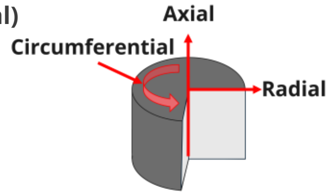



| Grain Average Diameter, microns | | | | |
|---|---|---|---|---|
| | **Whole Scan** | **R2** | **R3** | **R4** |
| **Longitudinal** | 29.72 | 33.02 | 32.53 | 31.12 |
| **Transverse** | 29.71 | 31.52 | 31.21 | 30.89 |

# Microstructure Computational Characterization

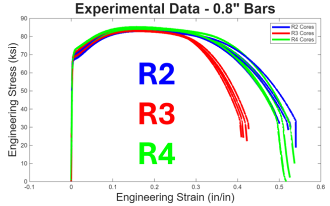
## Grain-wise ODF Comparison of 0.8" rotary forged bar

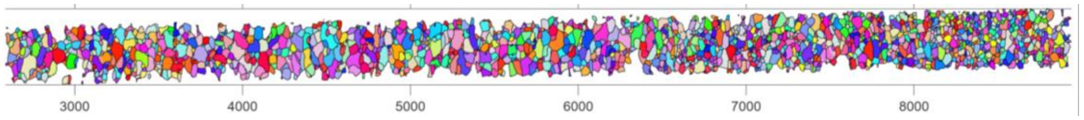


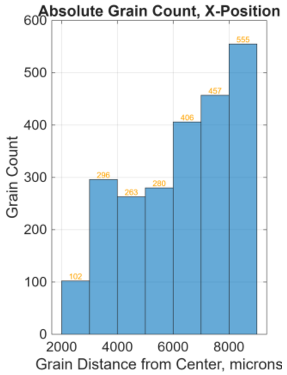



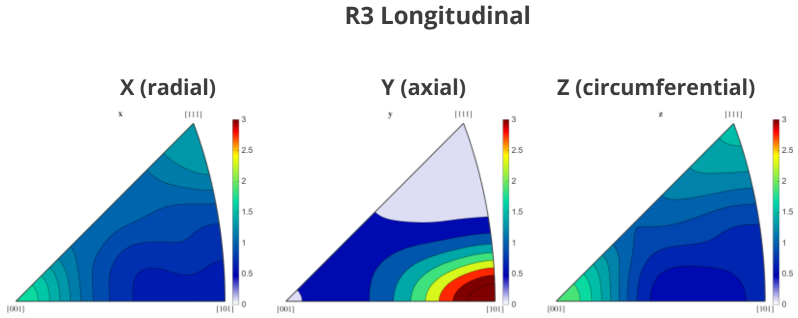

| Grain-wise ODF Max Intensity |
|---|
| **Longitudinal** |
| 6.97 |
| **Transverse** |
| 4.52 |

## R3 Tensile Bar Extraction Area




### Crystallographic Texture Analysis

- Tensile bar extraction locations show microstructural overlap within specimens while histograms confirm microstructural differences within each specimen depending on their regional location
- The 0.8" rotary forged bar exhibits a aligned texture along longitudinal direction with elevated texture index, indicating pronounced crystallographic orientation along forging axis

**Further investigation into all bar microstructure is needed to make conclusive results**

### Future Directions

- EBSD scan through thickness to capture whole cross-section texture evolution to confirm radial gradients patterns
- SEM fracture surface analysis
- Hardness testing of each tensile specimen extraction site

# Micromechanics Modeling - Summary

Crystal plasticity modeling allows us to model individual grains – we can use it to determine how the tensile properties arise from the microstructure.

This task is broken down into three steps:

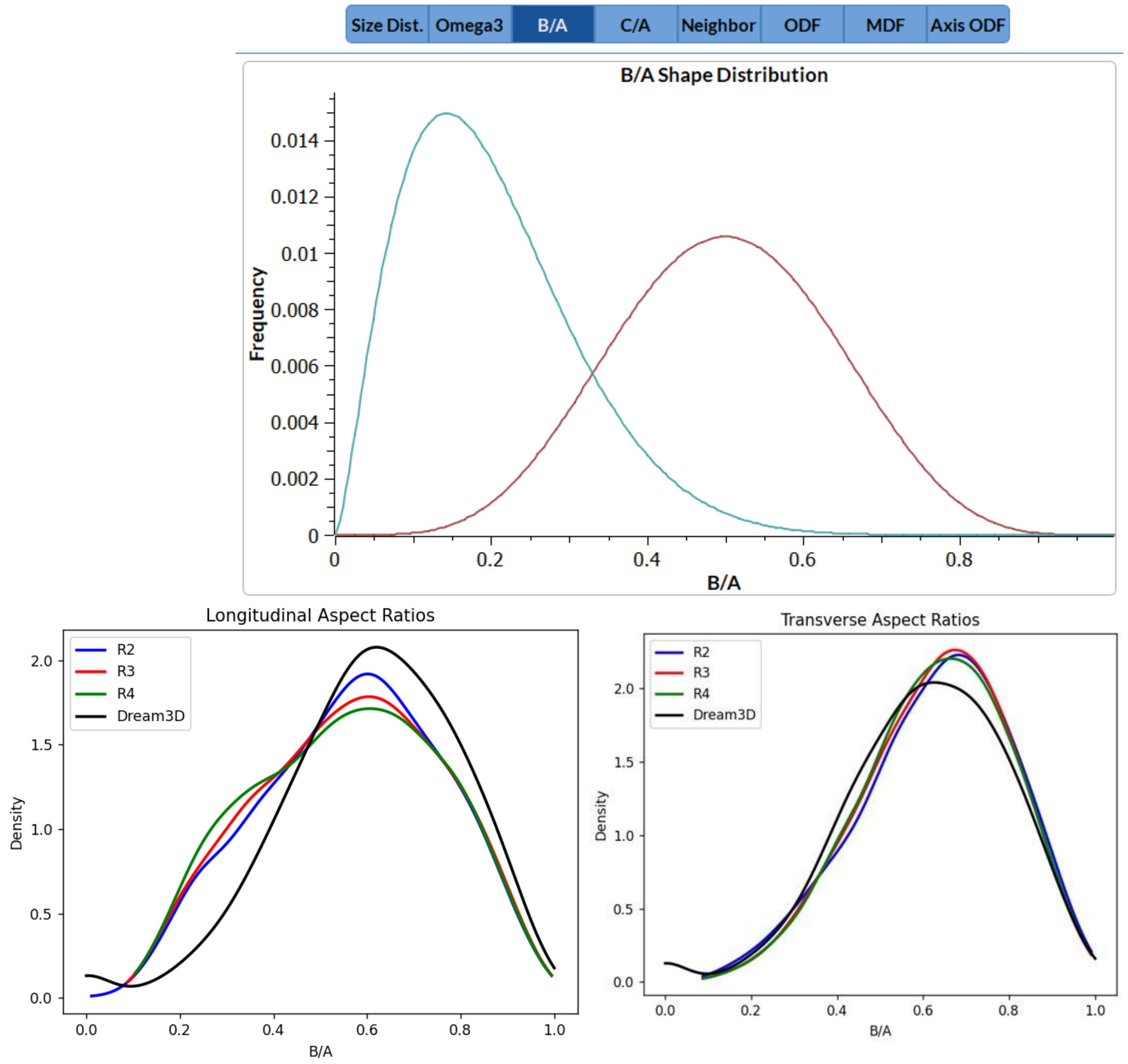
1. Measure how grain size, aspect ratio, crystallography, and morphological orientation vary throughout the sample.
2. Construct synthetic microstructure volumes with slices in the transverse and longitudinal directions statistically equivalent to the corresponding views in the EBSD data.
3. Run crystal plasticity FFT simulations to assess the tensile response produced by the previously generated microstructures.

Due to time constraints, we only examine the .8in Rolled R2 and R4 samples.

