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An analytical model for material strength accounting for microstructural variability

PRESENTED BY

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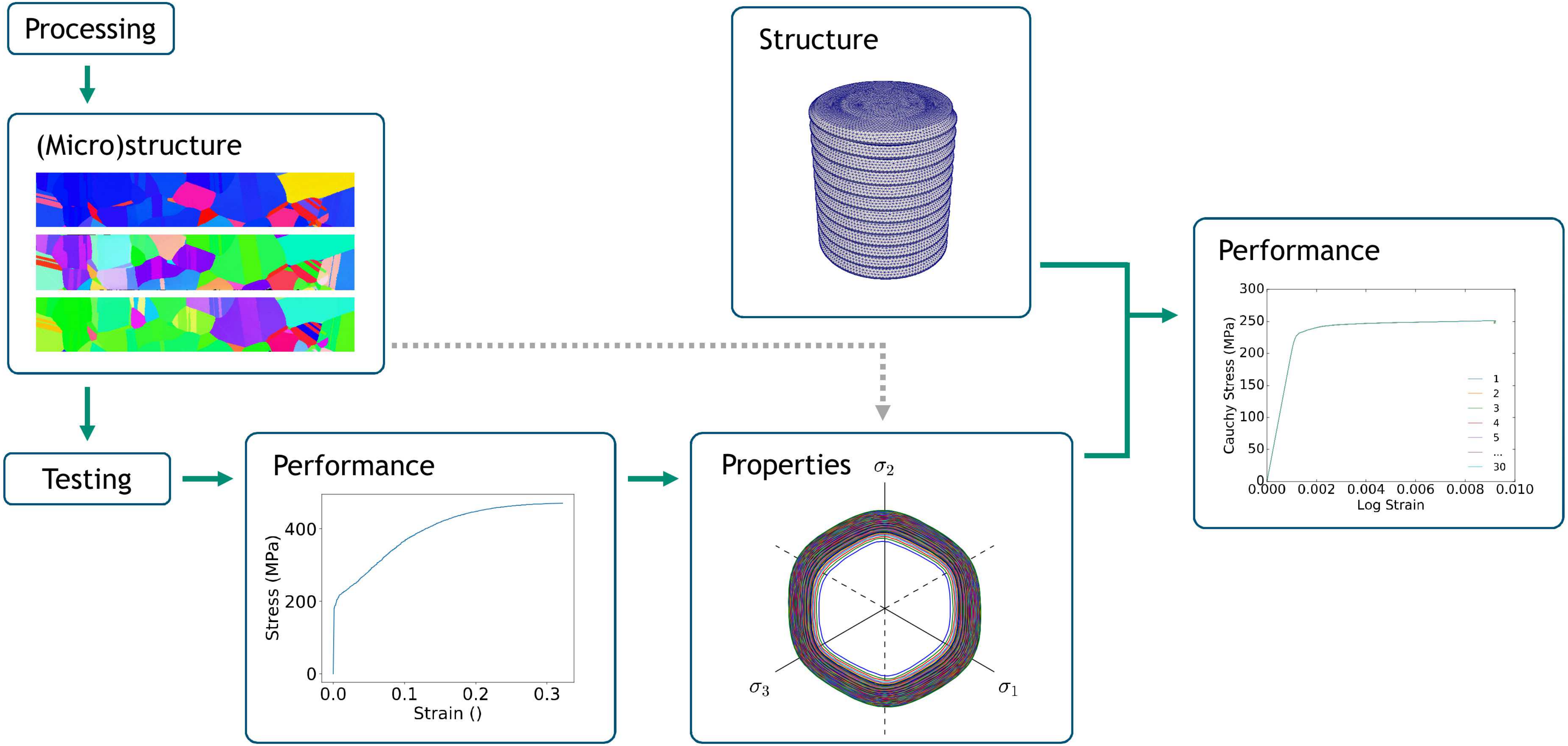
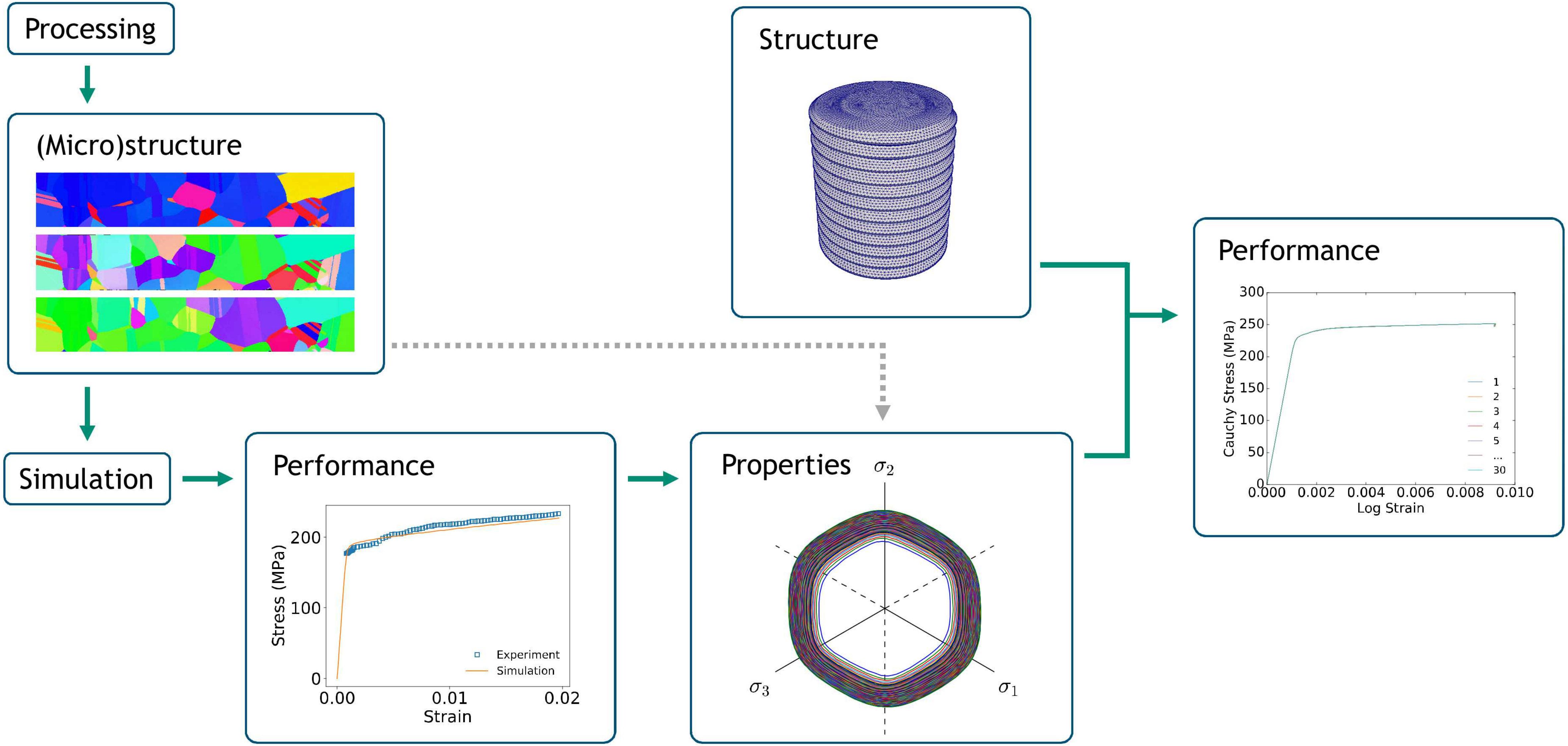
Connecting processing to performance (Testing paradigm)



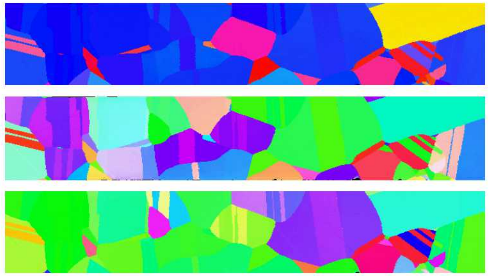
Connecting processing to performance (Simulation paradigm)



Connecting processing to performance (Calculation paradigm)

