

Kanapy: An open software tool for analyzing and processing of microstructure data

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Kanapy: Overview

Kanapy: Open-source python tool for microstructure analysis and generation of 3D microstructure models

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Features:

- Possibility to analyze experimental microstructures in form of EBSD maps
- Support of multiphase microstructures
- Generation of 3D microstructures based on statistical features as size distributions and aspect ratio distributions of grains and phase regions
- Crystallographic texture reconstruction using orientations from experimental data in form of Orientation Distribution Function (ODF).
- In-built hexahedral mesh generator for representation of complex polycrystalline microstructures in form of voxels
- Import and export of voxel structures according to following a modular materials data schema.

Kanapy: Installation and use

Installation:

The preferred method to install Kanapy is within a conda or any virtual environment by

```
$ conda install kanapy -c conda-forge
```

or

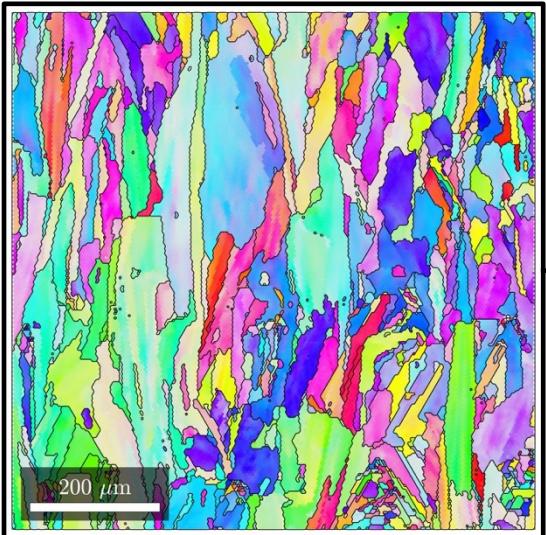
```
$ pip install kanapy
```

Use:

- Python Application Programming Interface (API) allows import of Kanapy functions into own python scripts by
`>>> import kanapy as knpy`
- Command Line Interface (CLI) supports administrative functions. Type
`$ kanapy –help`
for a complete list of CLI functions.
- Graphical User Interface (GUI) is under development. Start with
`$ kanapy gui`

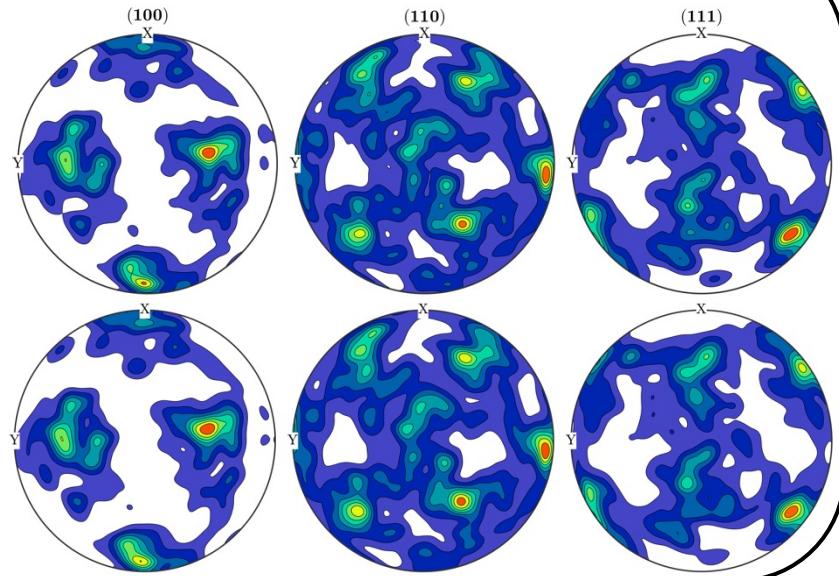
Kanapy: Work flow

EBSD



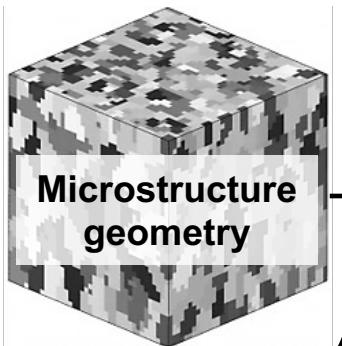
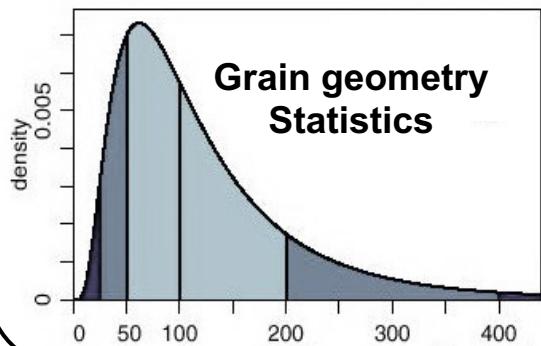
Texture module: ODF