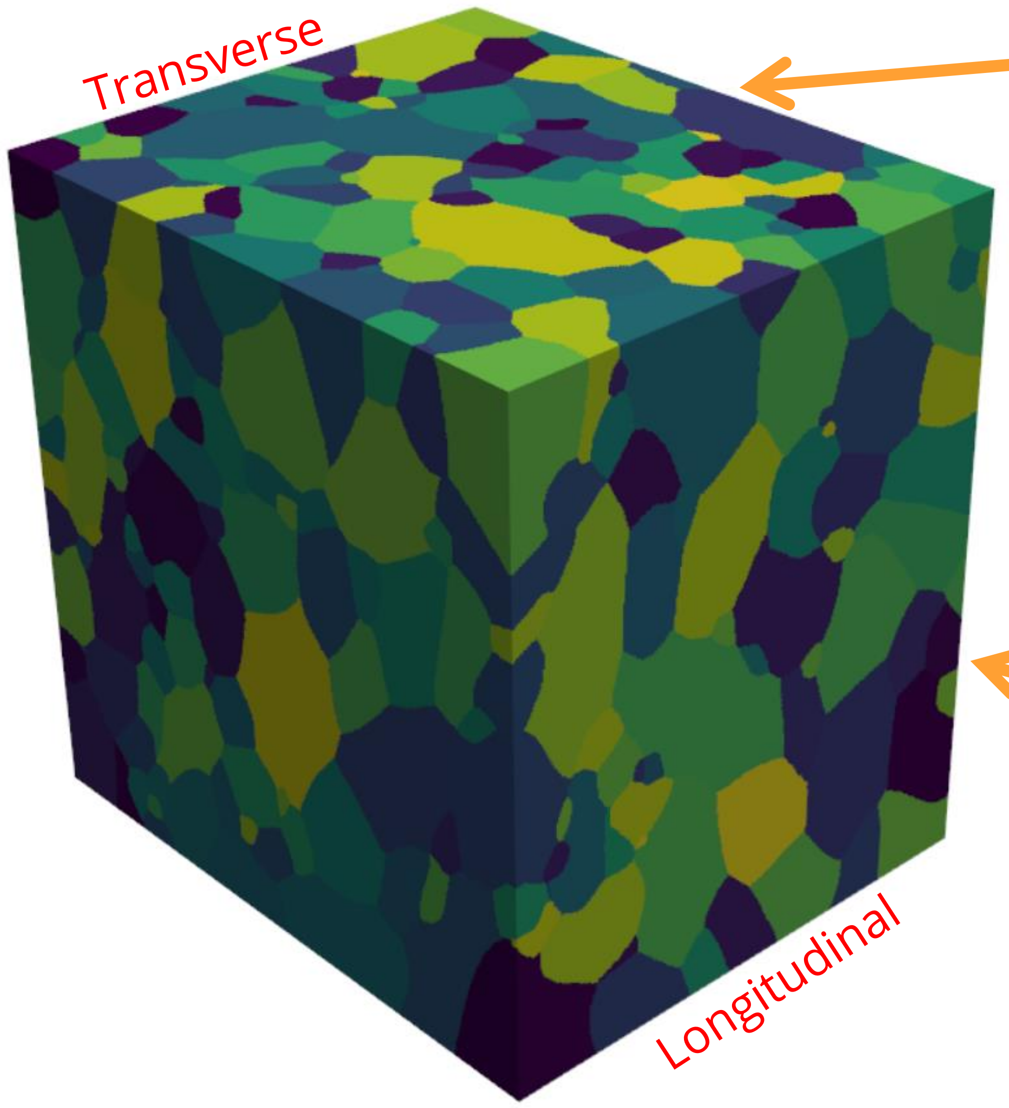
# Microstructure Generation Methodology

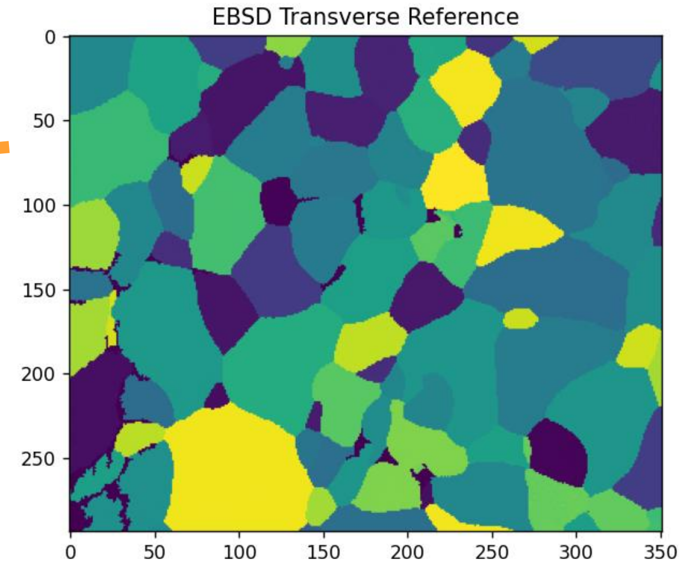
1. Adjust parameters in Dream3D (top image)
2. Generate a microstructure
3. Take slices of the generated microstructure volume in the transverse and longitudinal directions
4. Compare the output statistics to those obtained from the EBSD data (bottom images)
5. Repeat until agreement is obtained

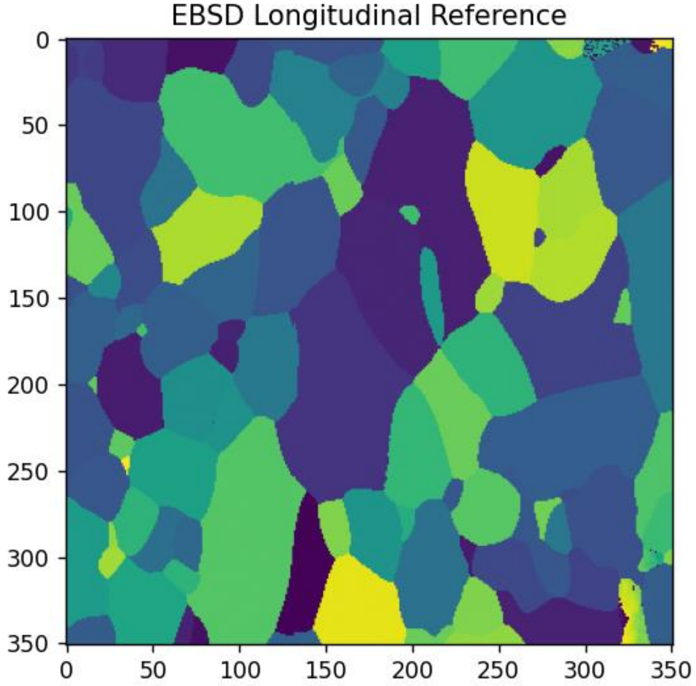
We attempted to create an optimization algorithm to solve this problem but could not get good results form this approach



# Synthetic Microstructure



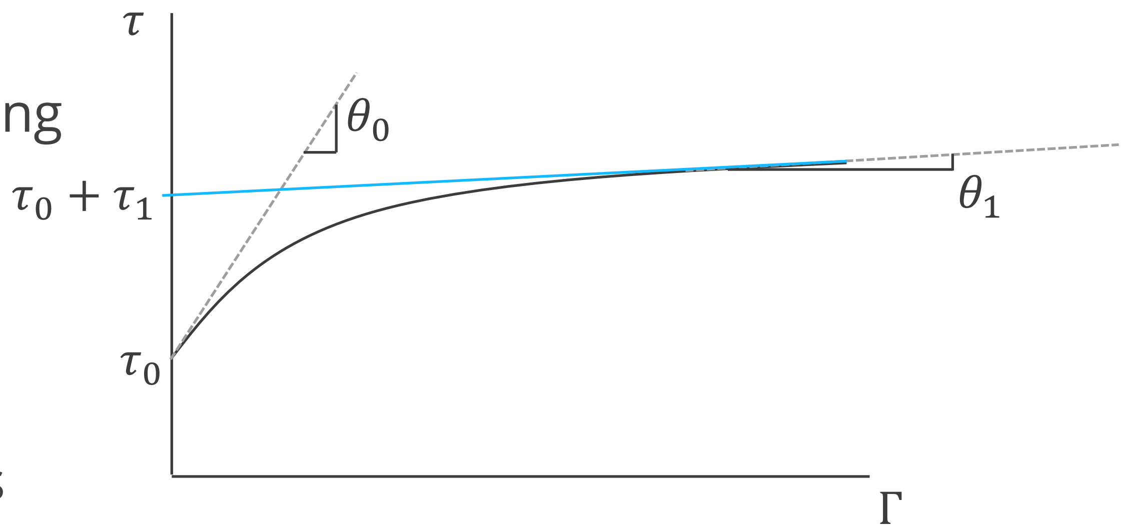

Reference images are from the 1.125 forged bar. The microstructure at left is an attempt to match the statistics of the reference.