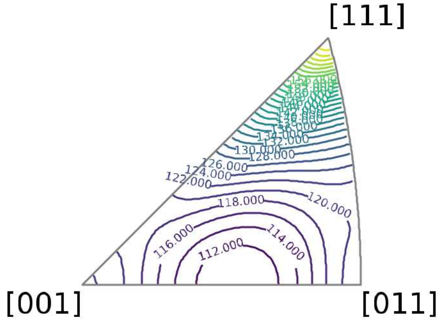
Processing

(Micro)structure

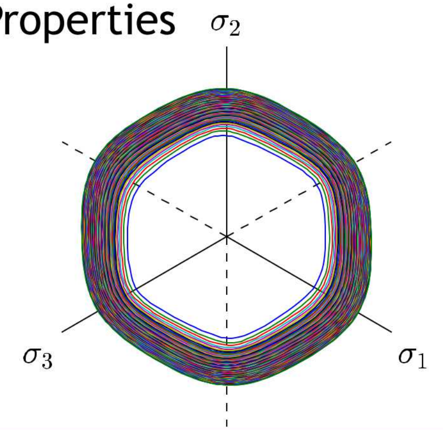


Calculation

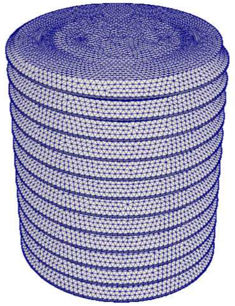
Properties



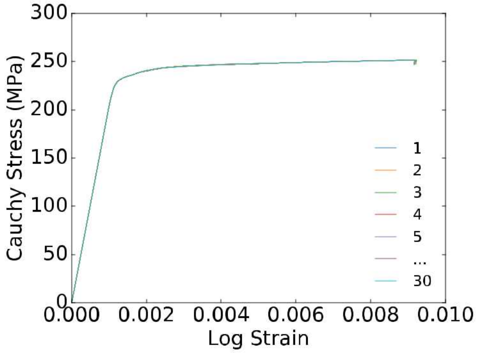
Properties



Structure



Performance



Enabling the calculation paradigm: Yield strength

We define the onset of plastic deformation (yielding) as the point when the plastic dissipation reaches a critical fraction of the applied power:

$$\mathcal{D}^p = \phi_{cr}\dot{W}$$

The applied power is the product of the applied stress and the rate of deformation:

$$\dot{W} = \underline{\underline{s}}:\underline{\underline{D}}$$

At a material point, the plastic dissipation is the sum of the products of resolved shear stresses, τ^α and slip rates, $\dot{\gamma}^\alpha(\tau^\alpha)$ on each slip system:

$$d^p = \sum_\alpha \dot{\gamma}^\alpha(\tau^\alpha)\cdot\tau^\alpha, \qquad \tau^\alpha = \underline{\underline{s}}:\underline{\underline{P}}^\alpha$$

Thus, stress at the onset of yielding satisfies:

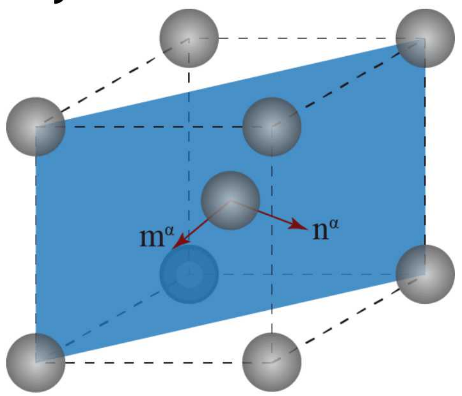
$$\sum_\alpha \dot{\gamma}^\alpha\left(\underline{\underline{s}}_y:\underline{\underline{P}}^\alpha\right)\cdot\underline{\underline{s}}_y:\underline{\underline{P}}^\alpha = \phi_{cr}\underline{\underline{s}}_y:\underline{\underline{D}}$$

The scalar yield strength, s_y is the norm of this stress:

$$s_y = \sqrt{\underline{\underline{s}}_y:\underline{\underline{s}}_y}$$

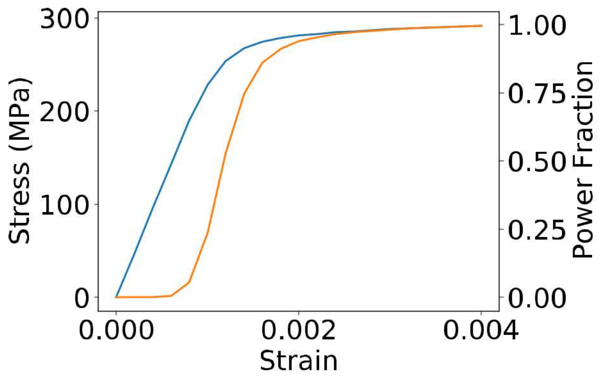
The yield strength is the magnitude of the stress at which plastic dissipation reaches a critical fraction of the applied power.

Slip system



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

Stress and dissipation



Enabling the calculation paradigm: Yield strength

We define the onset of plastic deformation (yielding) as the point when the rate of energy dissipation due to plastic work reaches a critical fraction of the applied power:

$$\sum_{\alpha} \dot{\gamma}^{\alpha}\left(s_y \underline{\underline{n}} : \underline{\underline{P}}^{\alpha}\right) \cdot \underline{\underline{n}} : \underline{\underline{P}}^{\alpha} = \phi_{cr} \underline{\underline{n}} : \underline{\underline{D}}, \qquad \underline{\underline{s}}_y = s_y \underline{\underline{n}}$$

In limited (but useful) situations, the stress direction $\underline{\underline{n}}$ and the rate of deformation $\underline{\underline{D}}$ can be approximately related to the loading conditions, so that s_y can be approximated via a closed-form algebraic equation, as follows.

The "Schmid Factor" is the ratio of the resolved stress to the applied stress:

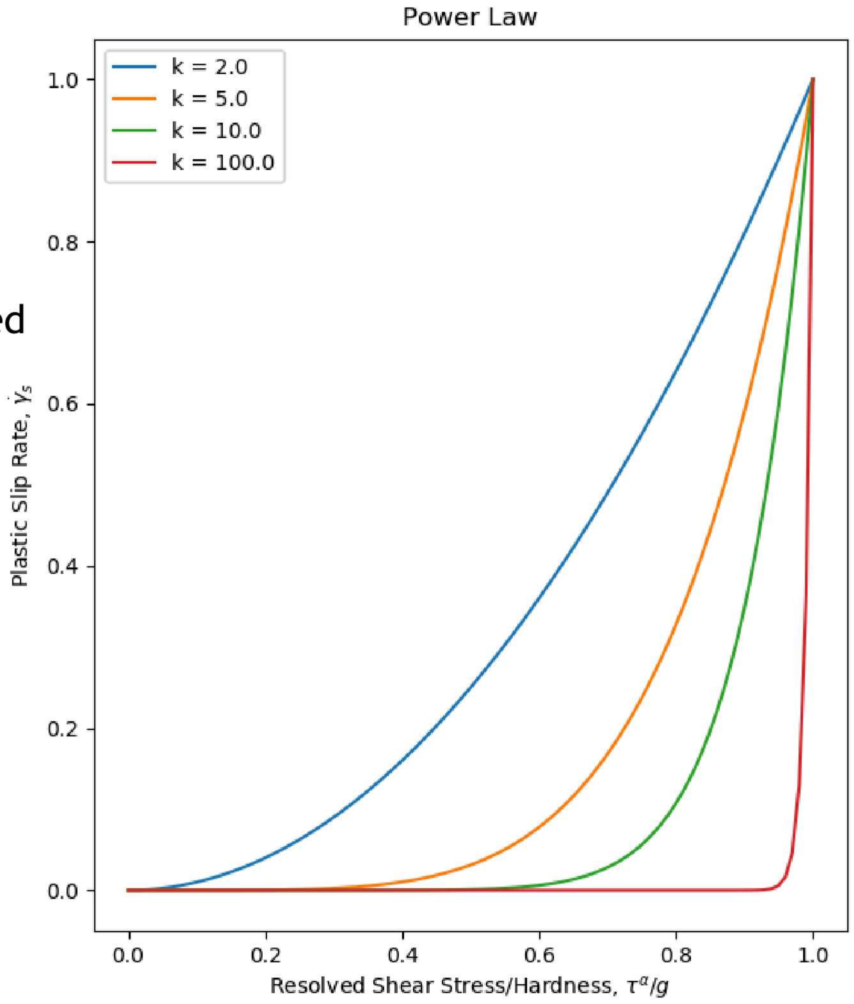
$$f^{\alpha} = \frac{\tau^{\alpha}}{s} = \underline{\underline{n}} : \underline{\underline{P}}^{\alpha} \Rightarrow \tau^{\alpha} = f^{\alpha} s$$