EBSD
ODF

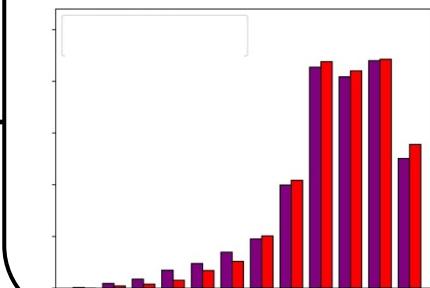


Reduced
ODF

Geometry module



Texture module: MDF

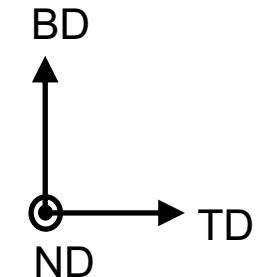
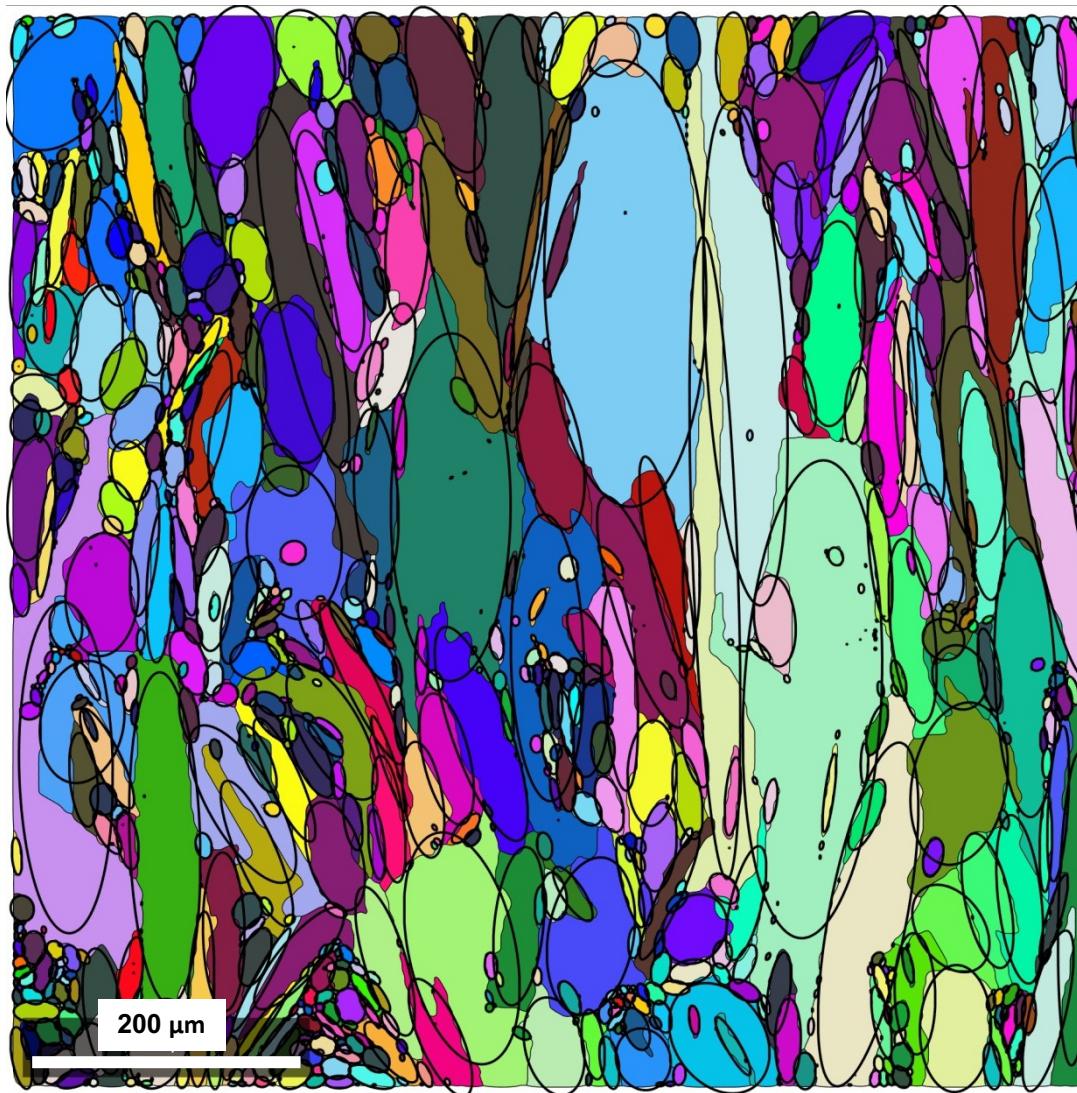
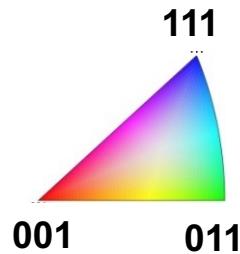


Synthetic Microstructure



<https://github.com/ICAMS/Kanapy>

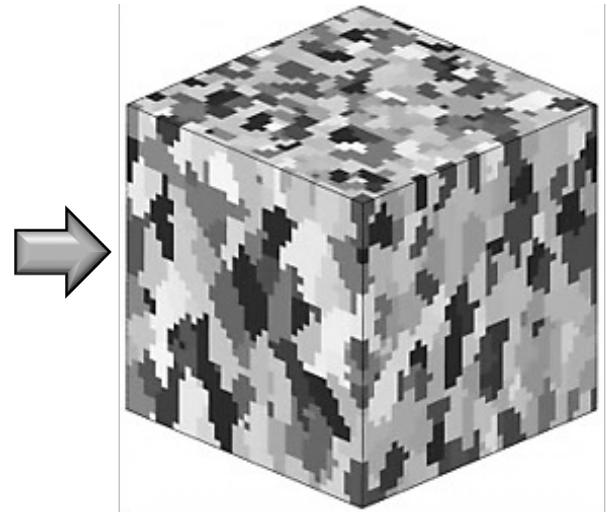
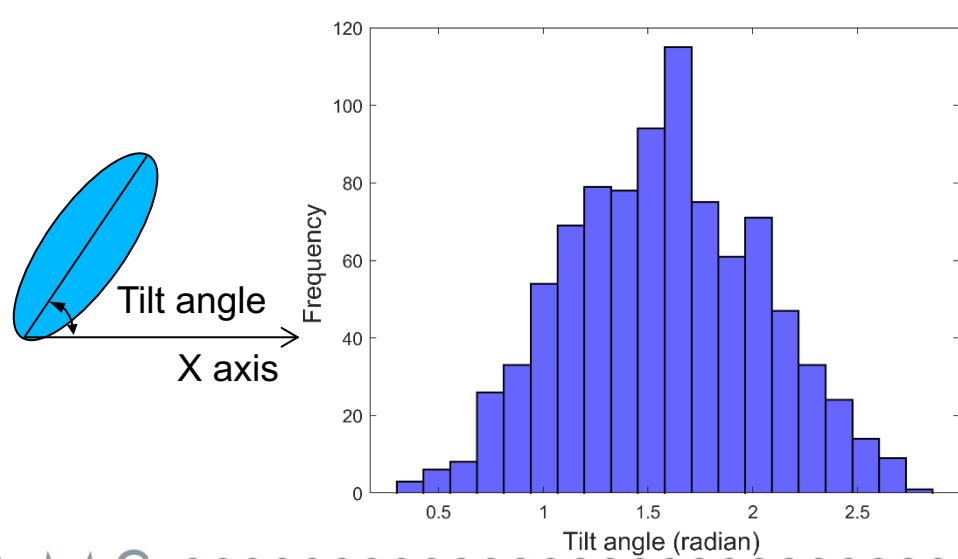
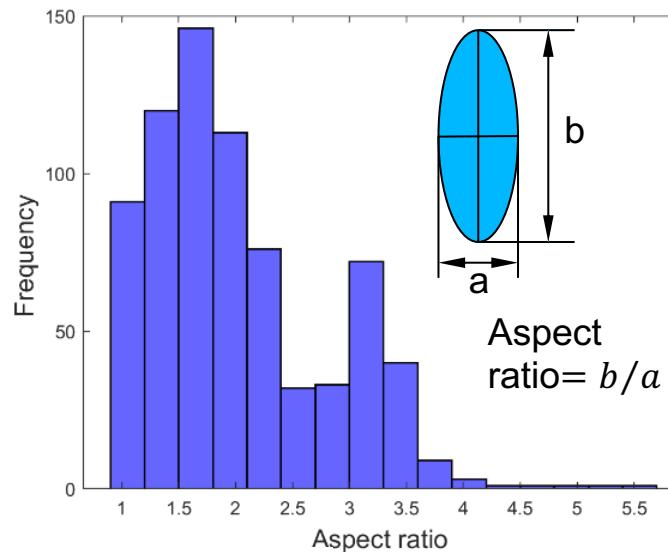
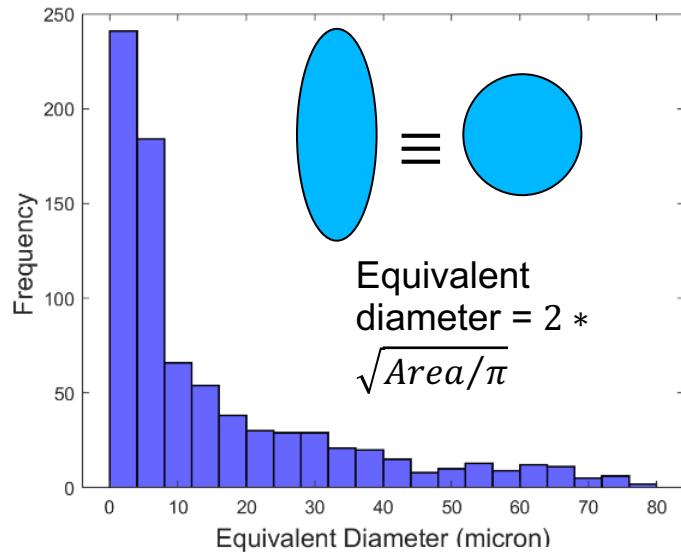
Elements of microstructure : Grains