# Crystal Plasticity Simulations – Parameter Fitting

Crystal plasticity simulation uses the Voce hardening law:

$$\tau = \tau_0 + (\tau_1 + \theta_1 \Gamma)\left(1 - \exp\left(-\Gamma\left|\frac{\theta_0}{\tau_1}\right|\right)\right)$$

$$\Gamma = \sum_N \gamma^\alpha$$

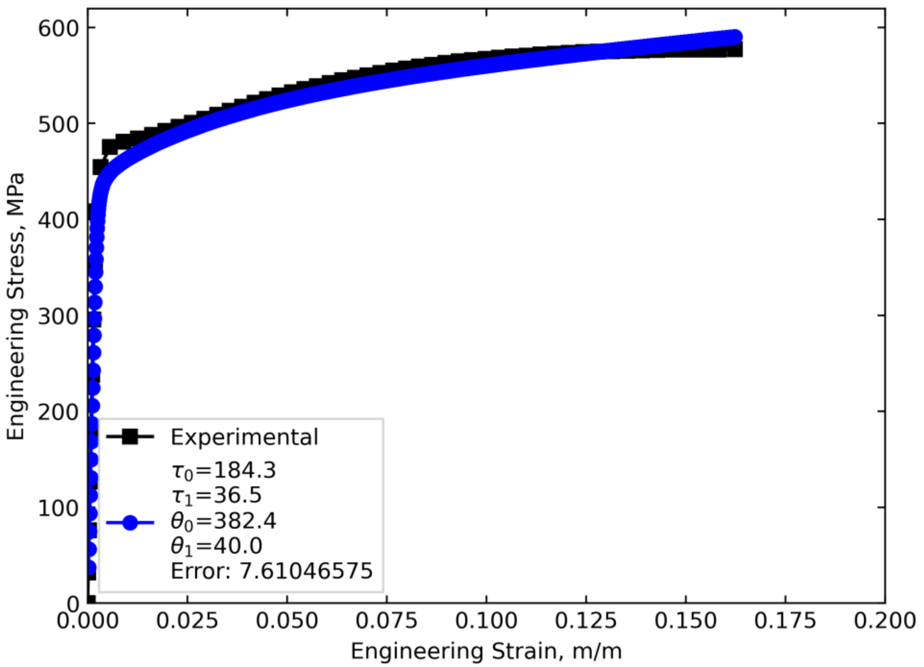



Elastic properties are taken from published values

Crystal plasticity parameters are fitted using a Bayesian optimizer

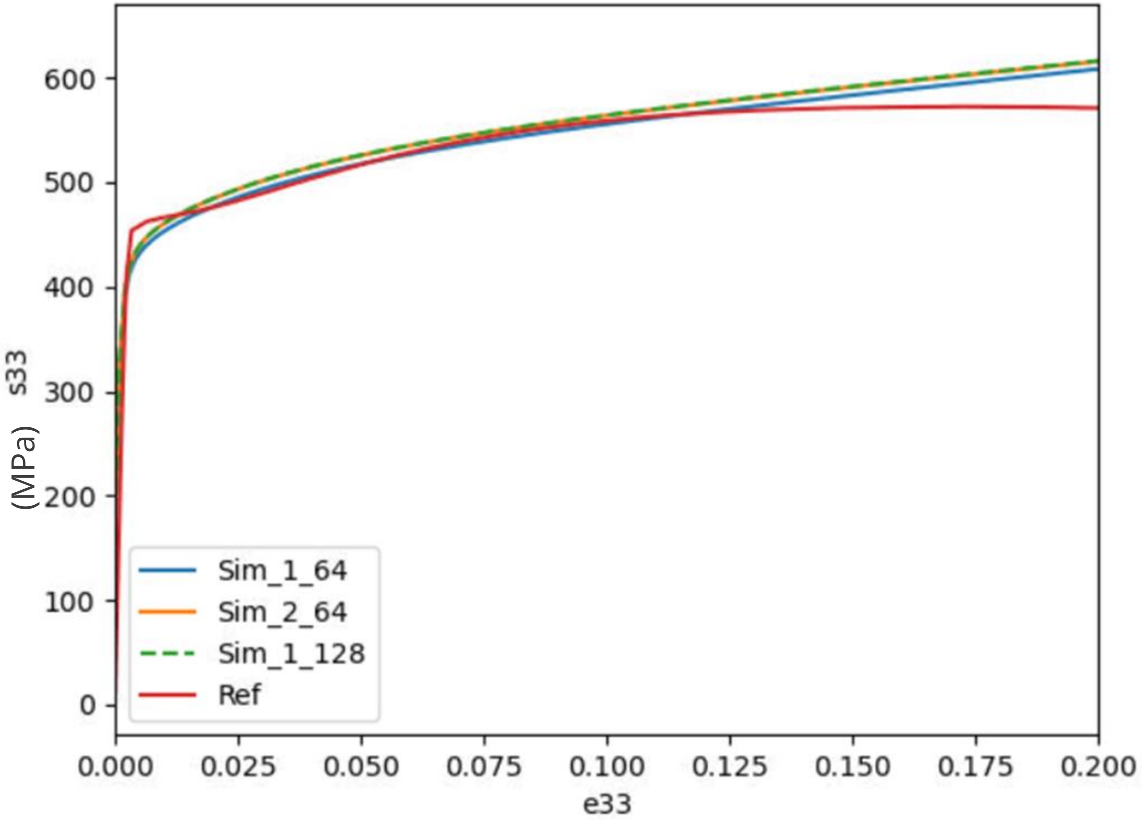
Parameters are fitted on a small microstructure with one voxel grains, with crystallographic orientation distribution matched to experimental data.

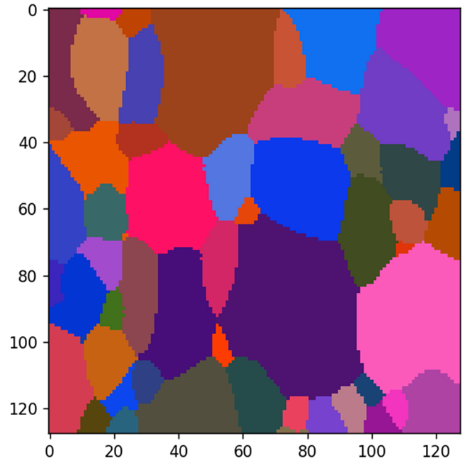
We obtain a close match (shown bottom right)

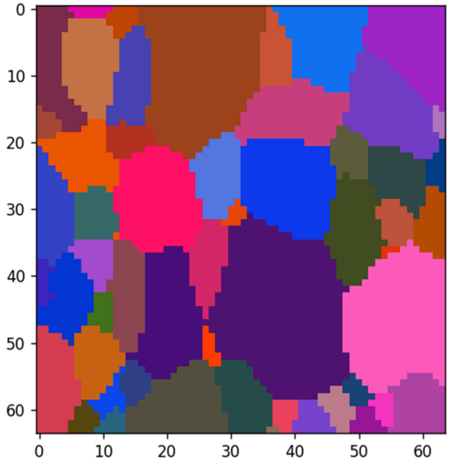


# Crystal Plasticity Simulations – Downsampling

- Ref is R2 from .8 in diameter rolled bar
- Sims 1 are the same microstructure, but sampled to a 64 cube or 128 cube
- Sim_2 is generated using the same Dream3D inputs as Sims 1.
- A microstructure with a length of 64 voxels produces an output very similar to a length 128 cube.