The plastic slip rate is commonly approximated via a power law:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left| \frac{f^{\alpha} s}{g} \right|^{k} \operatorname{sgn} \tau^{\alpha}$$

Assuming the stress at each point in the material is equal to the macroscopic applied stress, the yield strength is calculated:

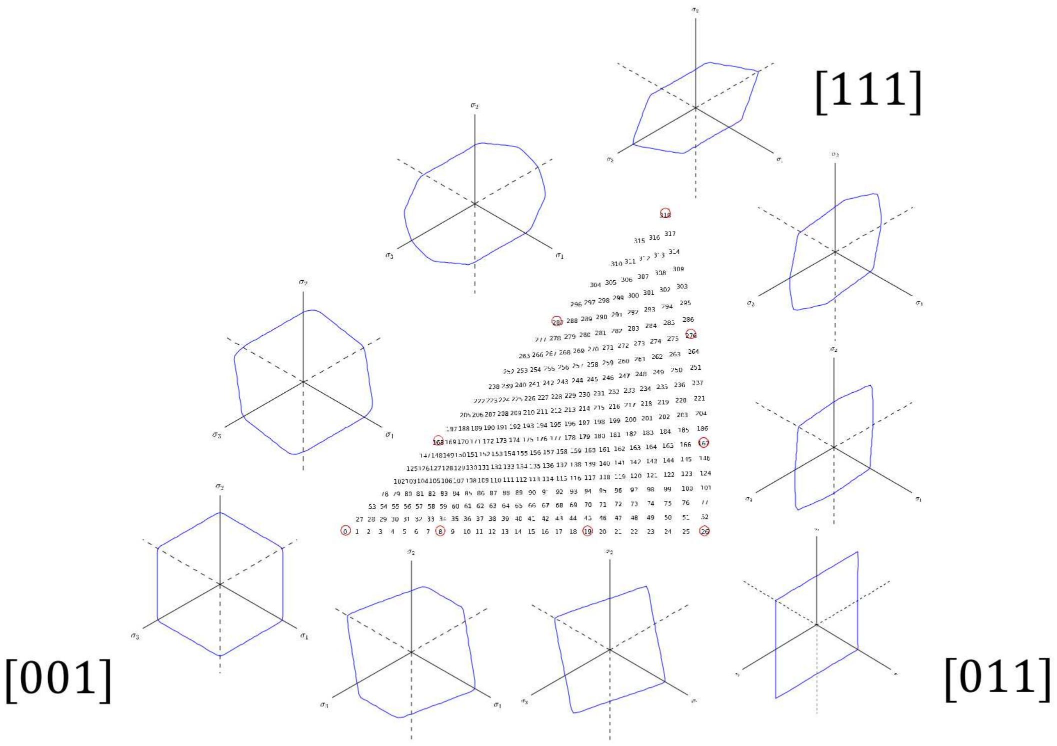
$$s_y = g \left[\frac{\phi_{cr} \underline{\underline{n}} : \underline{\underline{L}}}{\dot{\gamma}_0 \sum_i^{N_{grains}} v_i \sum_{\alpha}^{N_{slipsys}} |f^{\alpha}|^{k+1}} \right]^{\frac{1}{k}}$$



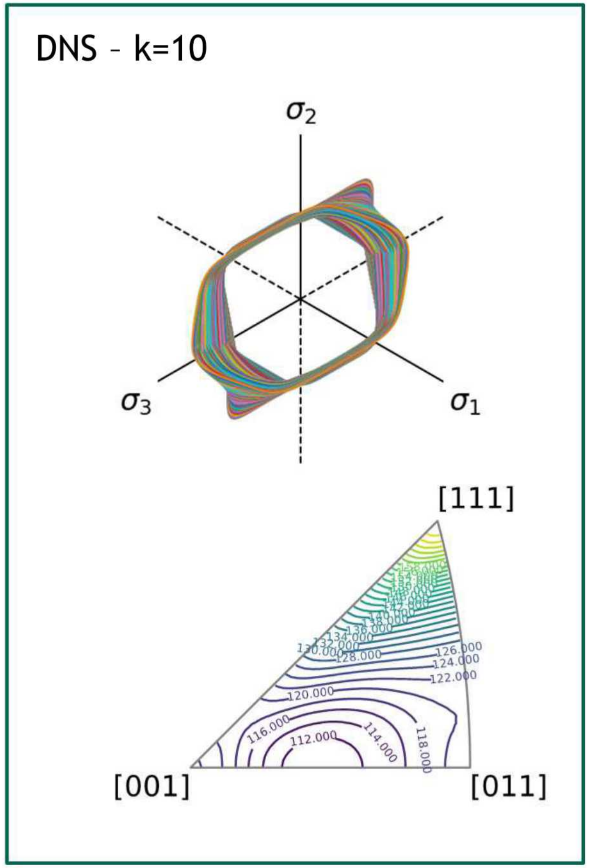
The yield strength can be approximated from properties of the microstructure and the loading scenario.

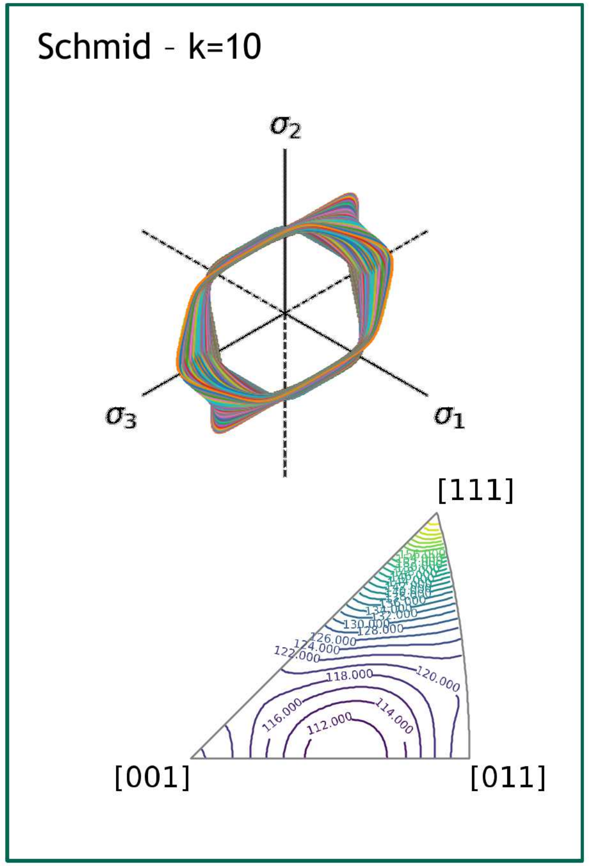
Replacing simulation with calculation: Single crystal yield strength

- **Verification**: for various measures of rate sensitivity k, run 319 simulations with orientations corresponding to discretized locations in the standard triangle
- Each orientation is subjected to 12 loading conditions with varying Lode angle, θ
- Yield surfaces are qualitatively compared between the direct numerical simulation (DNS) and analytical model



The 319 discretized orientations of the standard triangle. Each yield surface is built from 12 loading conditions according to the Lode angle.

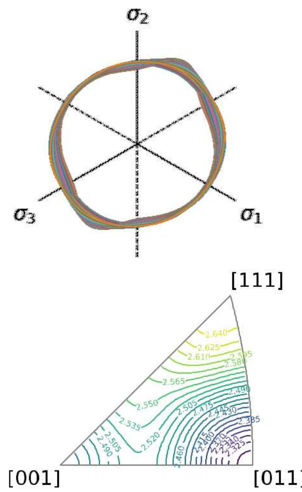




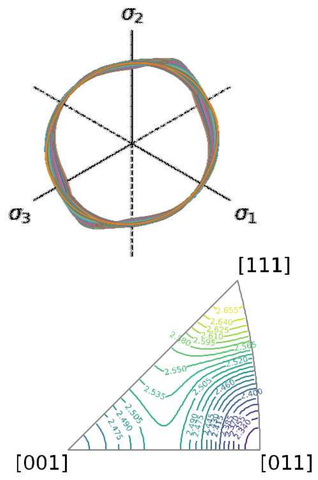
A comparison between the DNS and Generalized Schmid Factor approximation for k =10 showing good agreement.

