AN IMAGE BASED FINITE ELEMENT MODEL FOR NI-BASED SUPERALLOYS USING A TWO SCALE CONSTITUTIVE MODEL ACCOUNTING FOR MORPHOLOGICAL DISTRIBUTIONS OF γ' PRECIPITATES

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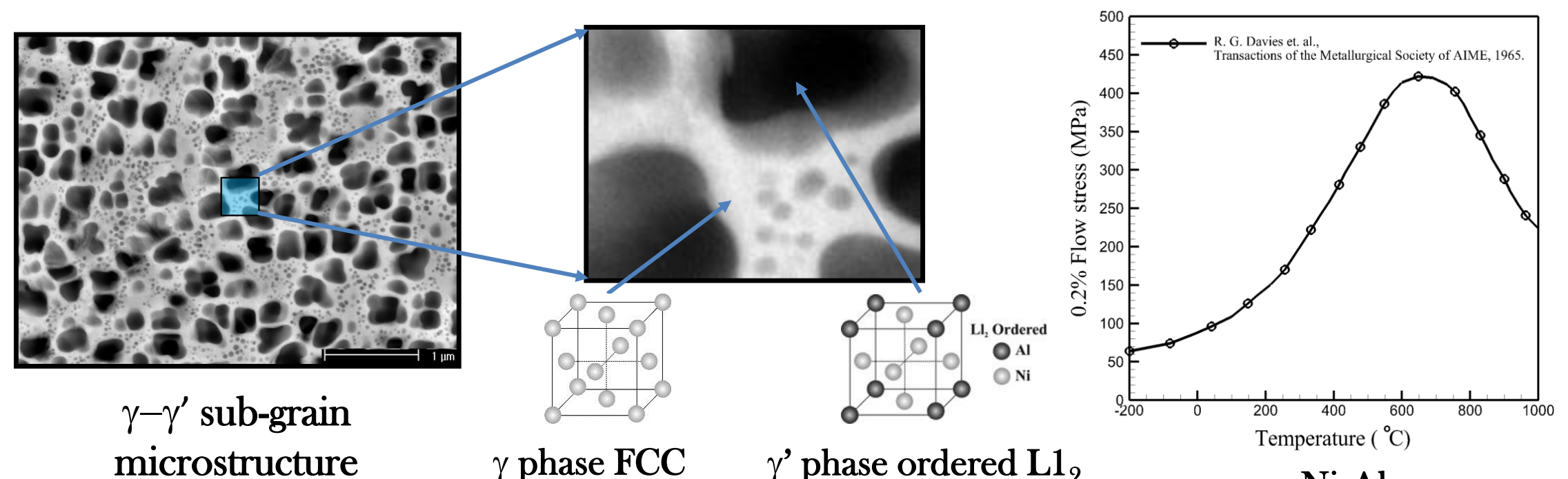
INTRODUCTION

Nickel-based superalloys are employed as one of the primary structural components in high temperature jet engine applications. Their unique ability to maintain mechanical strength and corrosion resistance over a wide range of temperatures highlights them as critically important engineering materials. However, modelling Ni-based superalloys is inherently a multiscale problem. The remarkable properties of the material are attributed to precipitate strengthening and other dislocation micromechanisms, which occur at the subgrain level. At this scale, the morphology and spacing of Ni_3Al γ' precipitates play a significant role in the thermo-viscoplastic behavior.