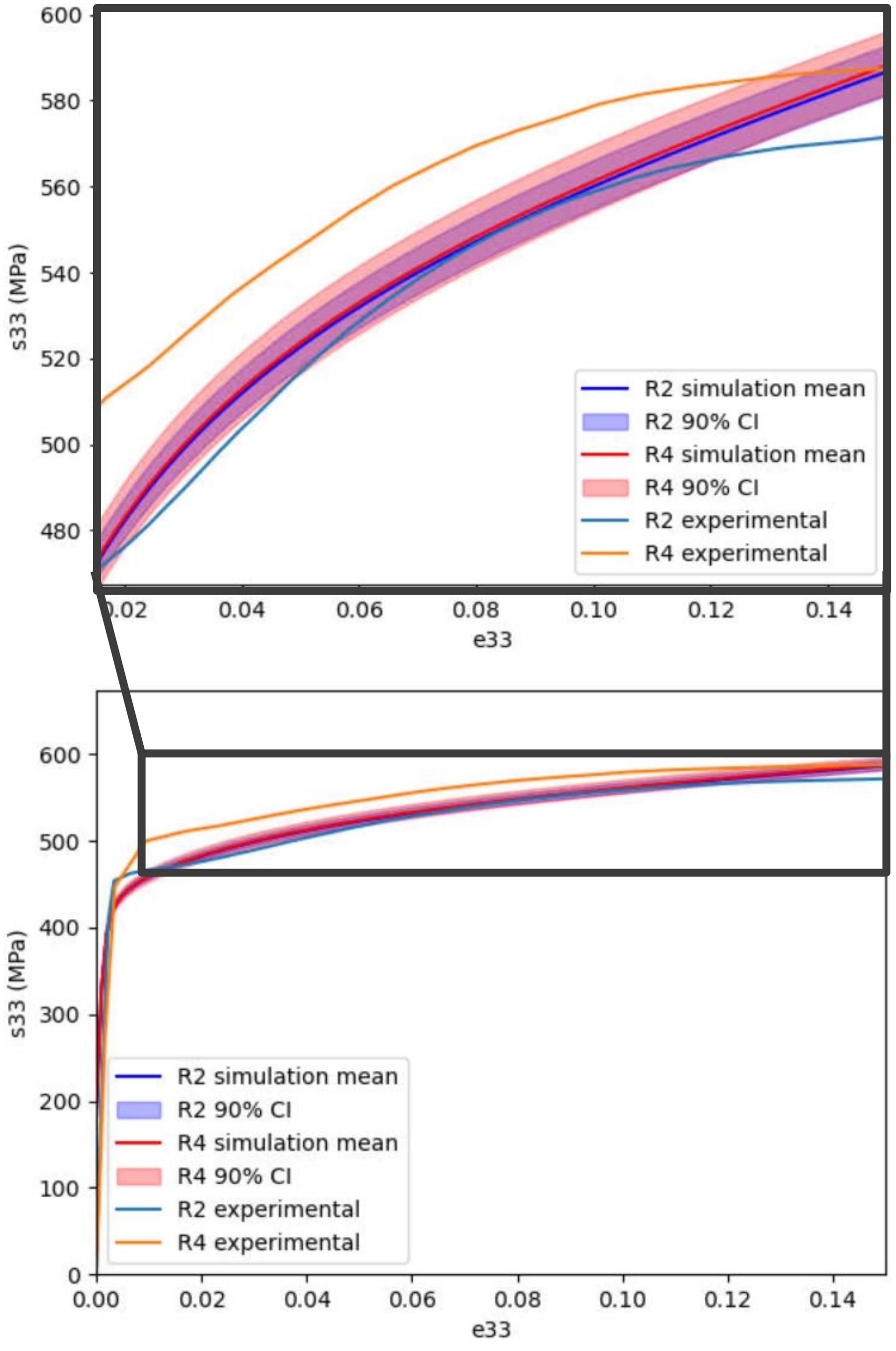


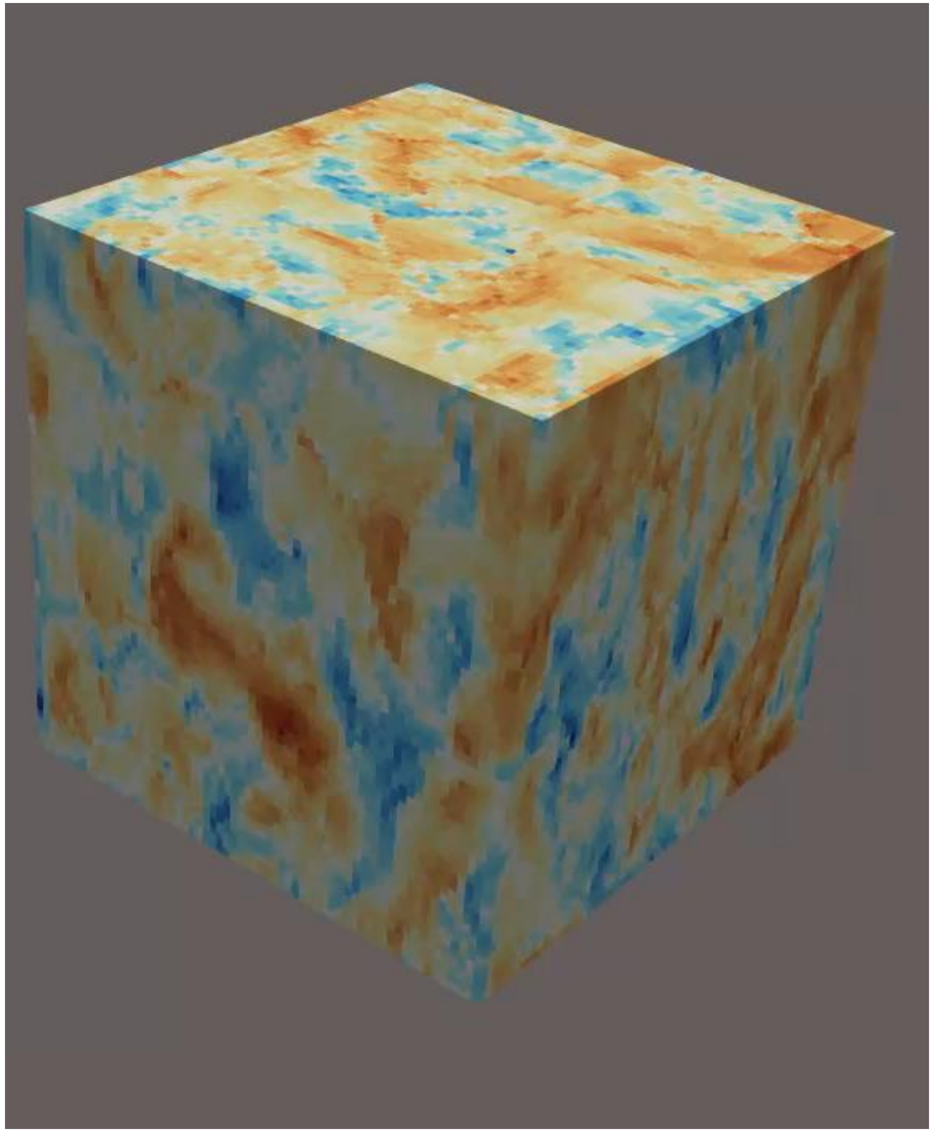
# Crystal Plasticity Simulations

- Ran simulations on 20 R2 and 20 R4 microstructures.
- Small difference between R2 and R4 simulations average, R4 is stiffer than R2, as observed in the experimental data
- Too much variation in the Dream3D outputs to capture the subtle variations present in the EBSD data?
- Non-homogeneity not captured by Dream3D might also produce different macro responses
- Various phenomena not modeled by Voce hardening: pre-stress, changes in dislocations, and others.