Replacing simulation with calculation: Single crystal yield strength

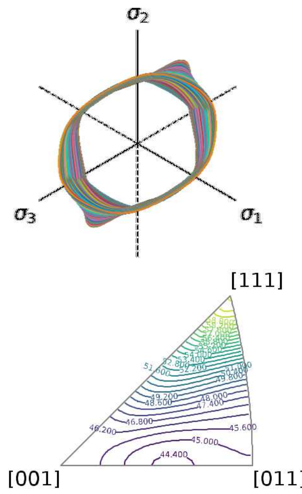
DNS – k=2



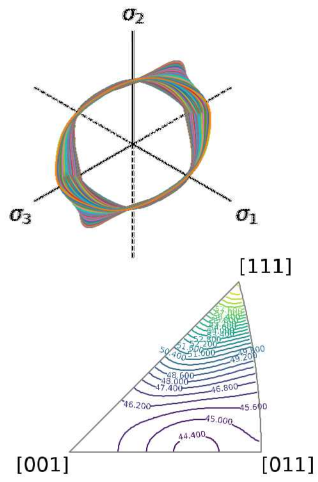
Schmid – k=2



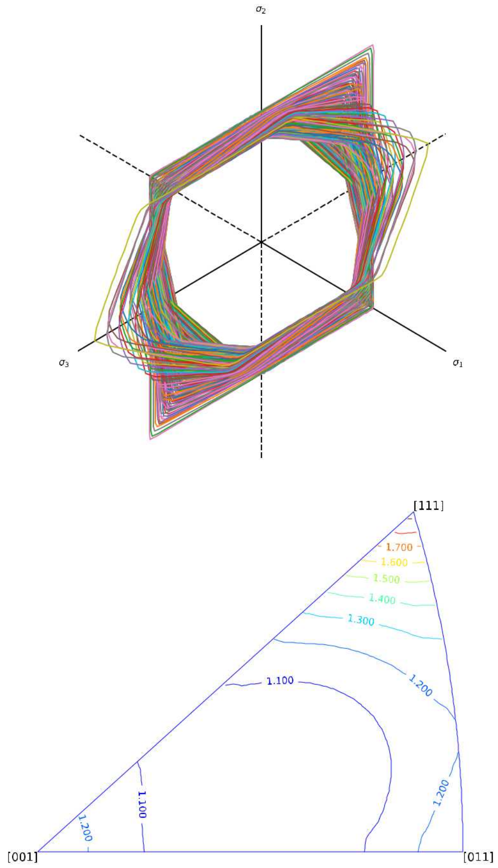
DNS – k=5



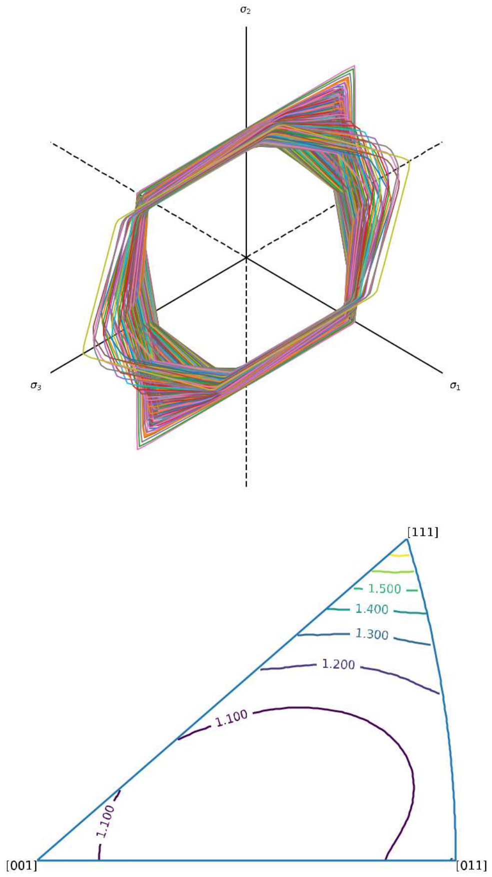
Schmid – k=5



DNS – k=100



Schmid – k=100



The analytical model can approximate the yield strength from single-crystal material orientation and loading scenario

Ongoing work: Polycrystalline yield strength

Recall the plastic dissipation due to slip:

$$d^p = \sum_\alpha \dot{\gamma}^\alpha(\tau^\alpha) \cdot \tau^\alpha , \qquad \tau^\alpha = \underline{\underline{S}} : \underline{\underline{P}}^\alpha$$

Hypothesis: the single grain case can be extended for the polycrystalline case via volume fractions

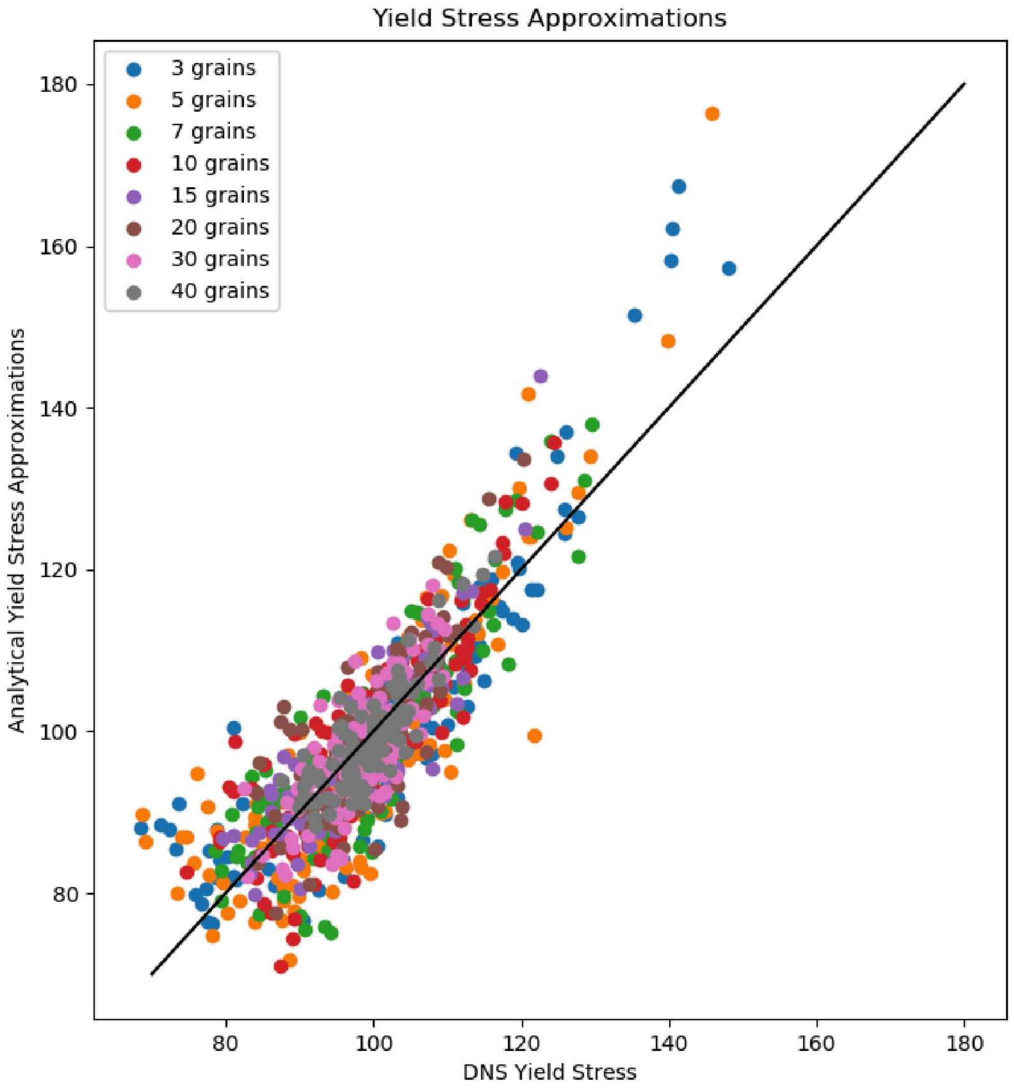
$$\sum_{i=1}^{N_{grains}} v_i d_i^p = \phi_{cr} \underline{\underline{S}} : \underline{\underline{D}}$$