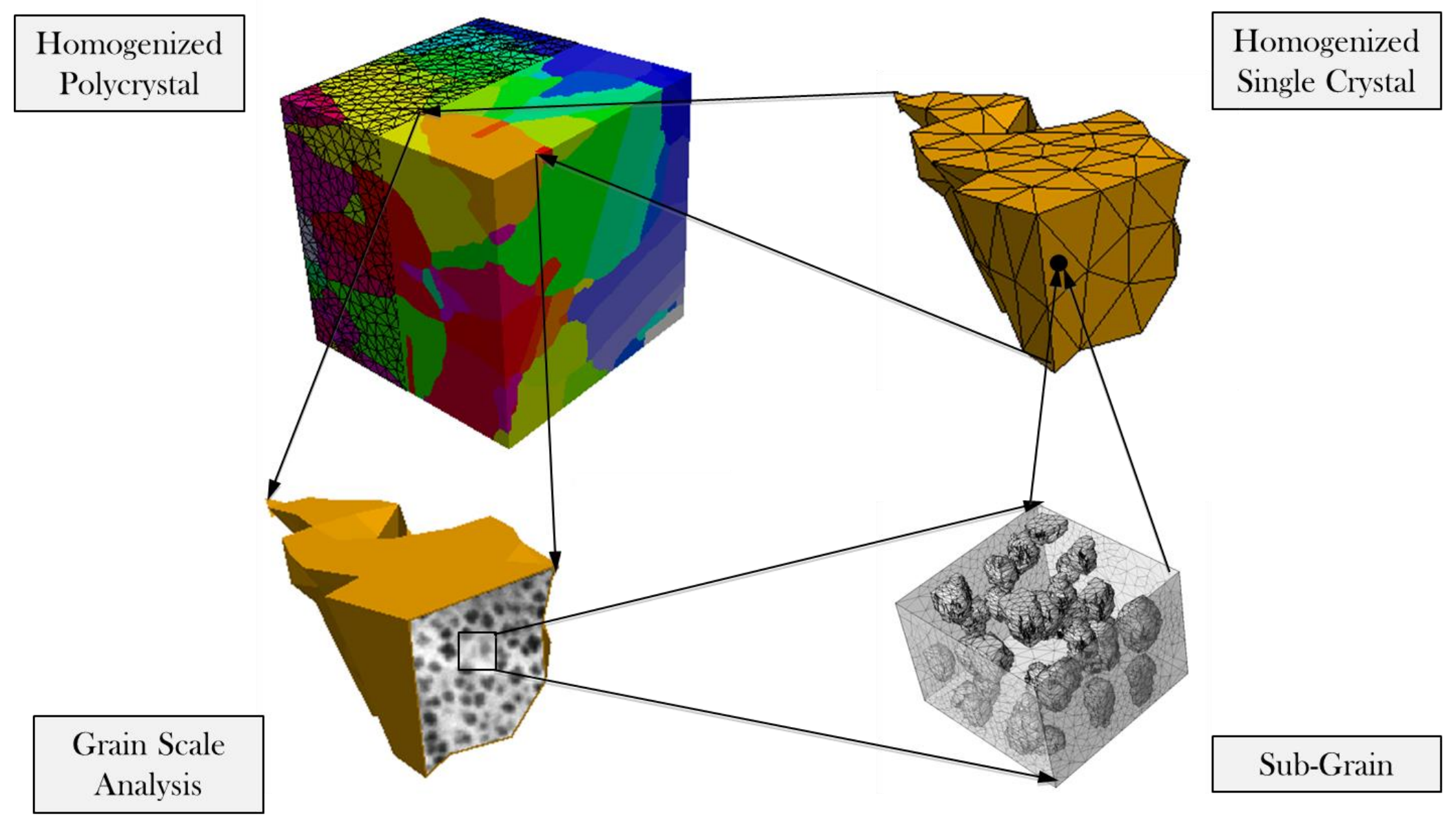
γ–γ' sub-grain microstructure

γ phase FCC structure (Pure Ni)

γ' phase ordered $L1_2$ structure (Ni_3Al)

Ni_3Al

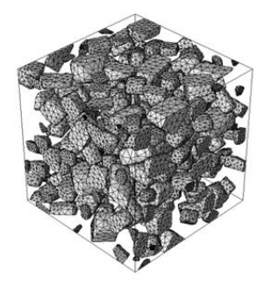
In order to develop a constitutive law for plastic deformation of polycrystalline Ni-based superalloys, a parametric homogenization scheme is utilized to elevate the mechanical effects of the γ' precipitate morphology to this higher scale. This multiscale framework permits the design and analysis of superalloy polycrystals by accounting for the complex mechanical behavior of the subgrain microstructure.



DISLOCATION DENSITY-BASED CRYSTAL PLASTICITY CONSTITUTIVE MODEL

Subgrain Crystal Plasticity Finite Element Model

A two phase dislocation density-based crystal plasticity model is developed to explicitly simulate the precipitate-matrix structures at the subgrain scale. (Keshavarz, Ghosh 2013)



Thermally Activated Flow Rule (Orowan equation)

$$\dot{\gamma} = \rho_m(\rho_0) b \lambda_{jw} \nu \exp\left(\frac{-Q_{act}}{kT}\right) sinh\left(\frac{|\tau| - \tau_{pass,tot}}{\tau_{cut}}\right)$$

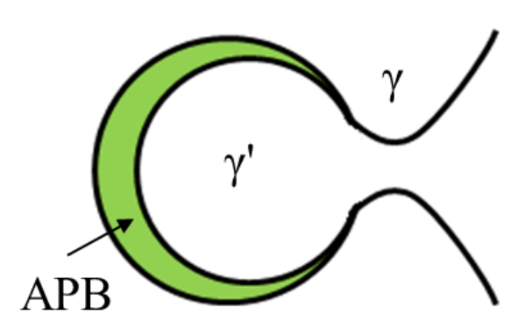
$$\tau_{pass} = c_{ps}\mu b\sqrt{\rho_p}$$

$$\tau_{cut} = \frac{kT}{c_{av}c_{jw}b^2}\sqrt{\rho_f}$$

γ' Phase Critical Resolved Shear Stress (Keshavarz, Ghosh. 2015)

$$\tau_c = \tau_c(\Gamma_{111}, \Gamma_{010}, \tau_{pe}, \tau_{se}, \tau_{cb})$$

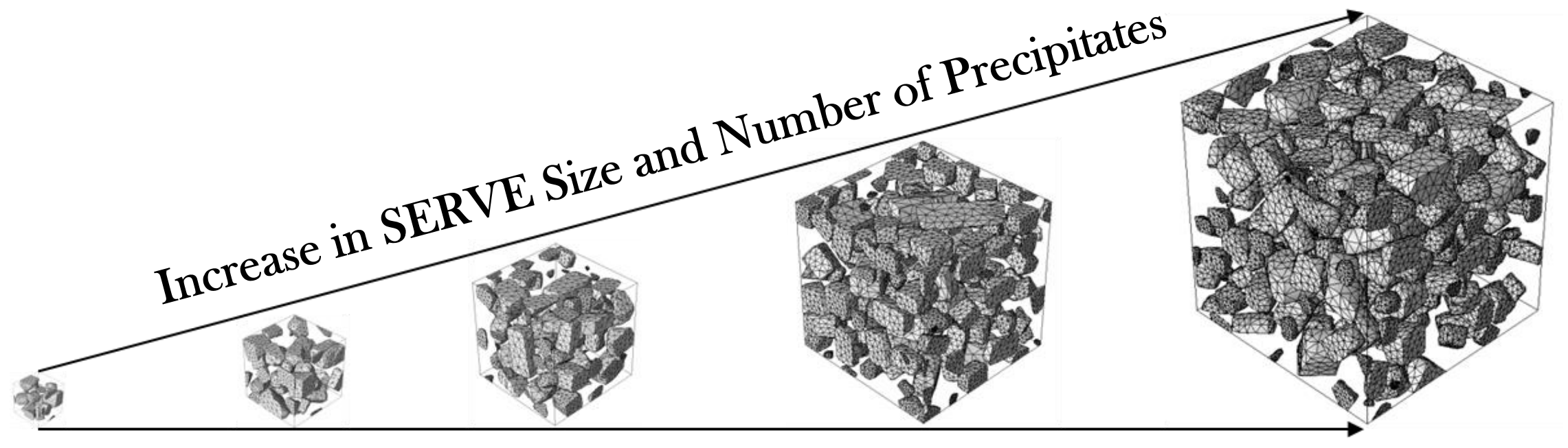
Comprised of two mechanisms
1. APB Shearing
2. K-W Locks