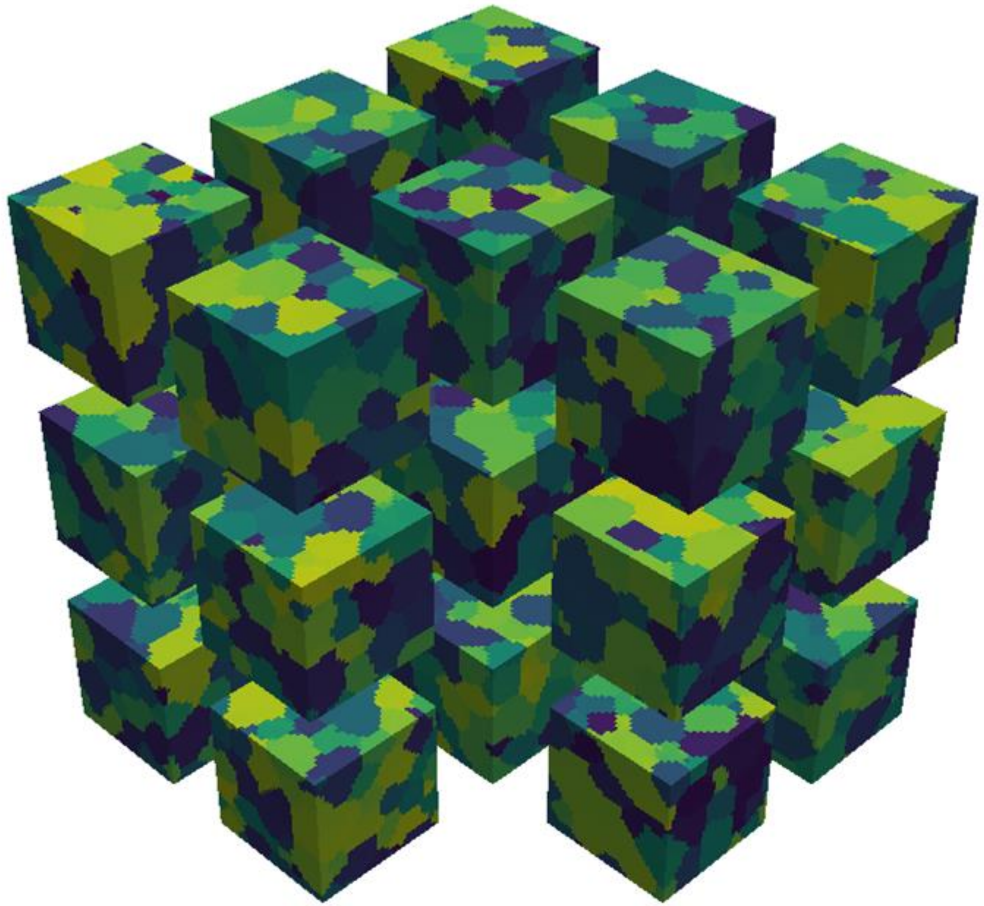
# Crystal Plasticity Simulations – Future Directions

- These crystal plasticity simulations do not model failure, so they are only accurate up to the ultimate tensile strength.
- Insight into behavior after failure can be gleaned from the distribution of stress concentrations in the microstructure.
- Also, the relationship between voxel size and tensile properties shown by the simulation has not been determined in detail.



# Synthetic Microstructure Generation - Future Directions

- Instead of Dream3D, use a generative machine learning model.
- My prior work demonstrated a close match in microstructure statistics (no need to tune microstructure statistics)
- May be possible to train a model for 2D to 3D reconstruction by only calculating loss on the slices of microstructure that we have.



Animation from: GrainPaint: A multi-scale diffusion-based generative model for microstructure reconstruction of large-scale objects, Hoffman et al.

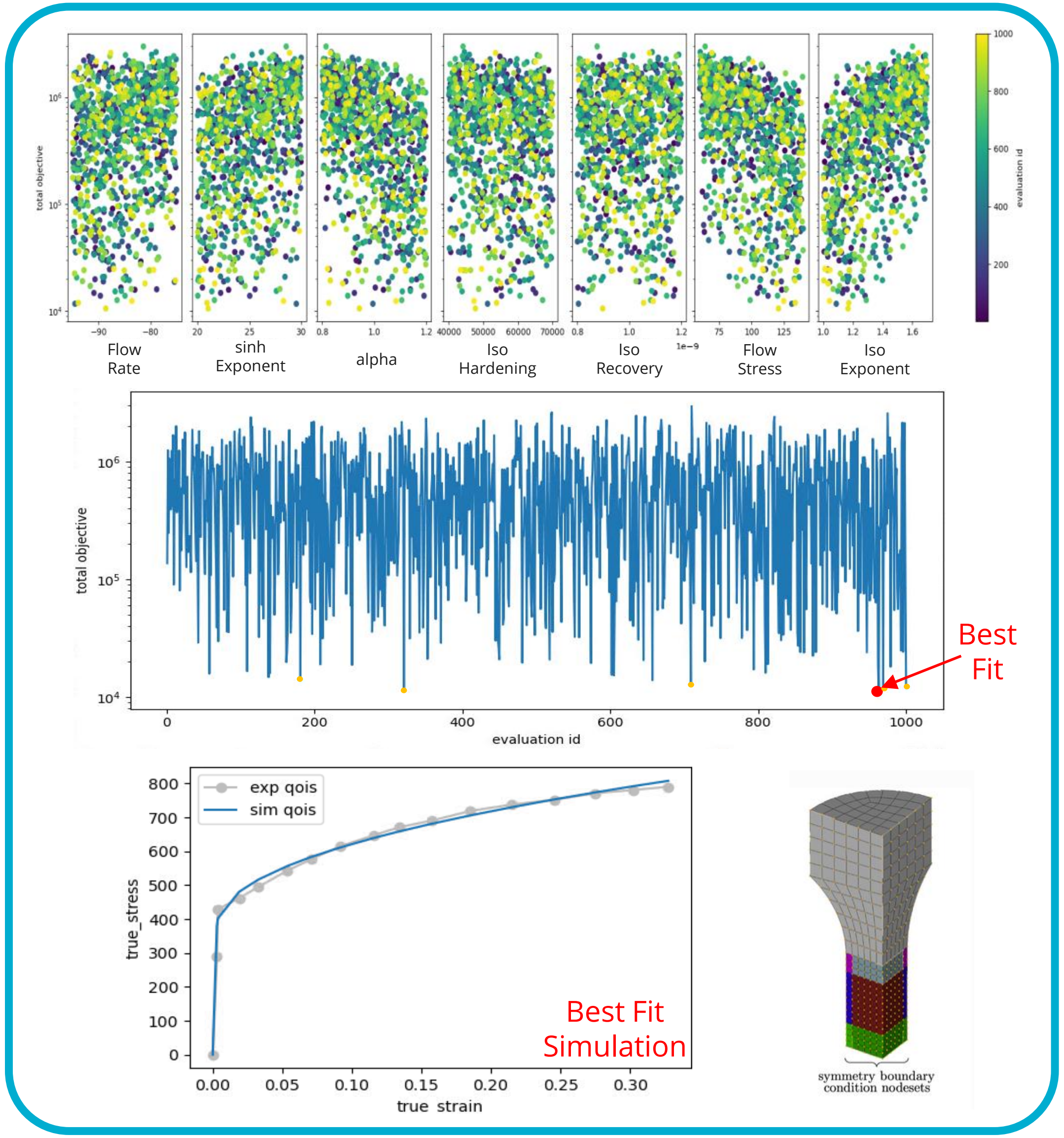
# Continuum Scale Characterization pre-Ultimate Strength

Refined fitment of experimental data up until ultimate stress

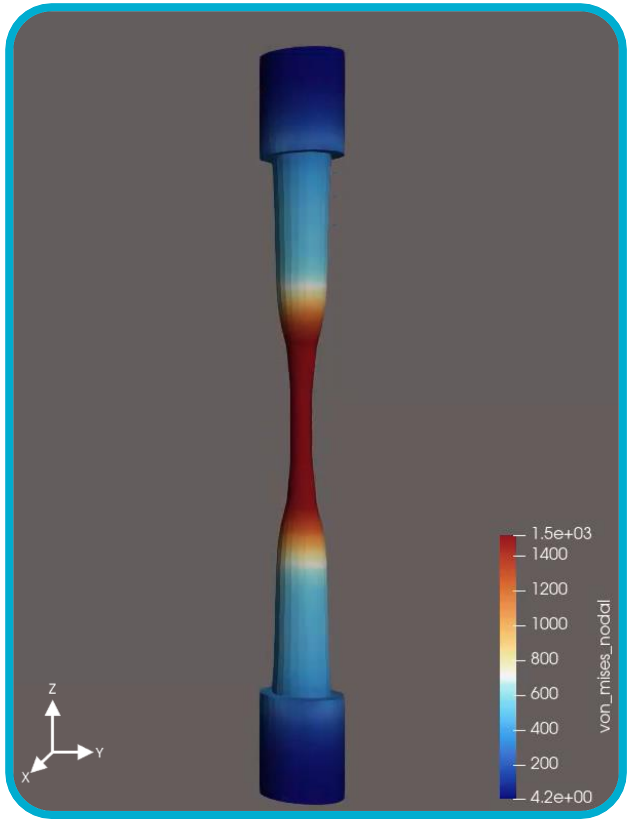
- Latin Hyper-Cube studies allow for parameterization based on fewer runs than full factorial
- Allows for finer tuning of viscoplastic parameters for non-failure mode applications