where v_i is a volume fraction

$$v_i = \frac{|\Omega_i|}{|\Omega|}$$

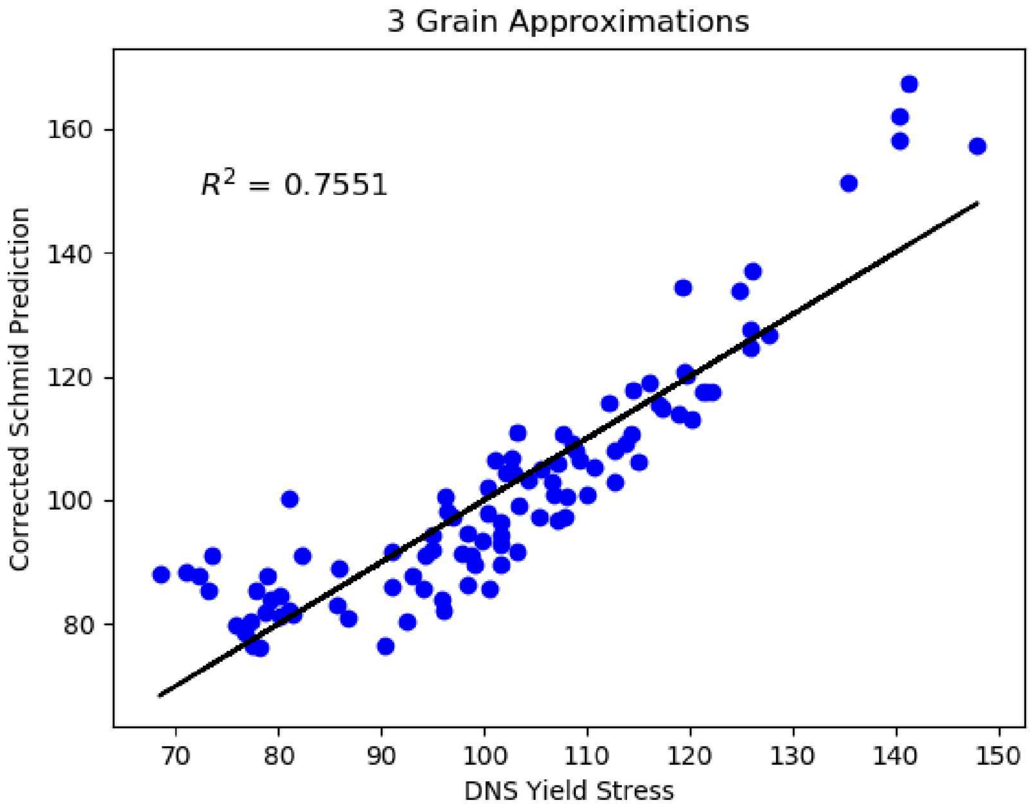
Testing Procedure: simulate multiple ensembles of grain structures and compare yield stress values from the analytical model to the DNS

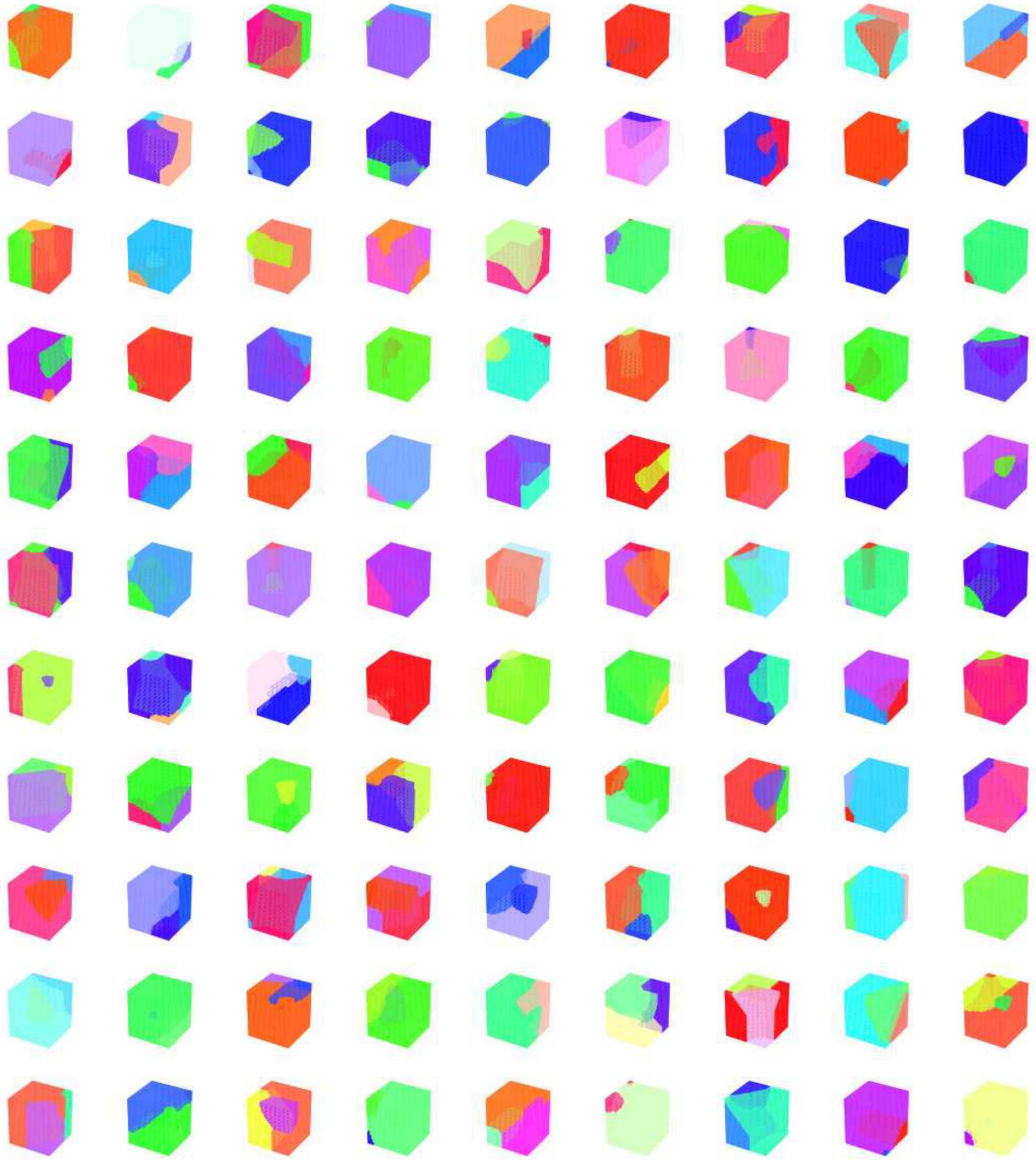
- 3, 5, 7, 10, 15, 20, 30, and 40 grain microstructures
- Run 100 unique microstructures generated using Spparks [1]
- Material parameters reminiscent of Austenitic stainless steel



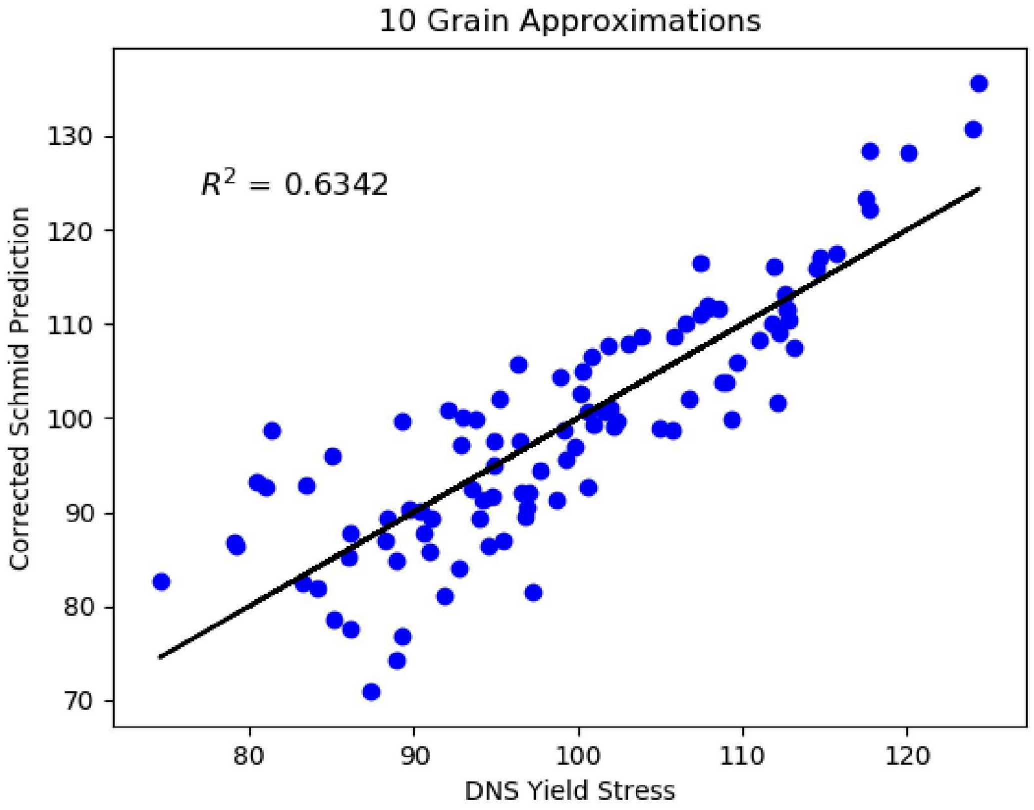
[1] S. Plimpton, et al. *SAND2009-6226* (2009). http://spparks.sandia.gov/