ESTABLISHMENT OF SERVES

SERVE Analysis

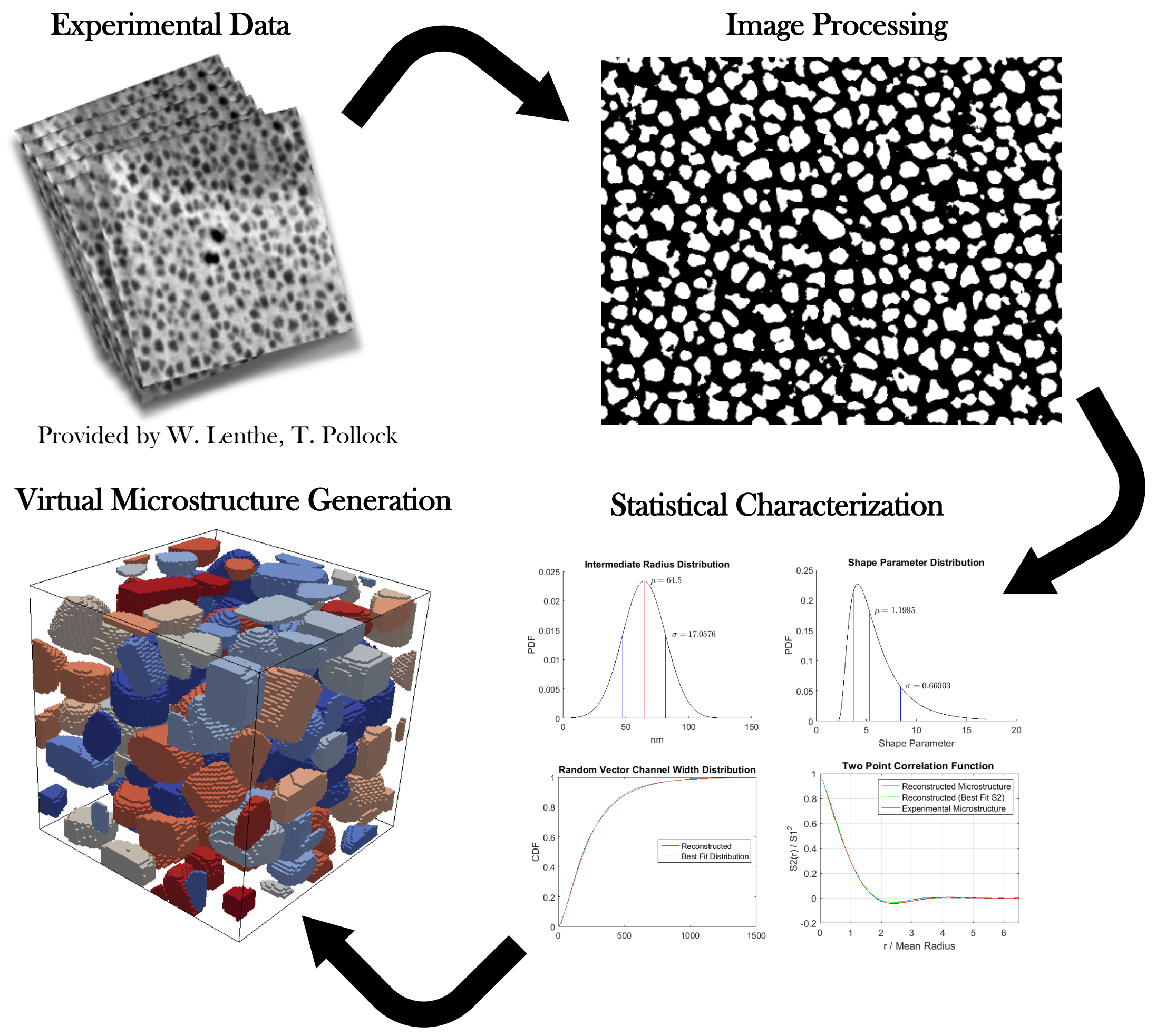
For the subgrain micromechanical analysis, it is important to generate statistically equivalent representative volume elements (SERVEs) for finite element simulation. The size of this SERVE is determined by studying the convergence of microstructural statistics, material parameters, and mechanical properties as the simulation volume is increased.