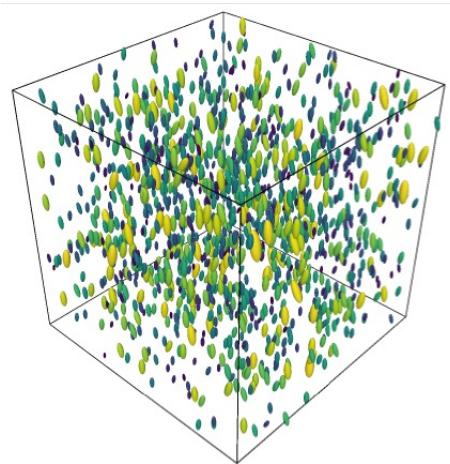
BD: Building direction
TD: Transverse direction
ND: Normal direction

MTEX documentation
<https://mtex-toolbox.github.io/Documentation.html>

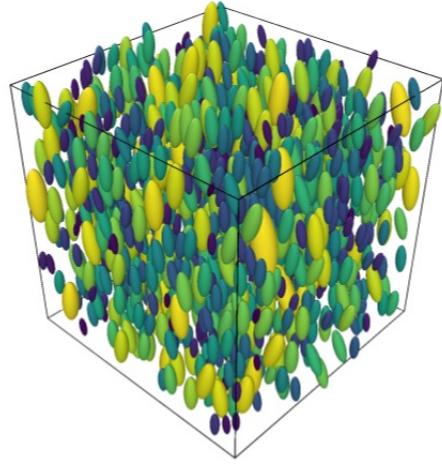
Elements of microstructure: Grain statistics



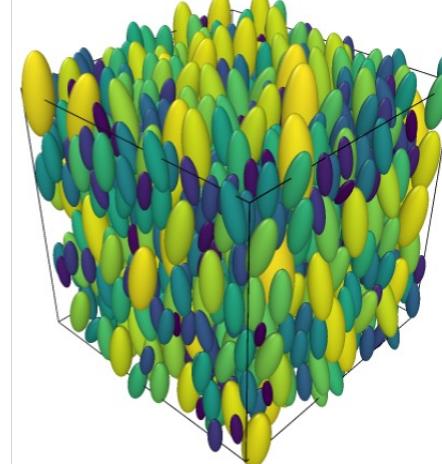
Geometry Module: Particle simulation



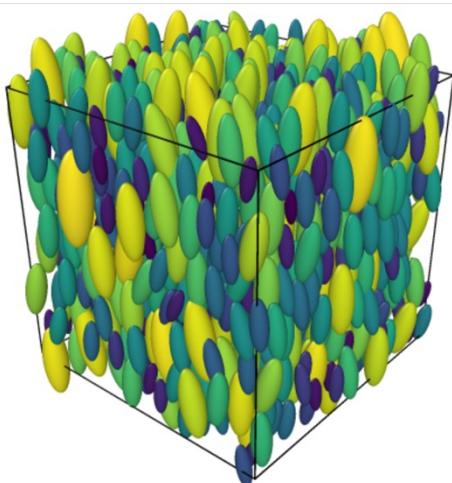
Time step : 250



Time step : 550



Time step : 850



Ellipsoid packing

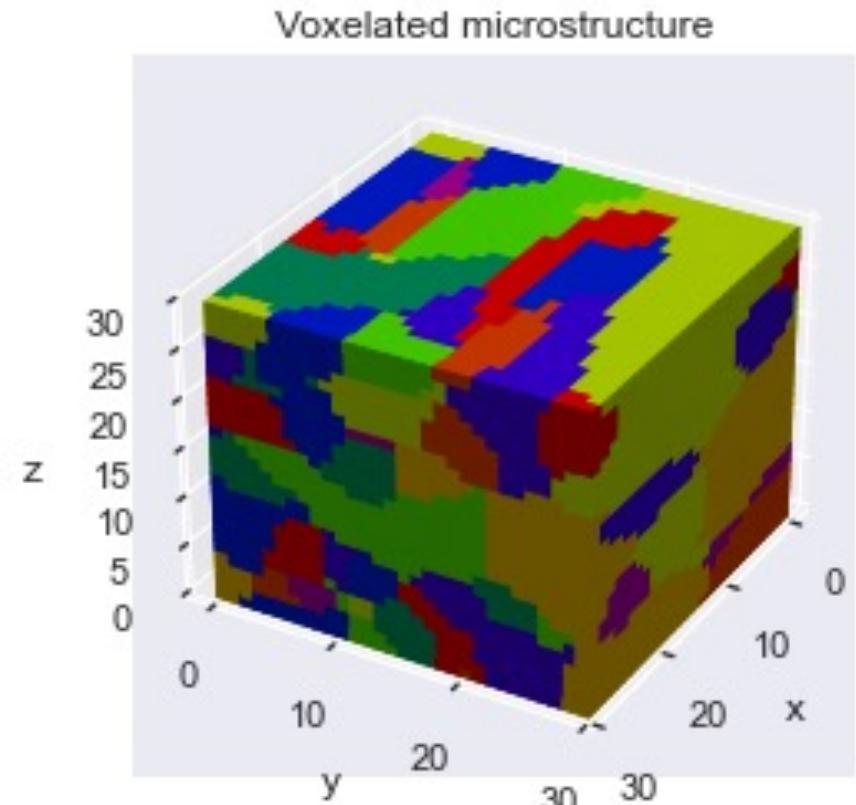
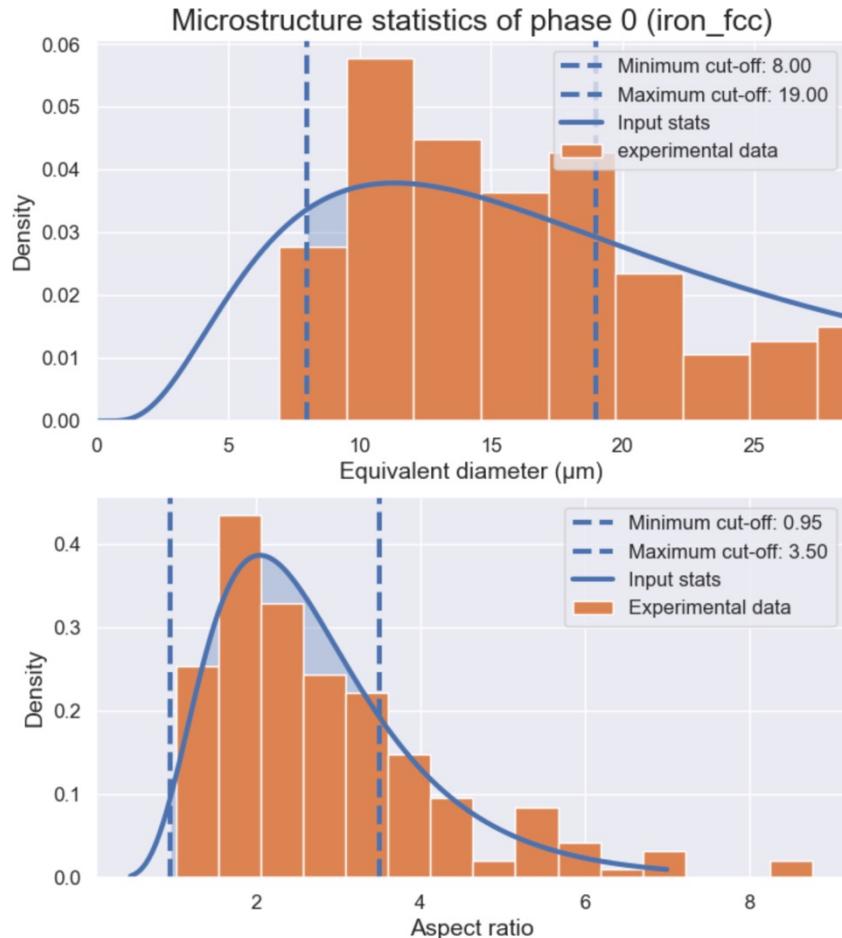