Analysis Method Possibilities:

- 1-to-1 comparison of pre-UTS data between Crystal Plasticity model and Viscoplasticity model
- Fitment of MatCal results to plastic deformation and failure



# Finite Element Modelling: Viscoplasticity

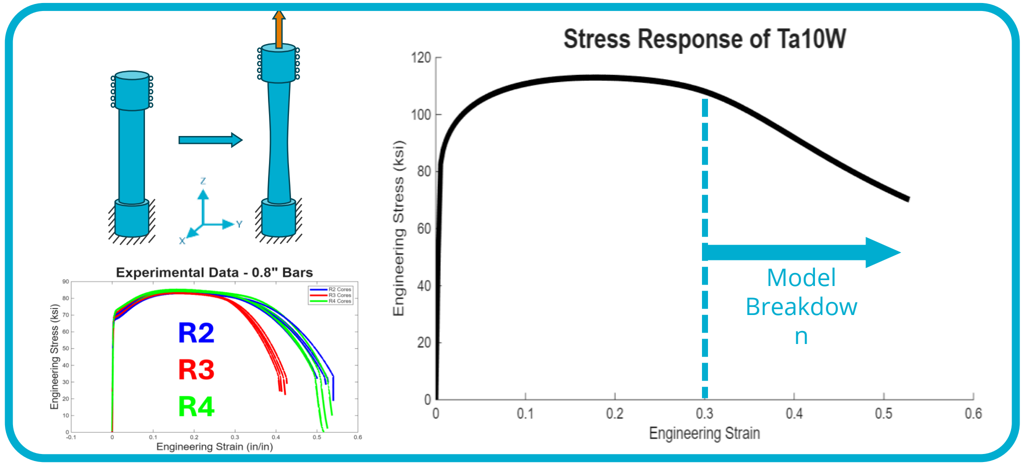



Viscoplastic Material Model

- Ta-10W alloys exhibit strain-rate dependent stress responses
- Interest in behavior under plastic deformation and failure

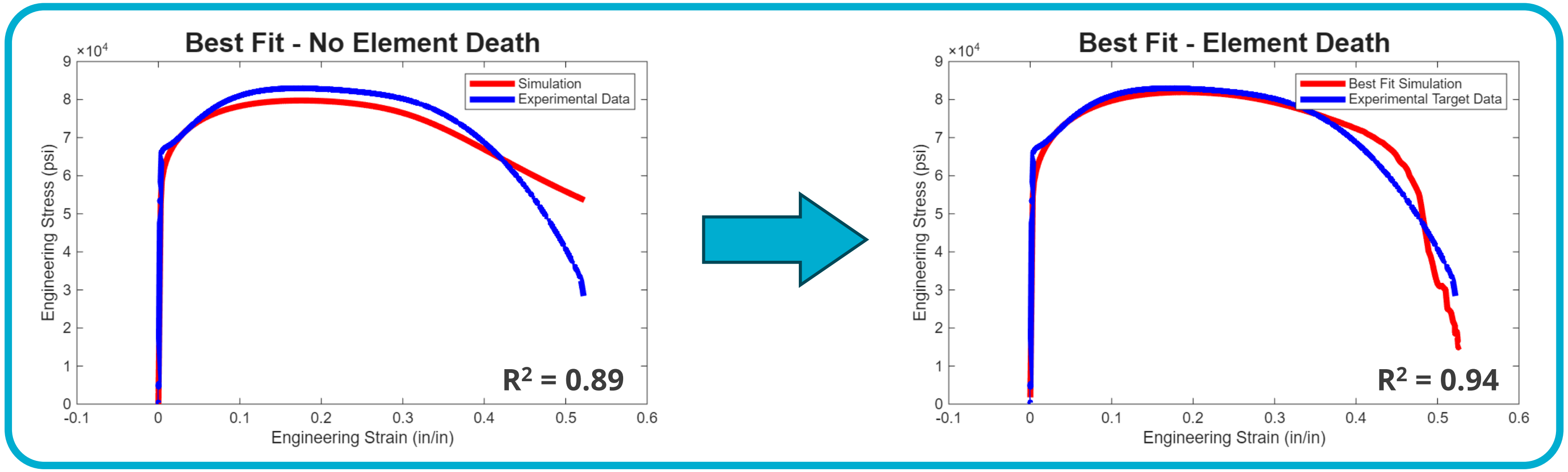
Limitations:

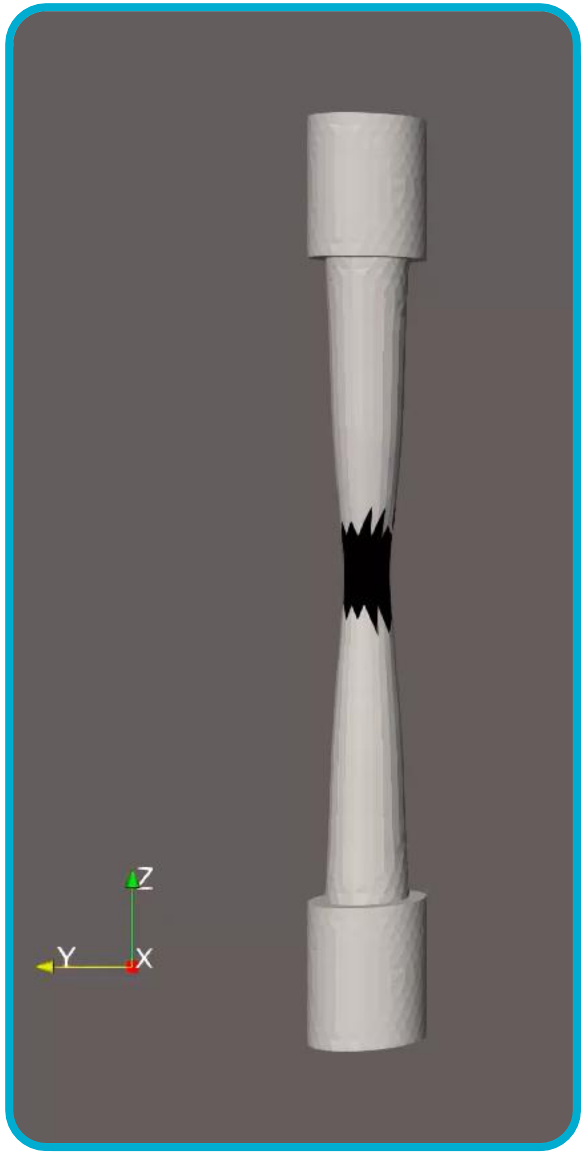
- Sierra Viscoplastic model incapable of modelling sample failure, as model has no addition of damage or disconnection
- Sample deforms continuously without ever breaking
- After ultimate stress, viscoplastic is not able to accurately model experimental data



# Capturing Sample Failure Behavior: Element Death

- To model failure behavior from experiments, Element Death is implemented
- Elements that reach aspect ratio threshold are deactivated, and can no longer contribute to sample stiffness
- This results in higher quality fitment of high-strain failure behavior when compared to models without element death