MICROSTRUCTURE SERVES

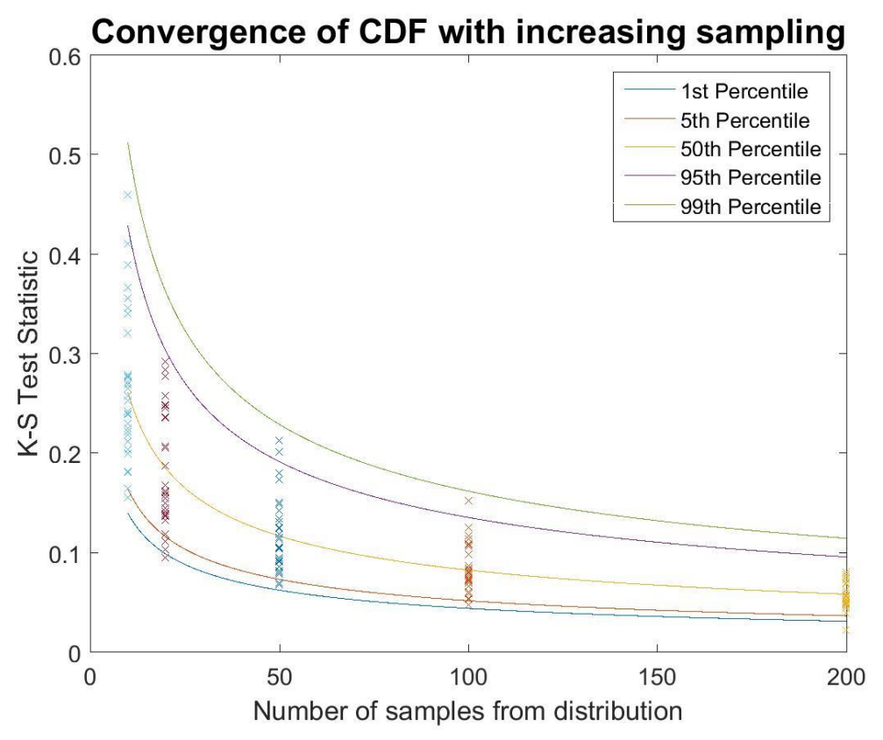
Microstructure SERVE (M-SERVE)

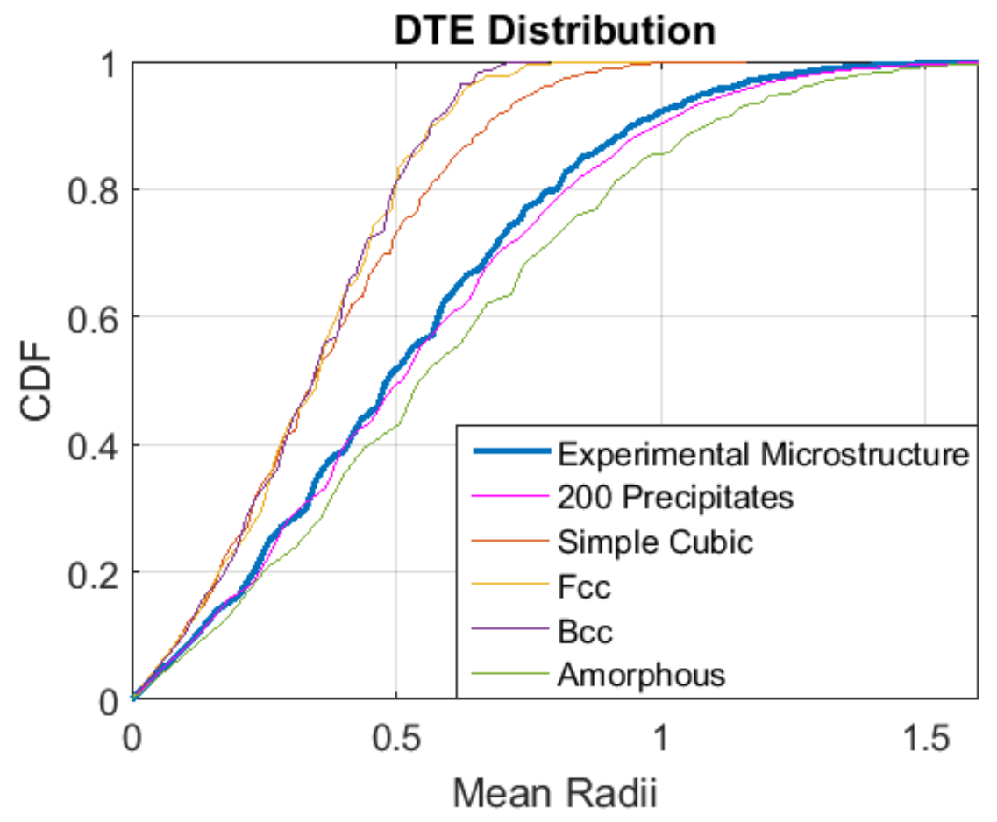
Experimental 3D subgrain γ-γ' microstructure data is collected through FIB-SEM serial sectioning and is statistically quantified in terms of precipitate morphology and spacing distributions.



M-SERVE Convergence and Validation

Virtual microstructures are generated for various SERVE sizes by matching the morphological statistics of the experimental data. The cumulative distribution functions (CDFs) of the experimental and virtual generation statistics are quantitatively compared using the Kolmogorov-Smirnov test.