Voxelization - Hexahedral meshing

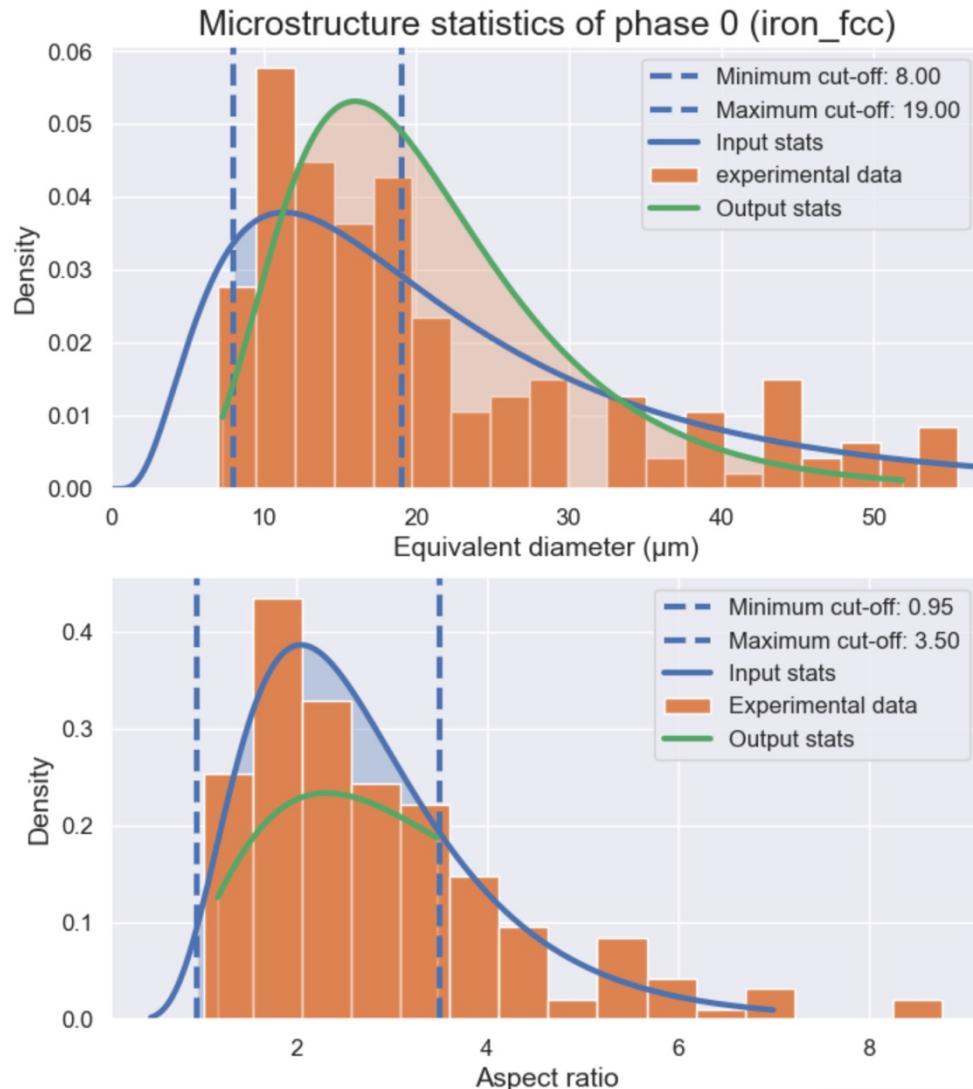


Micromechanical model

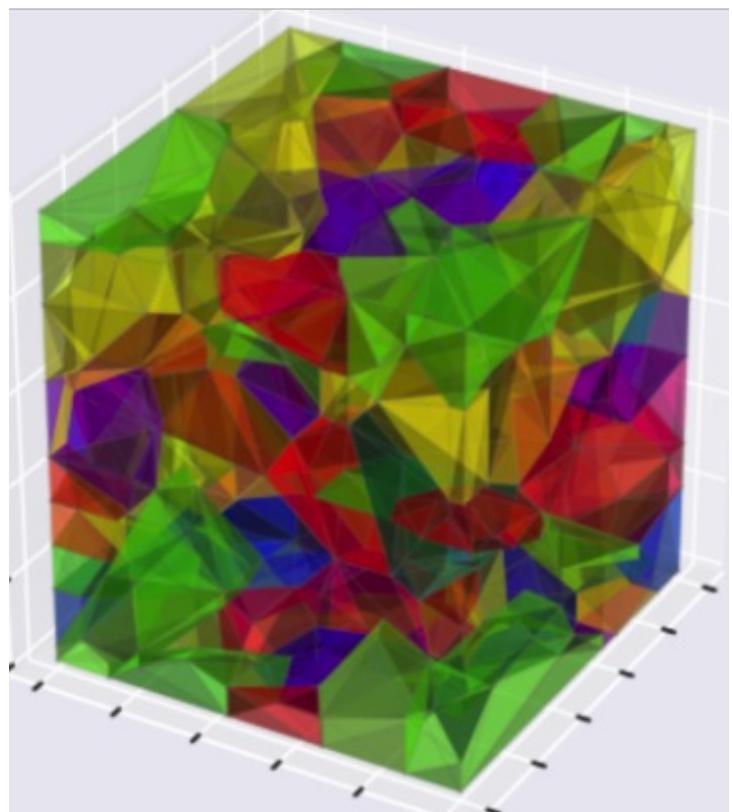
Statistically equivalent representative volume element (RVE)