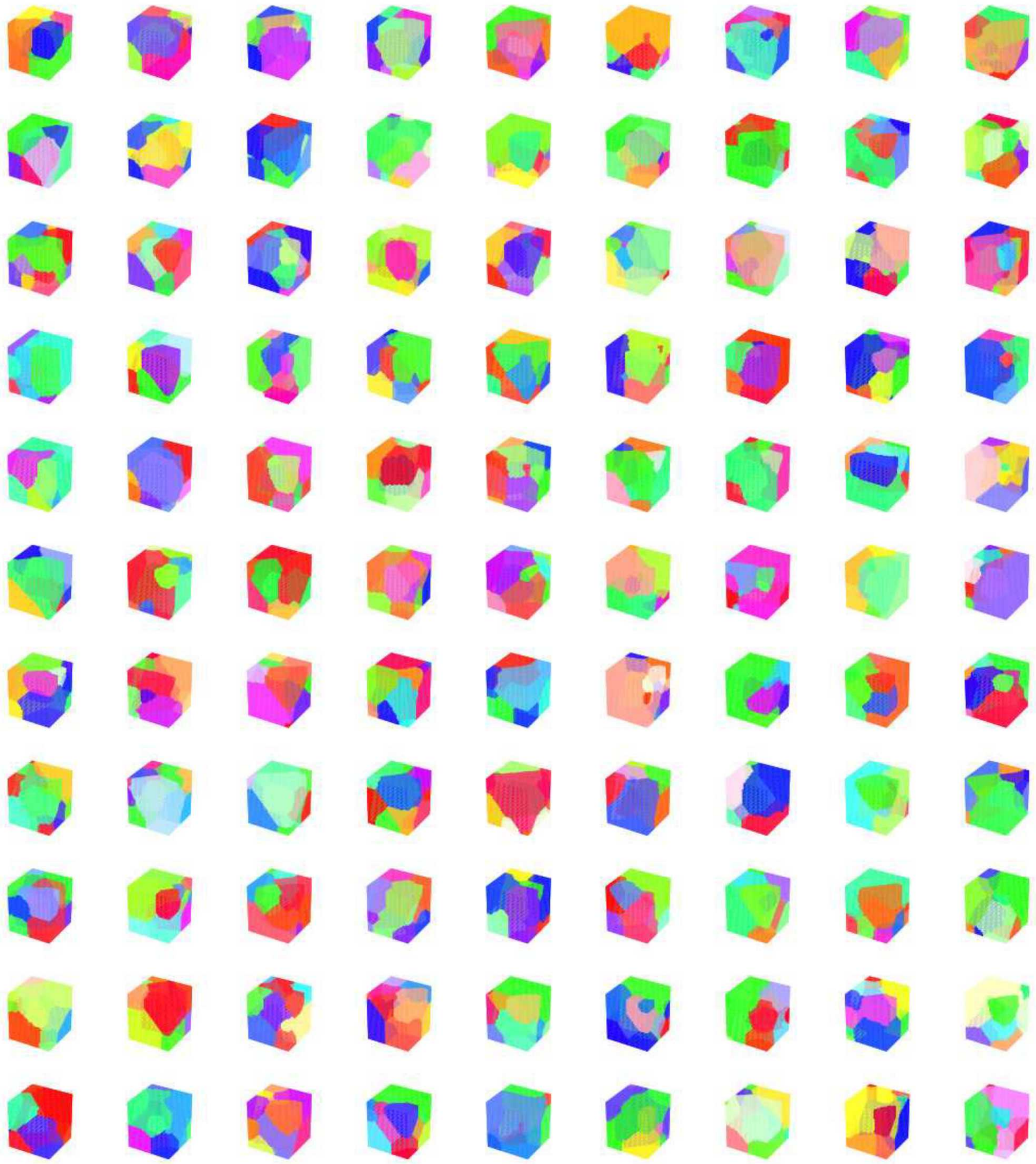
Polycrystalline results



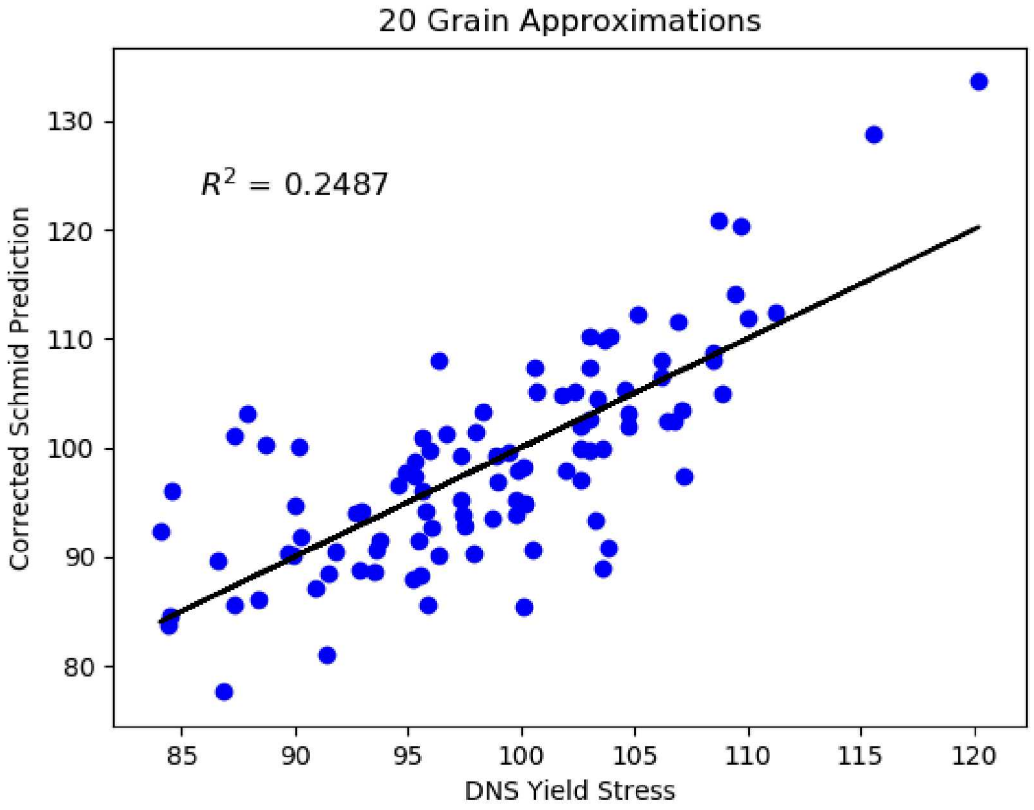


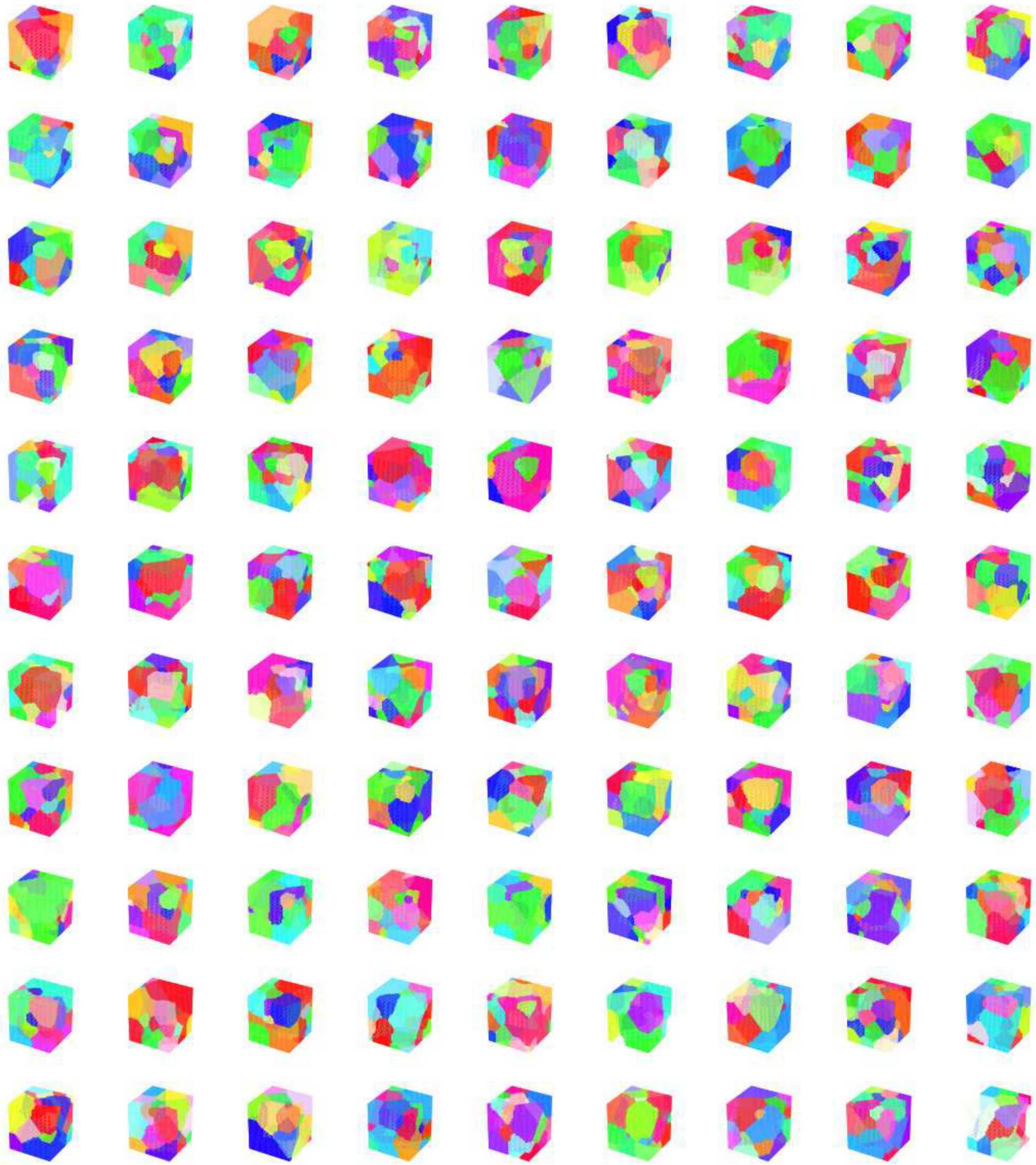
Polycrystalline results



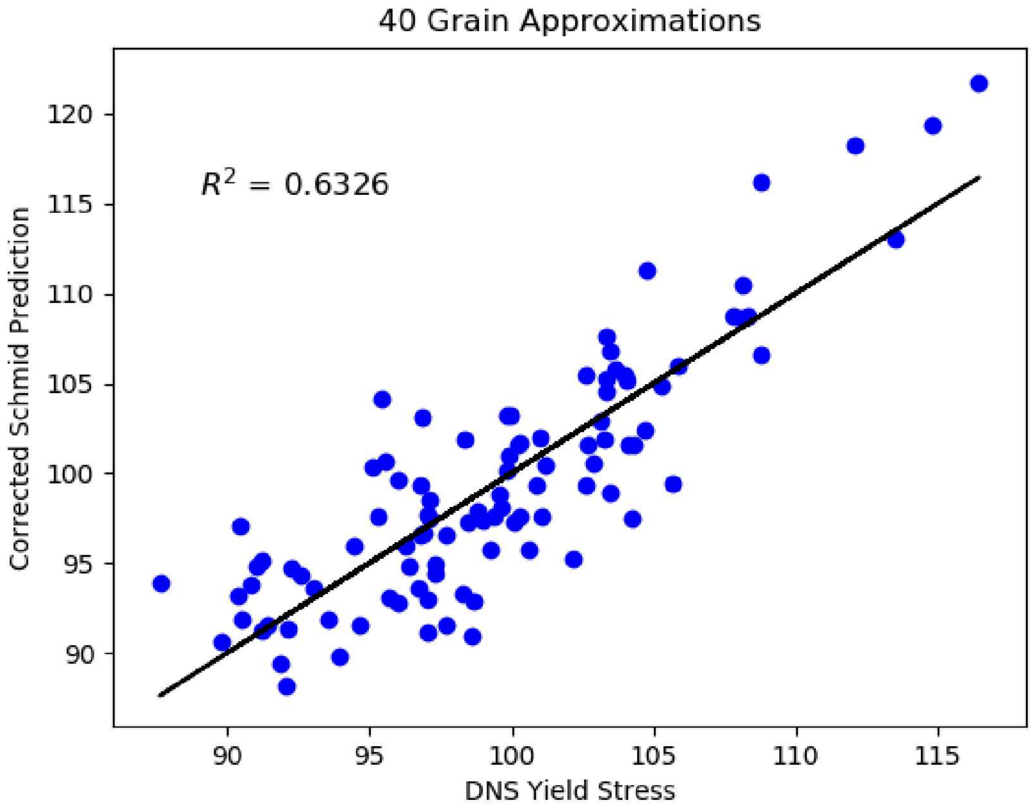


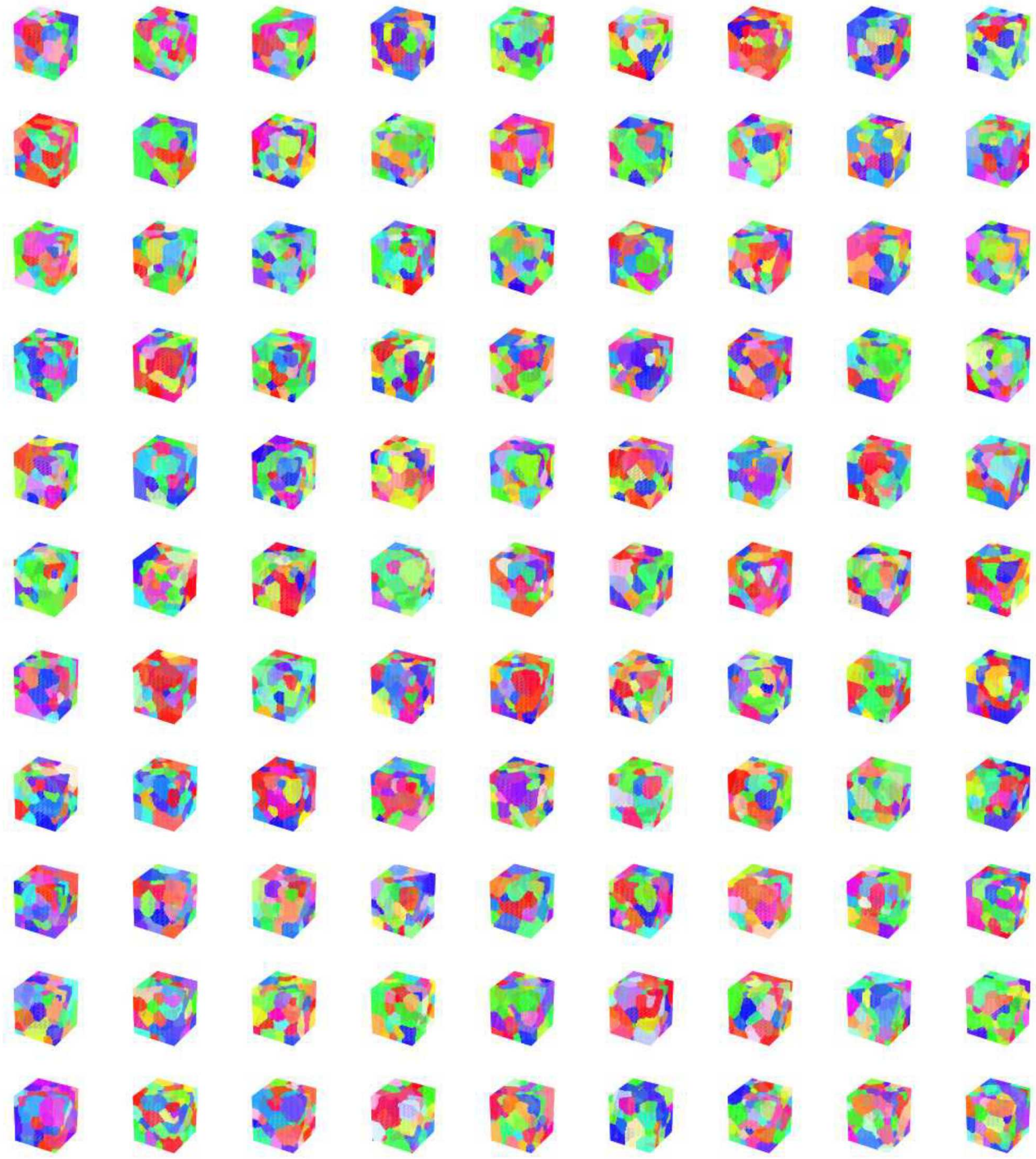
Polycrystalline results



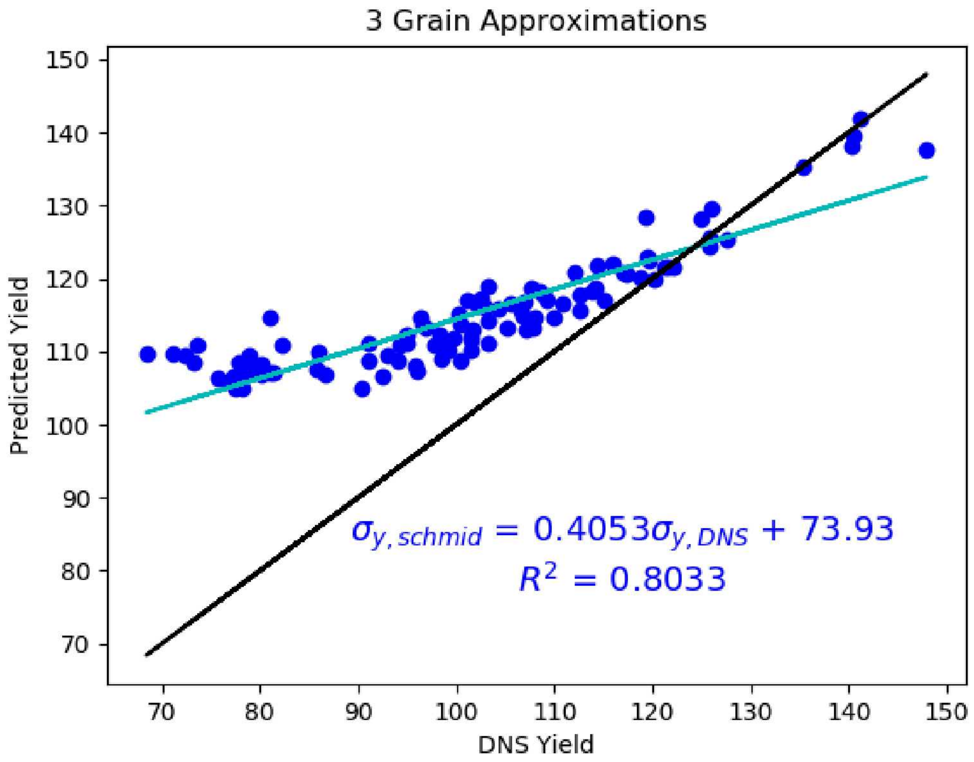


Polycrystalline results

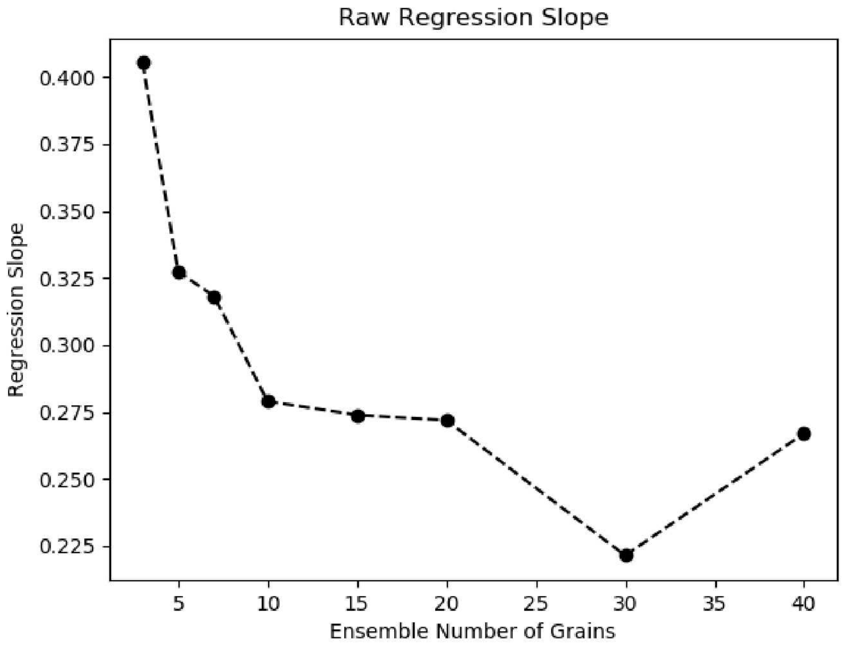