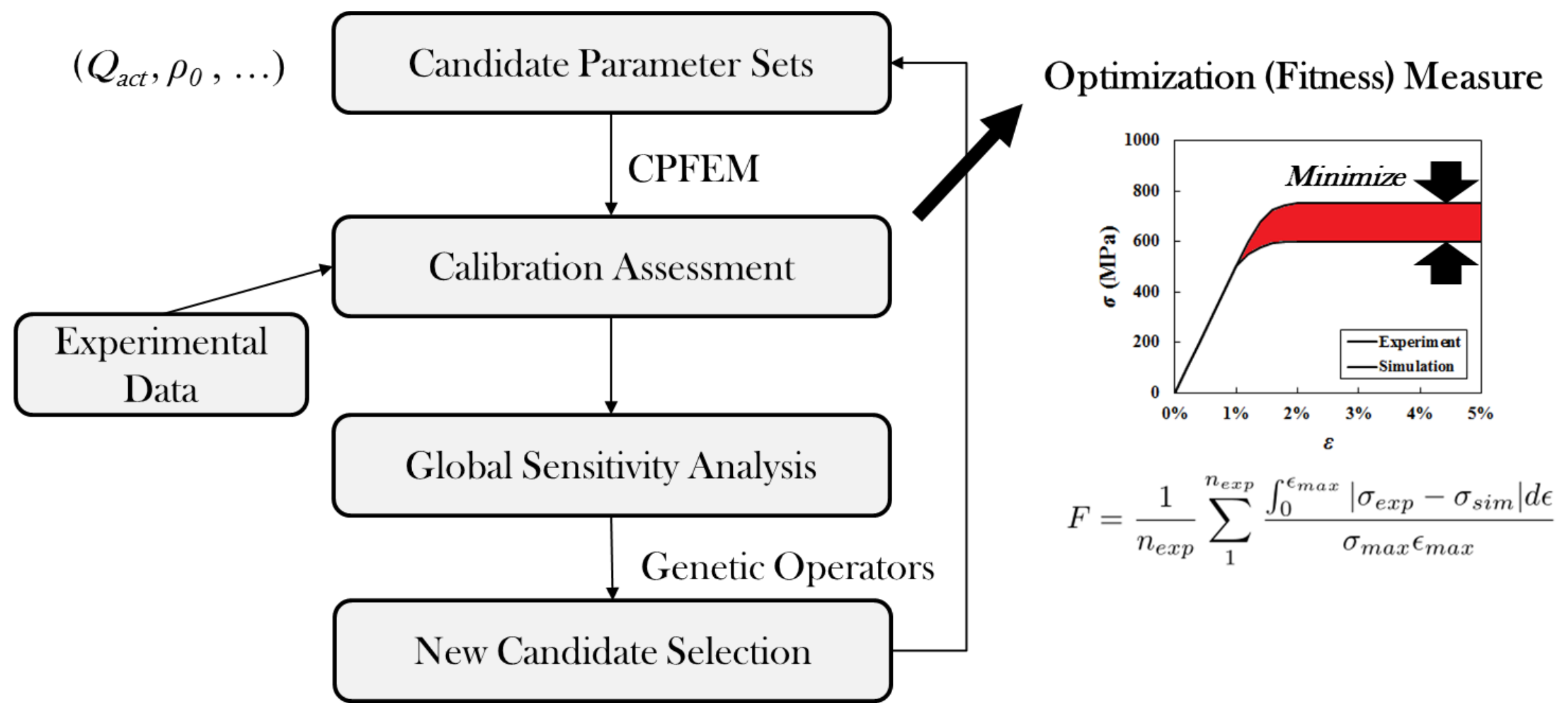


A distance to edge computation is performed to validate the virtual microstructure generation procedure.

CALIBRATION AND GLOBAL SENSITIVITY

Calibration of Constitutive Law Parameters

A genetic optimization procedure is executed to determine the constitutive law material parameters.



$$F = \frac{1}{n_{exp}}\sum_{1}^{n_{exp}}\frac{\int_0^{\epsilon_{max}}|\sigma_{exp} - \sigma_{sim}|d\epsilon}{\sigma_{max}\epsilon_{max}}$$

Global Sensitivity Analysis

Global sensitivity analysis is performed, in the form of Sobol' index computations, to understand which material parameters most influence the model and the calibration.

$$S_i = \frac{\mathrm{Var}_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i))}{\mathrm{Var}(\mathbf{Y})}$$

The "fraction" of output variance caused by a given input variance

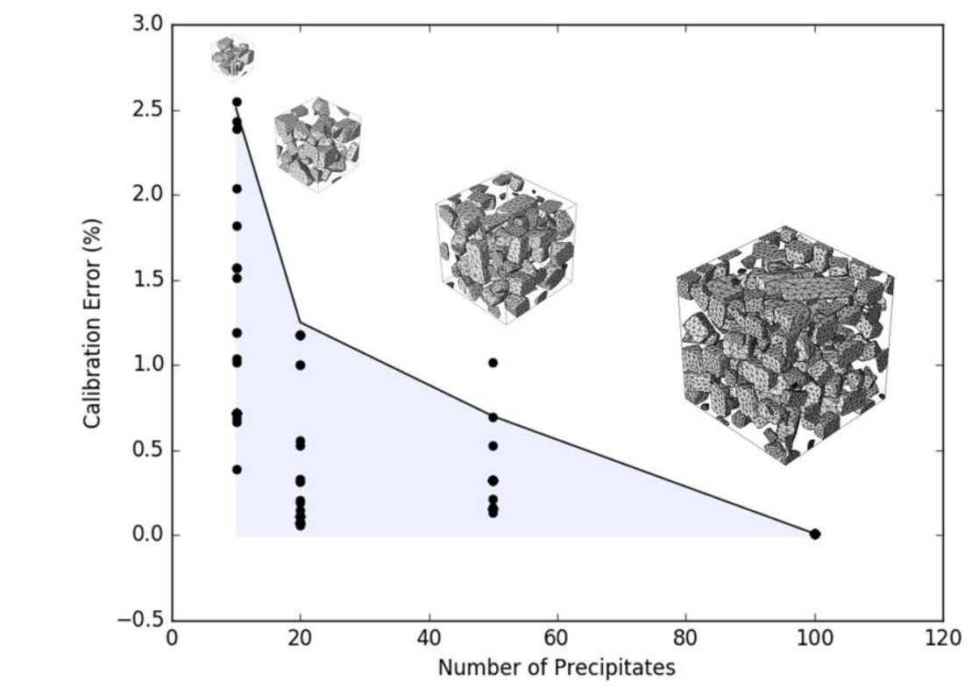
Which calibration parameters most influence the **yield strength** and **hardening rate**?

Uncertainty Added to Yield Strength
$S_{\rho_0} = 60.1\%$
$S_{Q_{act}} = 31.0\%$

Uncertainty Added to Hardening Rate
$S_{Q_{act}} = 44.2\%$
$S_{\rho_0} = 22.5\%$
(Another 16% from dislocation evolution parameters)

Is the calibration sensitive to SERVE instantiation?