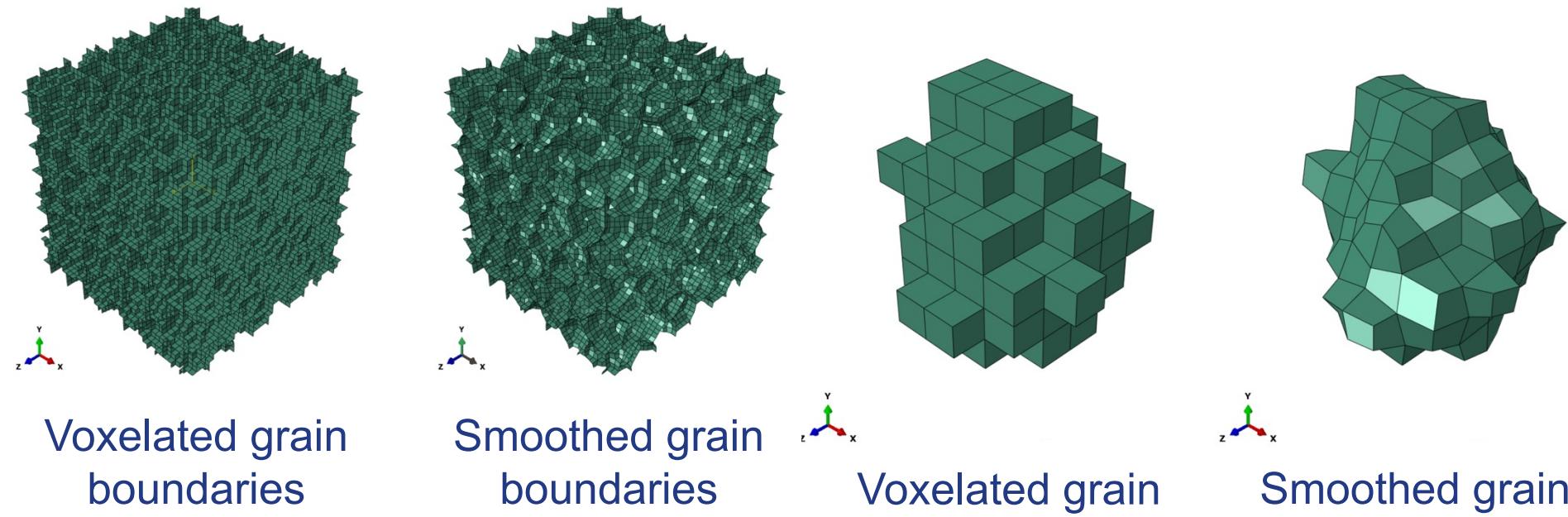
Analysis and processing of RVE



Statistics of RVE and polyhedral grains



Kanapy: Smoothing of grain boundaries



Source: <https://github.com/ICAMS/Kanapy>

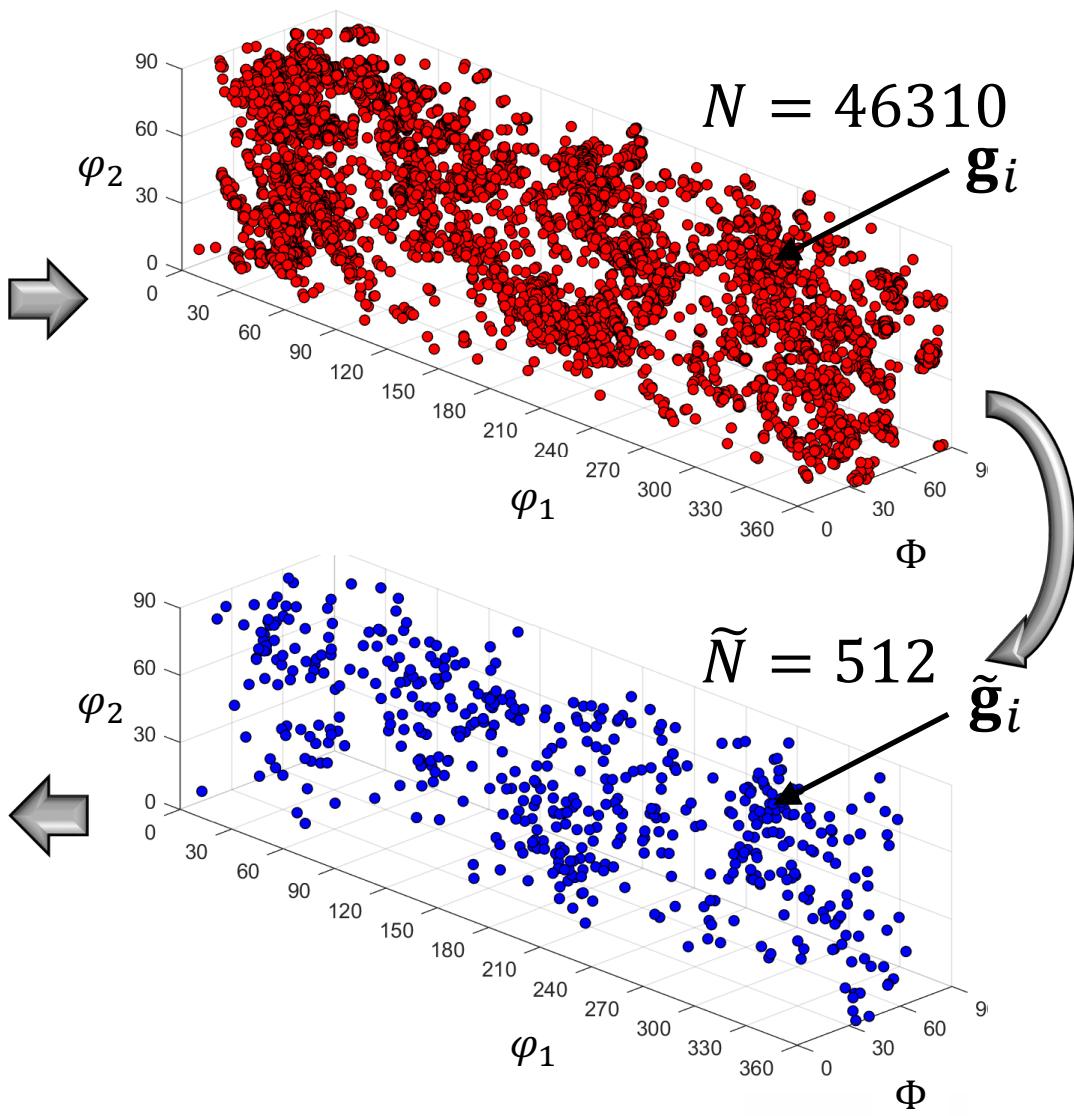
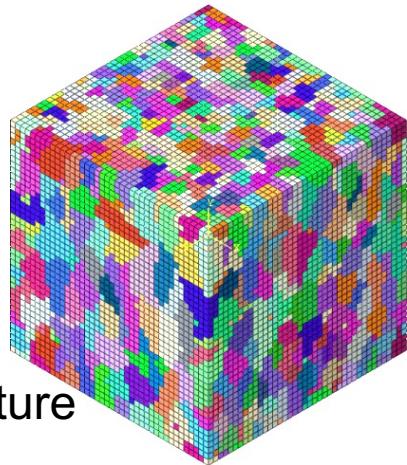