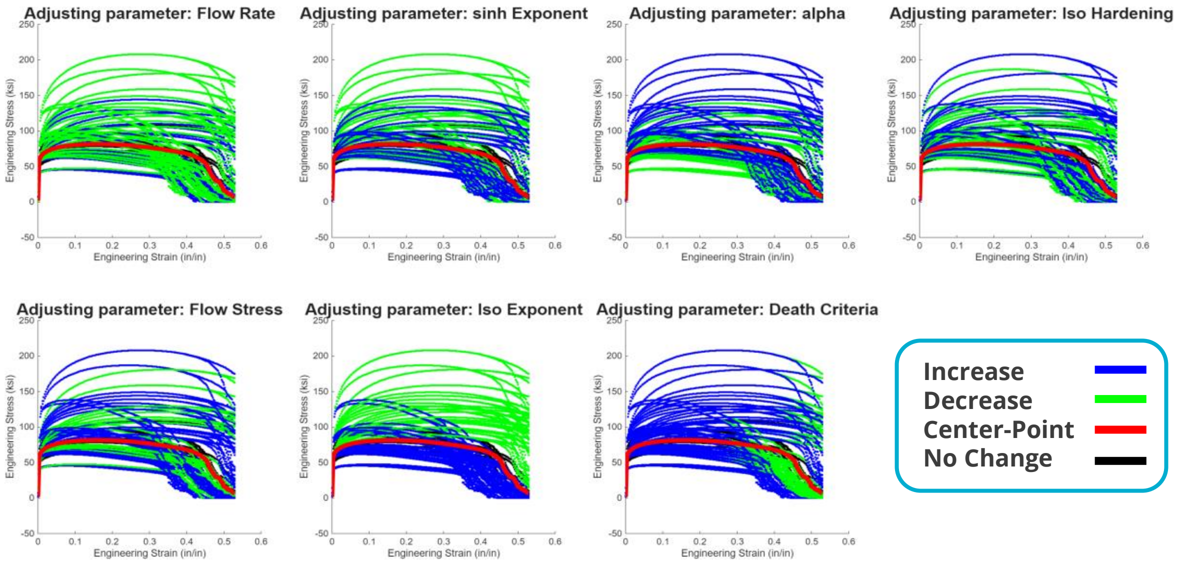


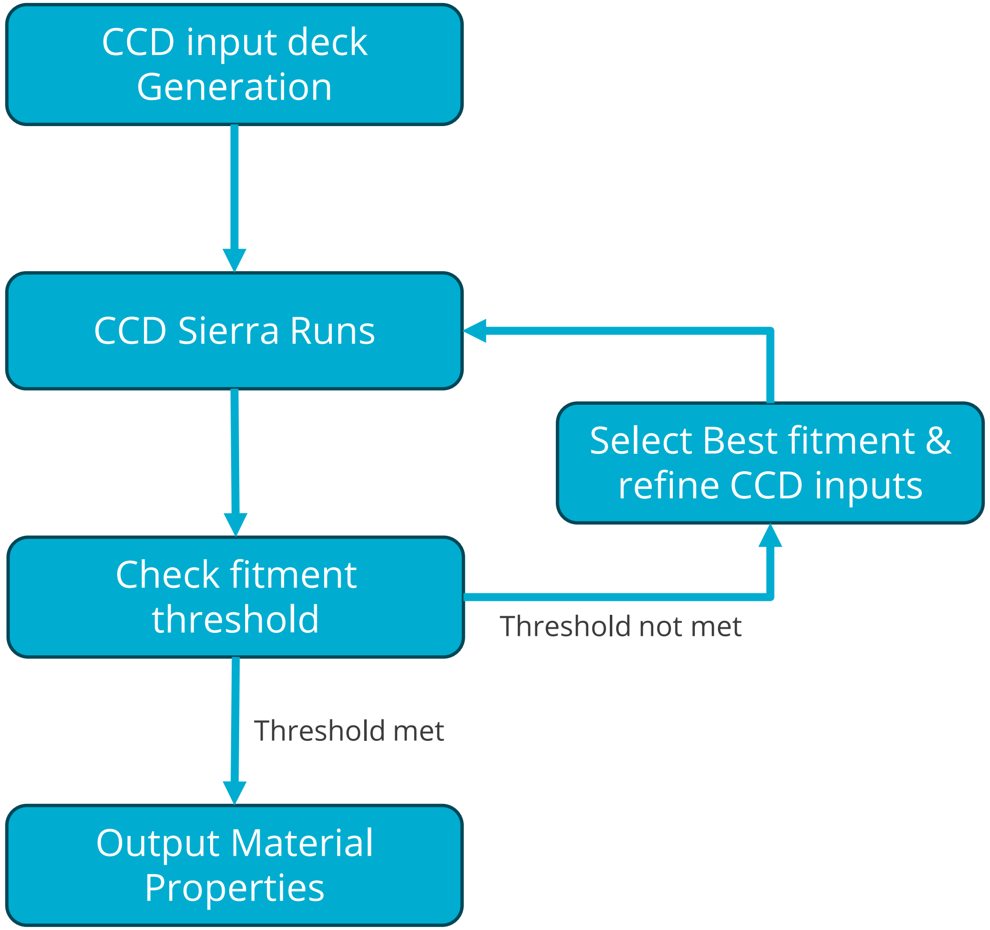



# Central Composite Design (CCD) Parameterization

If approximate starting values exist, CCD parameterization allows for characterization within a confidence margin

- Full-factorial simulation requires 500k+ simulations
- CCD parameterization requires only 275 simulations

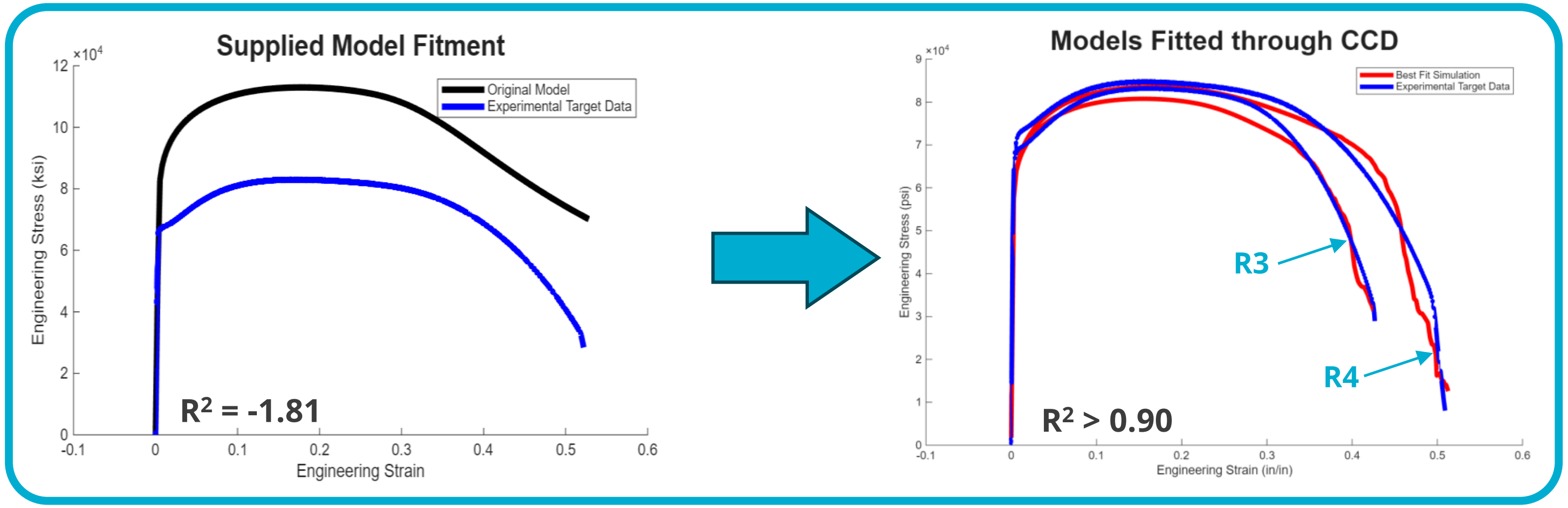


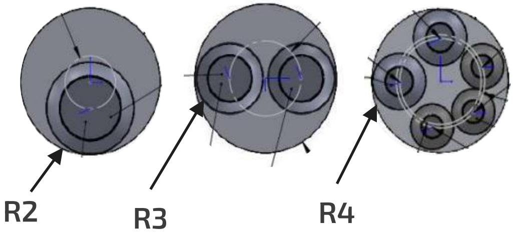

**Fitment to experimental data was improved when compared to the original model**

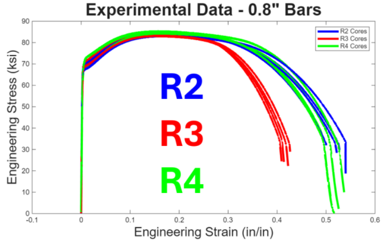
# Results: Continuum Scale Failure Model