It is observed that the calibration to experimental data is not strongly influenced by different microstructure realizations even at a low number of precipitates

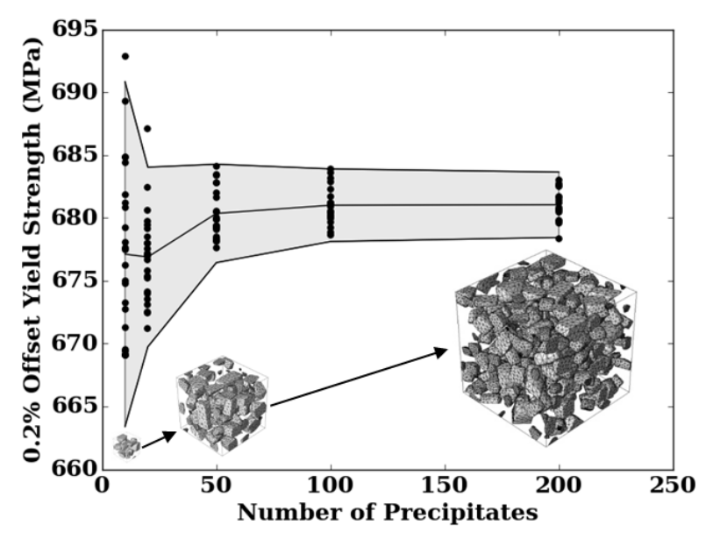


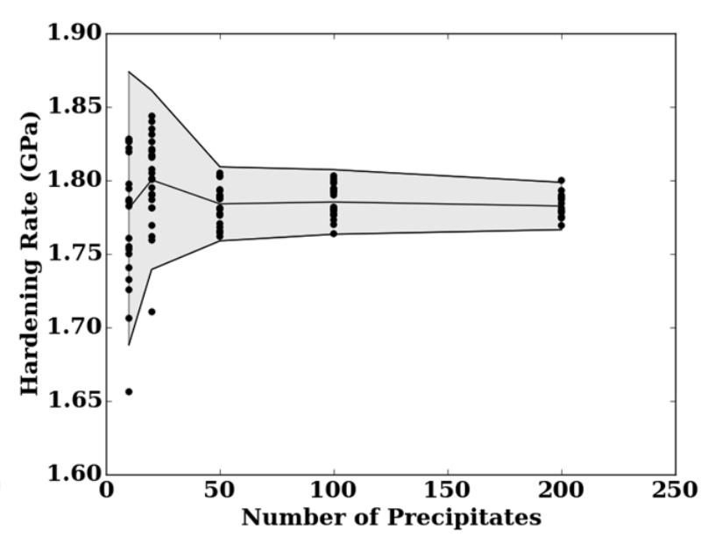
PROPERTY SERVES

Property SERVE (P-SERVE)

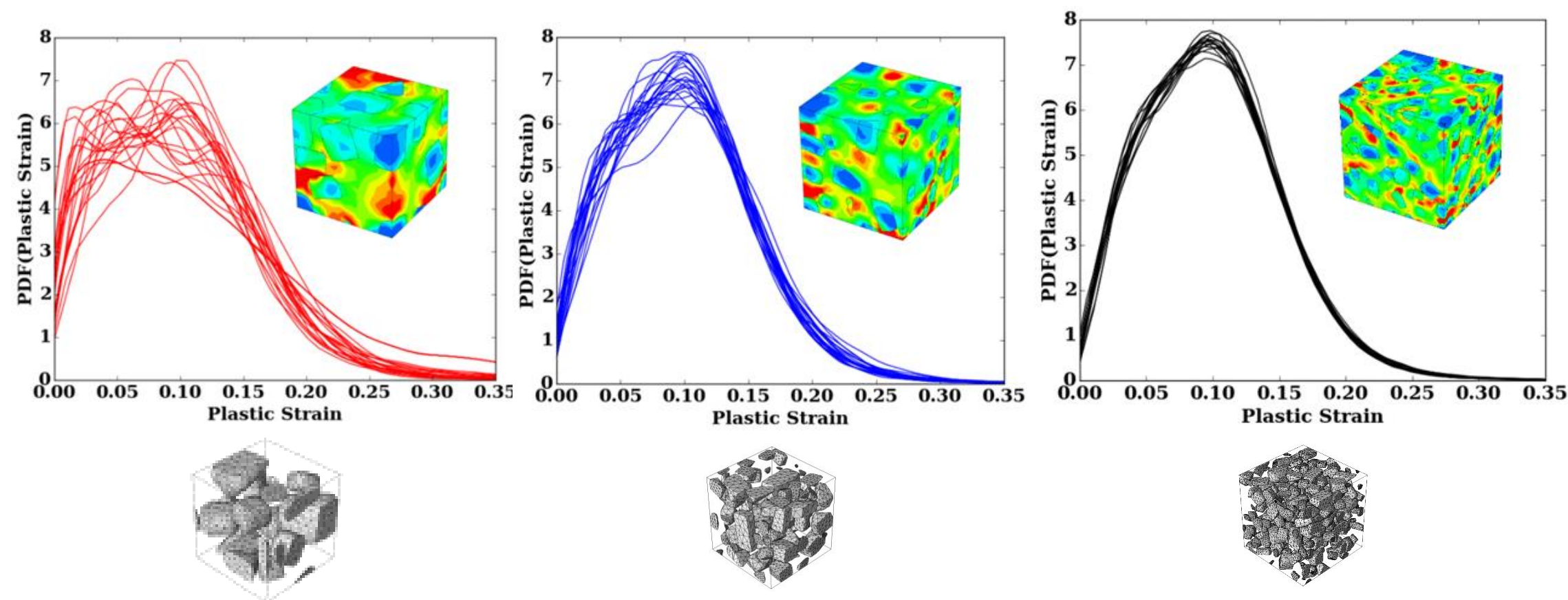
Defining the concept of a SERVE is ultimately linked to which mechanical property or microstructural feature is of interest. Yield and plastic strain behavior under monotonic loading is analyzed to determine the appropriate size of SERVE needed to represent these mechanical responses.