Orientation distribution reconstruction



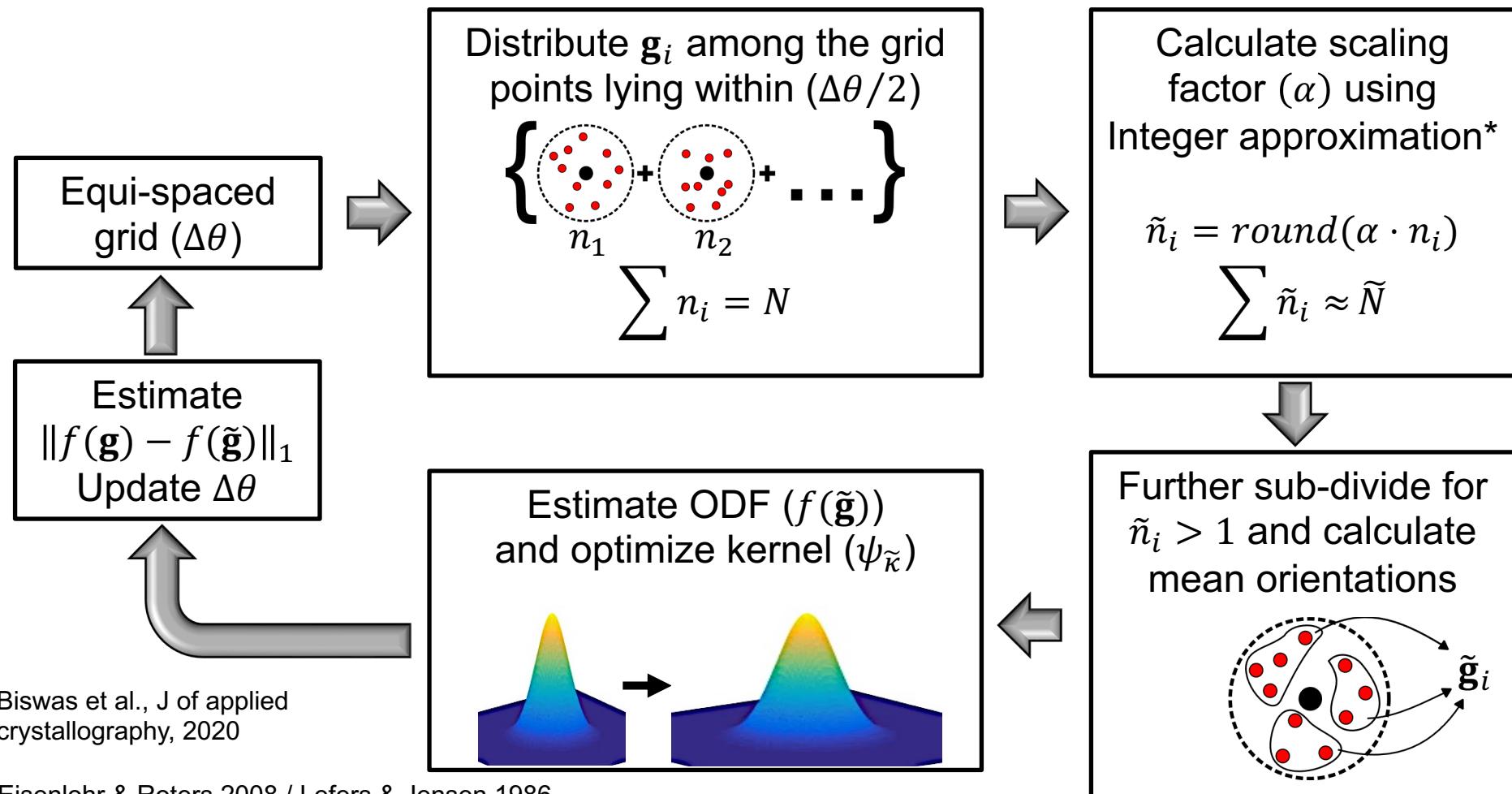
EBSD

Virtual
microstructure

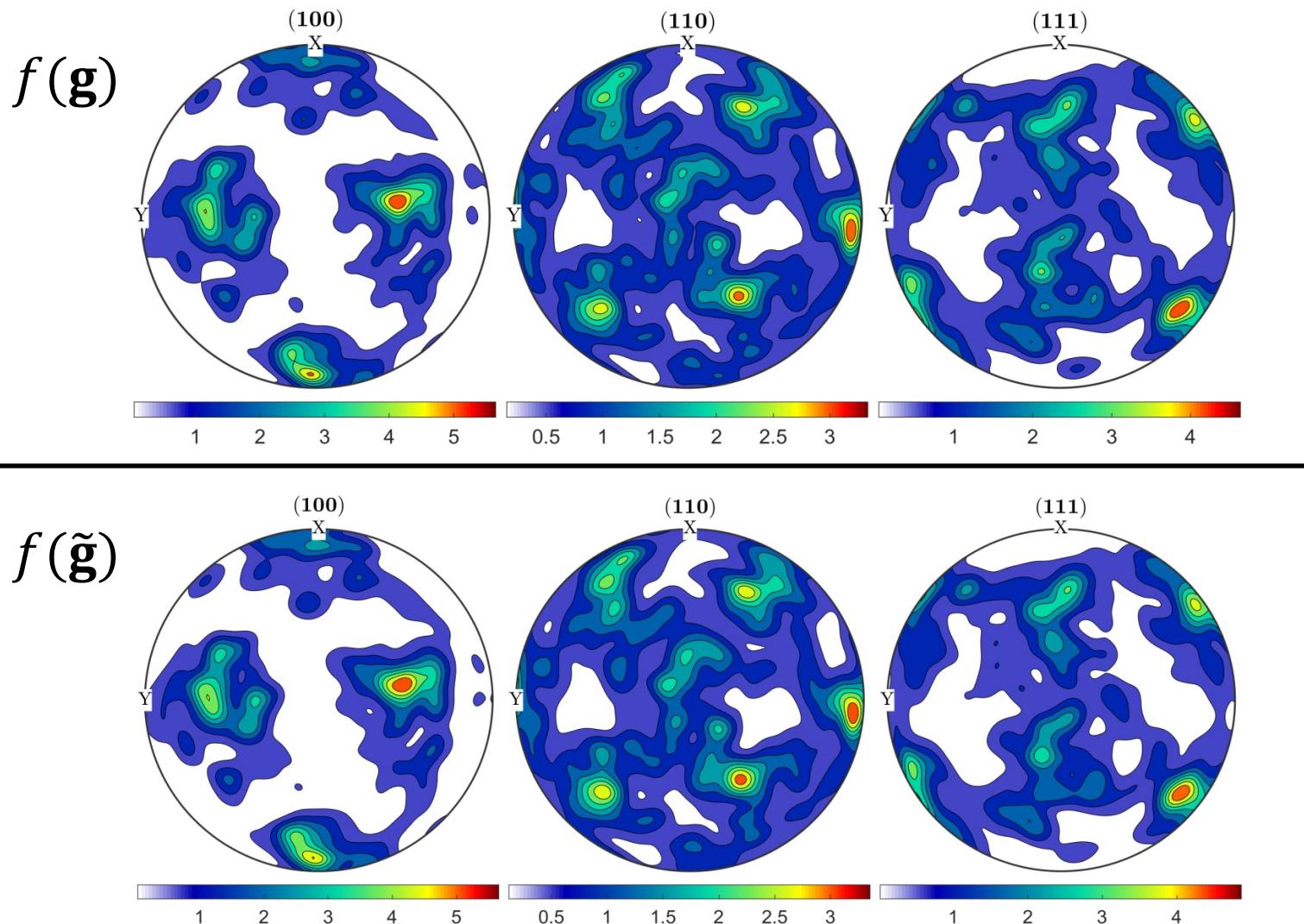


Orientation distribution reconstruction

L_1 Minimization scheme: $\min_{\Delta\theta, \psi_{\tilde{\kappa}}} \|f(\mathbf{g}) - f(\tilde{\mathbf{g}})\|_1$

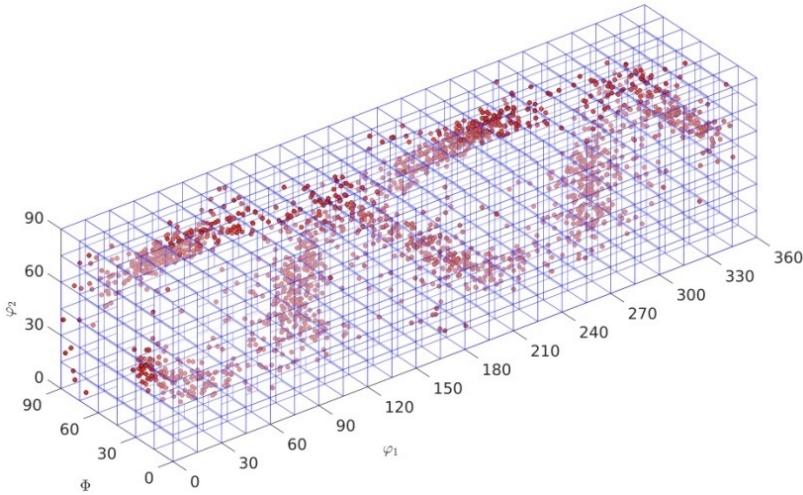