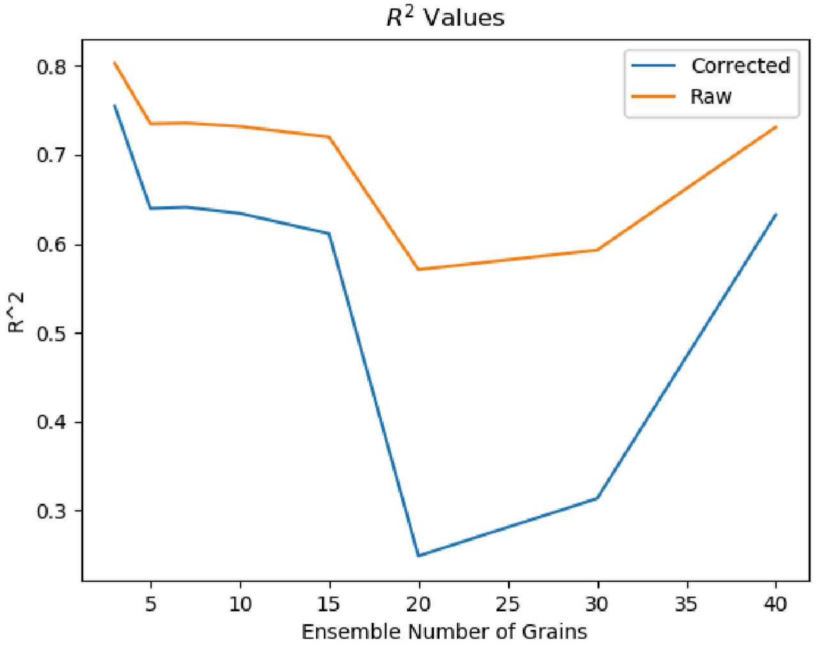


Systemic bias and preliminary trends



- Results shown are corrected for systemic bias
  - Sources of bias are to be investigated
- Analytical model underpredicts heterogeneity
- Regression slope shows decreasing trend as number of grains increase
- No conclusive trend in R^2 values





Conclusions and ongoing work

- The analytical model has been shown to:
  - Accurately predict yield stress in single crystal simulations
  - Capture the general effects of heterogeneity on yield stress for polycrystals

Ongoing Work

- Test statistical significance of ensembles
- Investigate and characterize sources of bias
- Apply the assumption that the strain (rather than stress) at each point in the material is equal to the macroscopic applied stress (i.e. “Taylor factor”)