Convergence of macroscopic response occurs before M-SERVE





Distributions of mechanical fields converge near 100-200 precipitates



10 Precipitates

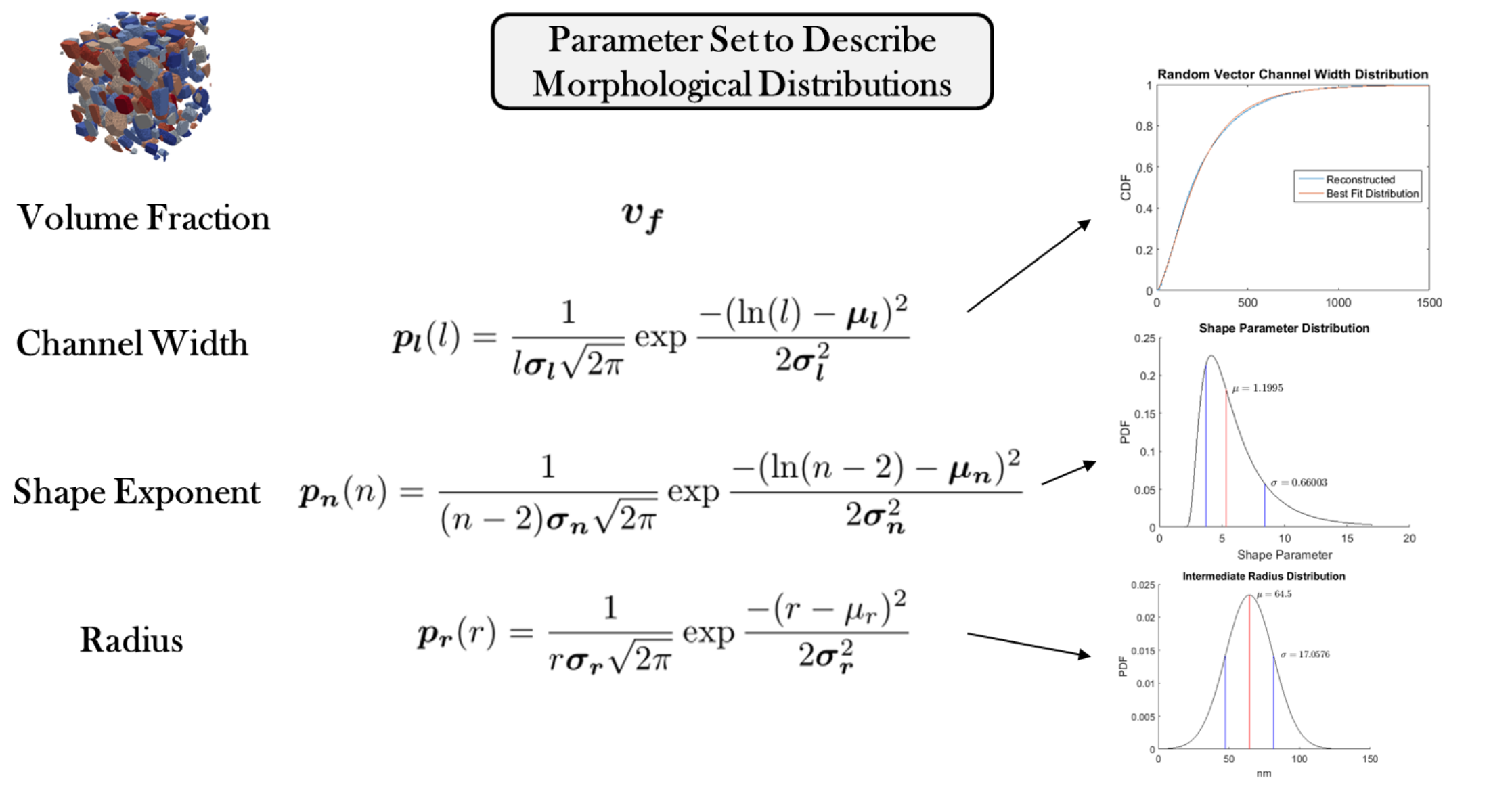
50 Precipitates

200 Precipitates

PARAMETRIC HOMOGENIZATION

Morphological Distribution Parameters

The morphological distributions of γ' precipitates critically influence the dislocation mechanics at the subgrain scale. The effects of these statistics are brought to the polycrystalline scale by parameterizing the distributions into lower order representations.



Volume Fraction $\boldsymbol{v_f}$

Channel Width $$\boldsymbol{p_l}(l) = \frac{1}{l\boldsymbol{\sigma_l}\sqrt{2\pi}}\exp\frac{-(\ln(l)-\boldsymbol{\mu_l})^2}{2\boldsymbol{\sigma_l^2}}$$

Shape Exponent $$\boldsymbol{p_n}(n) = \frac{1}{(n-2)\boldsymbol{\sigma_n}\sqrt{2\pi}}\exp\frac{-(\ln(n-2)-\boldsymbol{\mu_n})^2}{2\boldsymbol{\sigma_n^2}}$$

Radius $$\boldsymbol{p_r}(r) = \frac{1}{r\boldsymbol{\sigma_r}\sqrt{2\pi}}\exp\frac{-(r-\mu_r)^2}{2\boldsymbol{\sigma_r^2}}$$

The constitutive model at the higher scale is constructed as a function of these morphological descriptors (volume fraction, logmean/logvariance of channel width, logmean/logvariance of shape exponent, and variance of mean radius).