Orientation distribution reconstruction

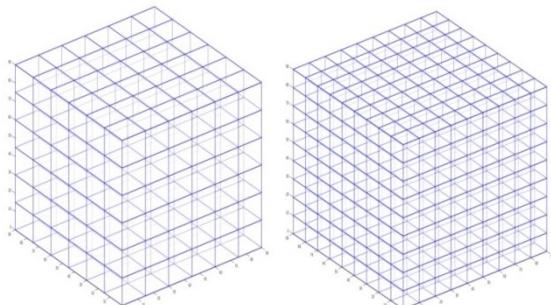


Kanapy: Synthetic microstructure generator

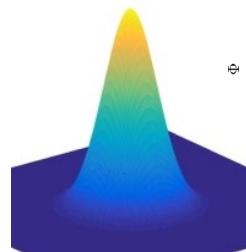
Kanapy ODF reconstruction module



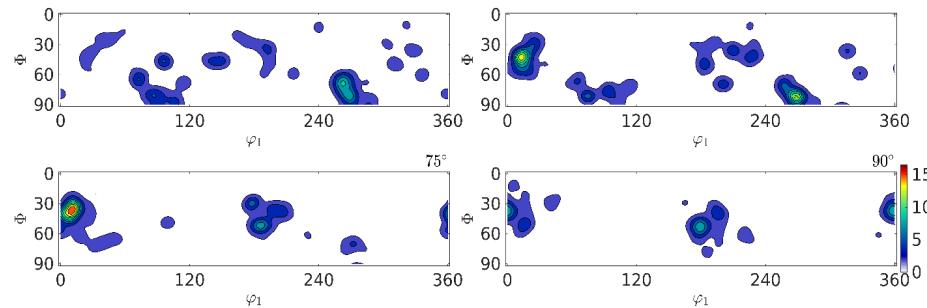
Integer Approximation (IA)



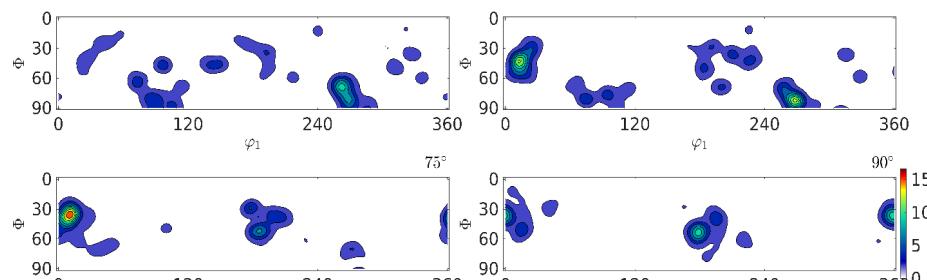
Grid spacing $\Delta\theta$ optimization