- Viscoplastic Model improvement in low-strain modelling
- With implementation of Element Death, high-strain/failure behavior modelled
- Treating element death criteria as 8th parameter results in higher quality fit
- Fitment quality surpassed $R^2 > 0.90$ in all experimental datasets




0.8" Rotary Forged Bar:
Tensile Specimen Extractions

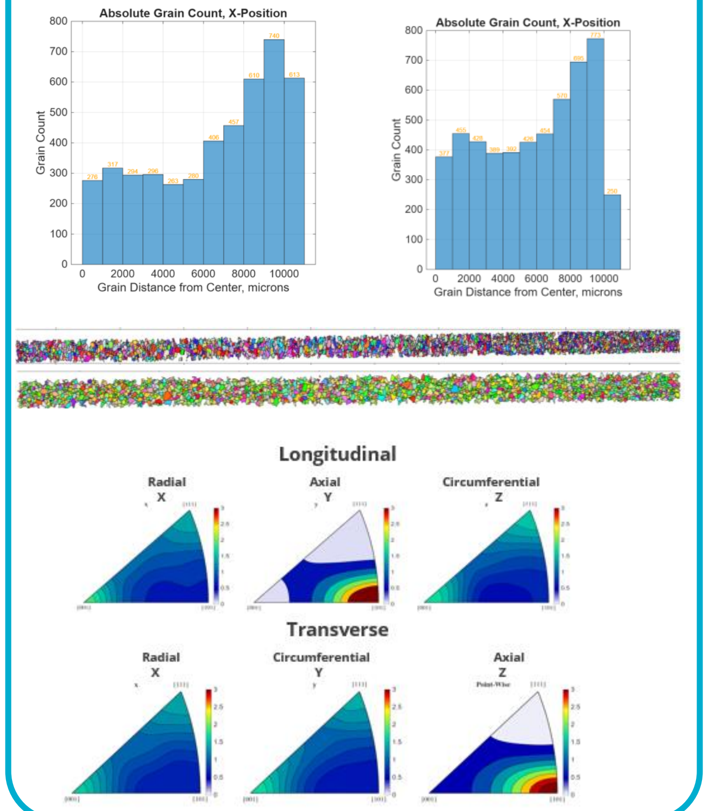


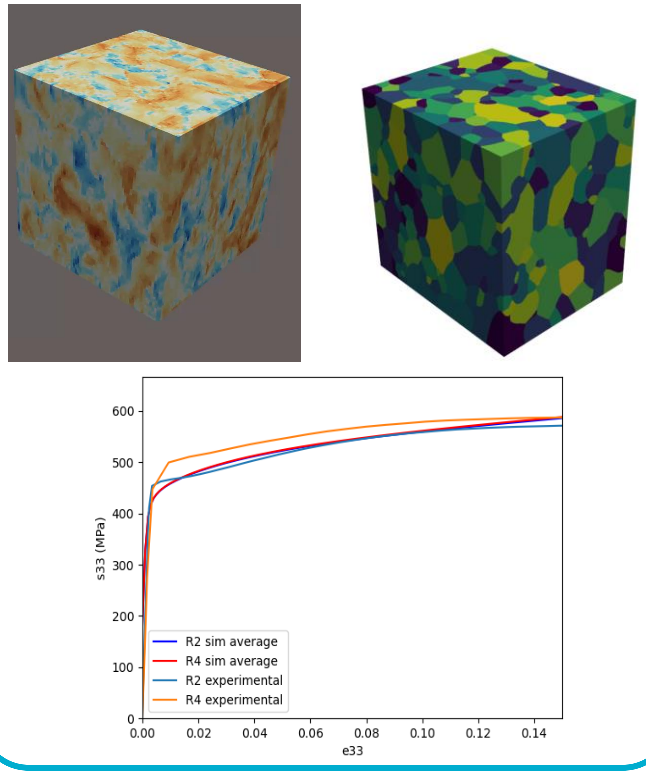

| Sample Set | Flow Rate | sinh exponent | alpha | Isotropic Hardening | Isotropic Recovery | Isotropic Exponent | Flow Stress |
|---|---|---|---|---|---|---|---|
| Rolled-R2 | -84.77 | 25.99 | 1.03 | 51008 | $1.03\cdot10^{-9}$ | 1.252 | 95.7 |
| Rolled-R3 | -63.92 | 20.84 | 1.20 | 77706 | $0.80\cdot10^{-9}$ | 1.113 | 132 |
| Rolled-R4 | -85.24 | 25.87 | 1.04 | 50832 | $1.03\cdot10^{-9}$ | 1.277 | 99.4 |
| Forged-R2 | -86.12 | 26.51 | 1.02 | 49571 | $1.04\cdot10^{-9}$ | 1.263 | 98.7 |
| Forged-R3 | -63.32 | 20.94 | 1.20 | 77859 | $0.80\cdot10^{-9}$ | 1.121 | 132 |
| Forged-R4 | -86.49 | 25.15 | 0.98 | 51423 | $.99\cdot10^{-9}$ | 1.294 | 101 |

# Project Summary: Ta-10W Alloy Characterization

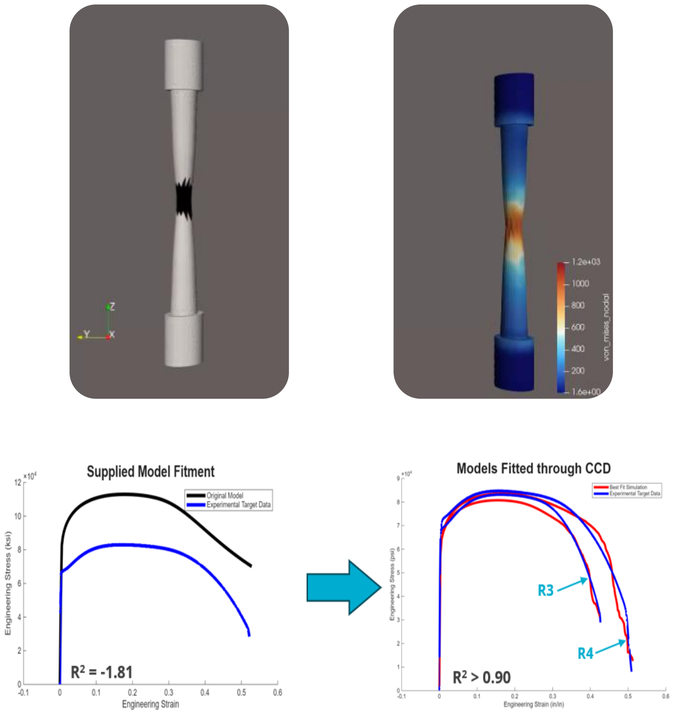
## Microstructural Characterization

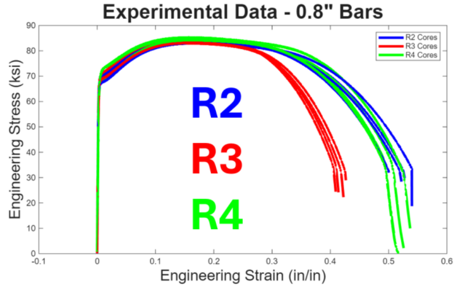



## Micro-Mechanics & Crystal Plasticity




## Continuum Scale Finite Element Modelling




Experimental data indicated abnormal behavior in R3 samples

- Upon analyzing the microstructure, further investigation is needed to tie mechanical property differences
- Crystal Plasticity simulations show that microstructure differences explain the higher stiffness of the R4 sample.
- On the continuum length-scale, R3 exhibited significantly different mechanical properties than R2 & R4

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## Questions?

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