Homogenized Constitutive Model

A thermally activated crystal plasticity constitutive law is adopted for the single crystal behavior of the higher scale. Two critical parameters (cutting stress $\tau_{cut,0}$ and hardening constant h_0) are selected to become functions of the γ' morphological descriptors.

Flow Rule

$$\dot{\gamma}^\alpha = \dot{\gamma}_*^\alpha \exp\left\{-\frac{Q}{K_B T}\left(1-\left[\frac{|\tau^\alpha| - \tau^\alpha_{pass}}{\tau^\alpha_{cut}}\right]^p\right)^q\right\}\mathrm{sign}(\tau^\alpha)$$

Hardening Evolution

$$h_\beta = \left[h_0\left(1-\frac{s^\beta}{s^\beta_{sat}}\right)^r\right] sign\left(1-\frac{s^\beta}{s^\beta_{sat}}\right)$$

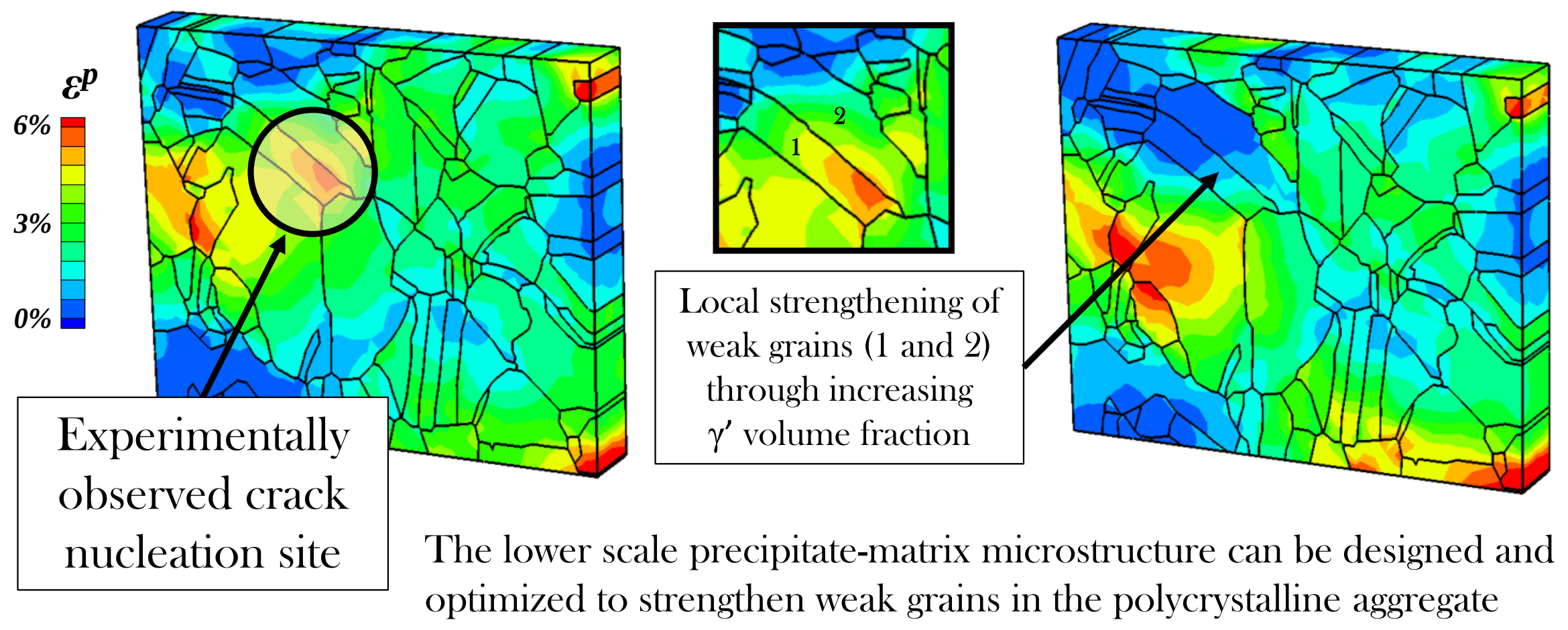
Parametric Homogenization

By simulating a number of microstructural realizations at the subgrain scale with various γ' microstructures, functional forms for the initial cutting stress and hardening constant are derived. The connection between scales is enforced through Hill's conditions.

$$\tau_{cut,0}(\boldsymbol{v_f}, \boldsymbol{p_l}, \boldsymbol{p_n}, \boldsymbol{p_r}) = A_0 + A_1\boldsymbol{v_f}\boldsymbol{\mu_n} + A_2\boldsymbol{v_f^2} + A_3\boldsymbol{v_f}\boldsymbol{\sigma_l}\boldsymbol{\sigma_n^2} + A_4\boldsymbol{v_f} + A_5\boldsymbol{\mu_n}\boldsymbol{\sigma_n}$$

$$h_0(\boldsymbol{v_f}, \boldsymbol{p_l}, \boldsymbol{p_n}, \boldsymbol{p_r}) = B_0 + B_1\boldsymbol{\sigma_l} + \frac{B_2}{\boldsymbol{\sigma_l}} + B_3\boldsymbol{\sigma_r}\boldsymbol{\mu_n}\boldsymbol{\mu_l} + B_4\boldsymbol{\sigma_r}\boldsymbol{\mu_n} + B_5\boldsymbol{\sigma_r}\boldsymbol{\mu_n^3} + B_6\boldsymbol{v_f}$$

Precipitate Strengthening at Polycrystalline Scale



Experimentally observed crack nucleation site

Local strengthening of weak grains (1 and 2) through increasing γ' volume fraction

The lower scale precipitate-matrix microstructure can be designed and optimized to strengthen weak grains in the polycrystalline aggregate

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