Kernel optimization



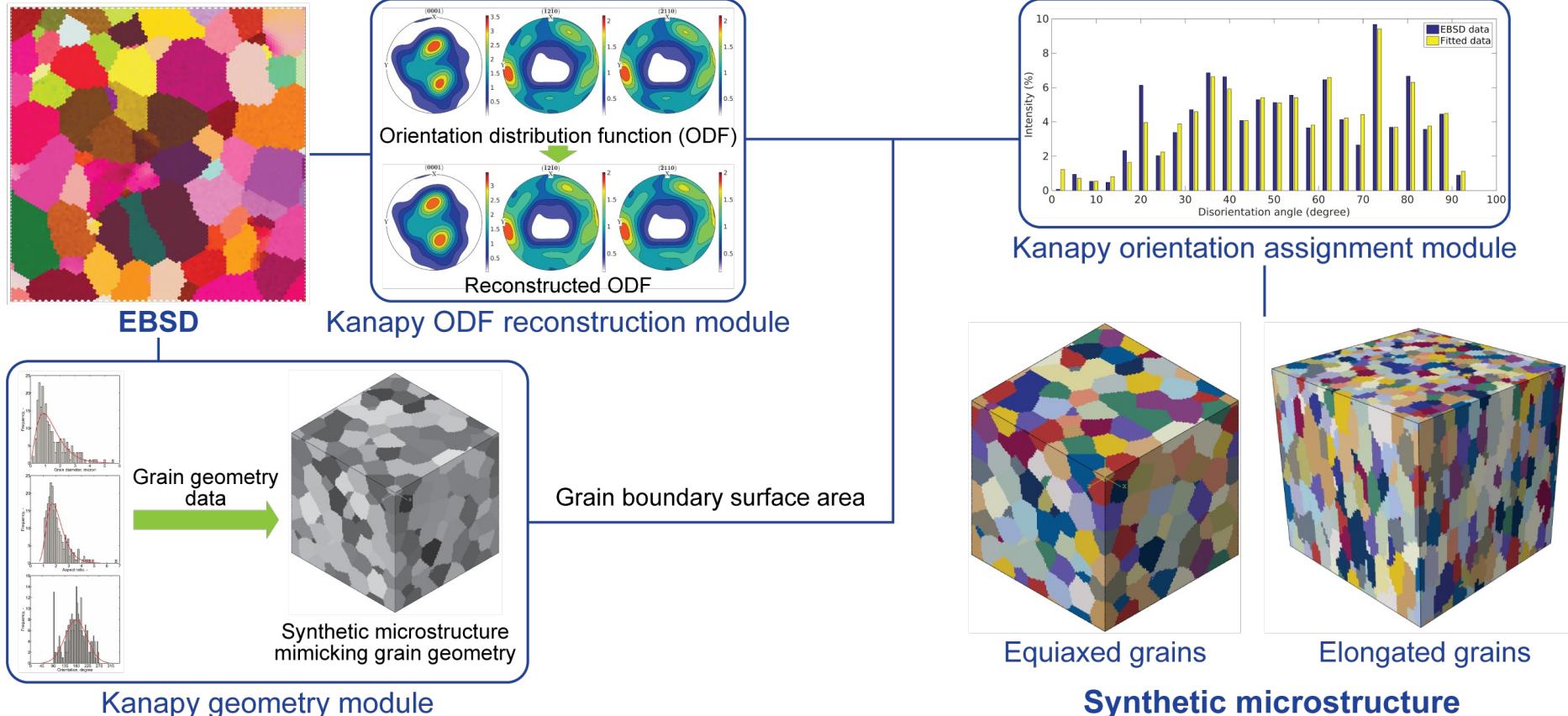
Experimental ODF



Discretized ODF



Kanapy: Synthetic microstructure generator

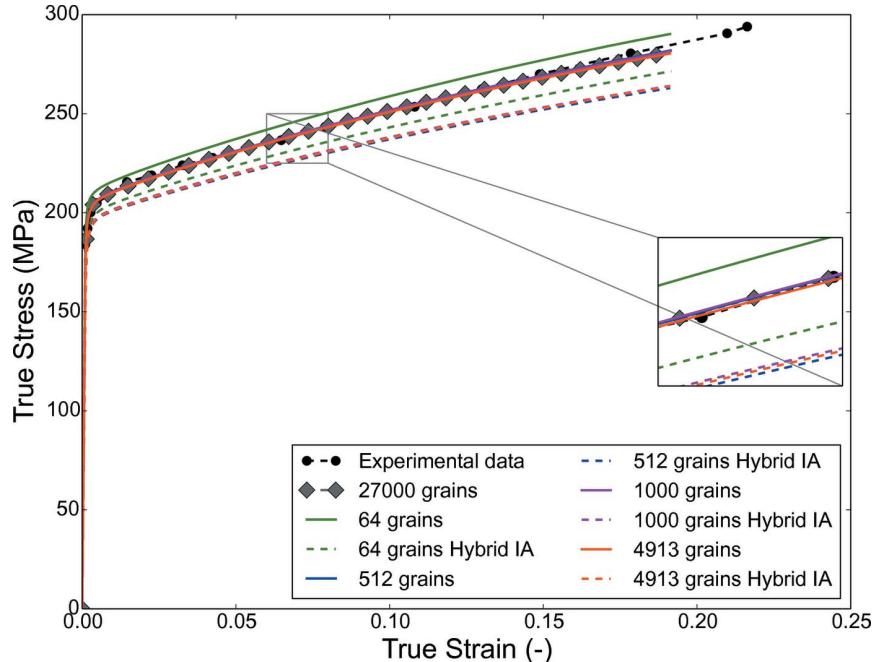


Source: <https://github.com/ICAMS/Kanapy>

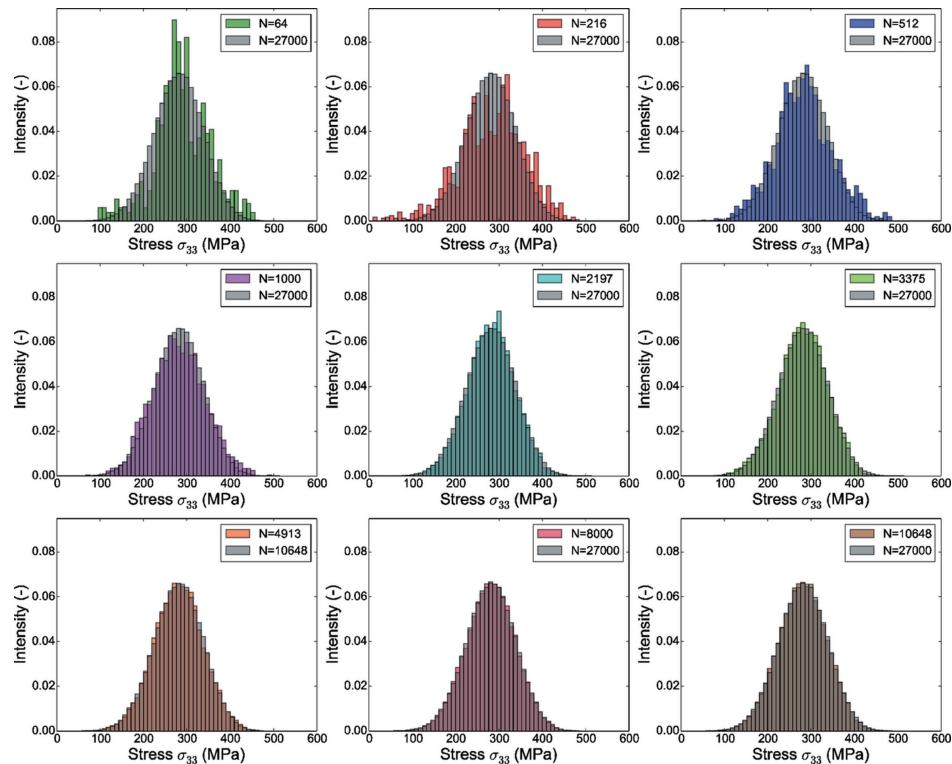


Kanapy: Synthetic microstructure generator

Kanapy ODF reconstruction module



Flow curves comparison

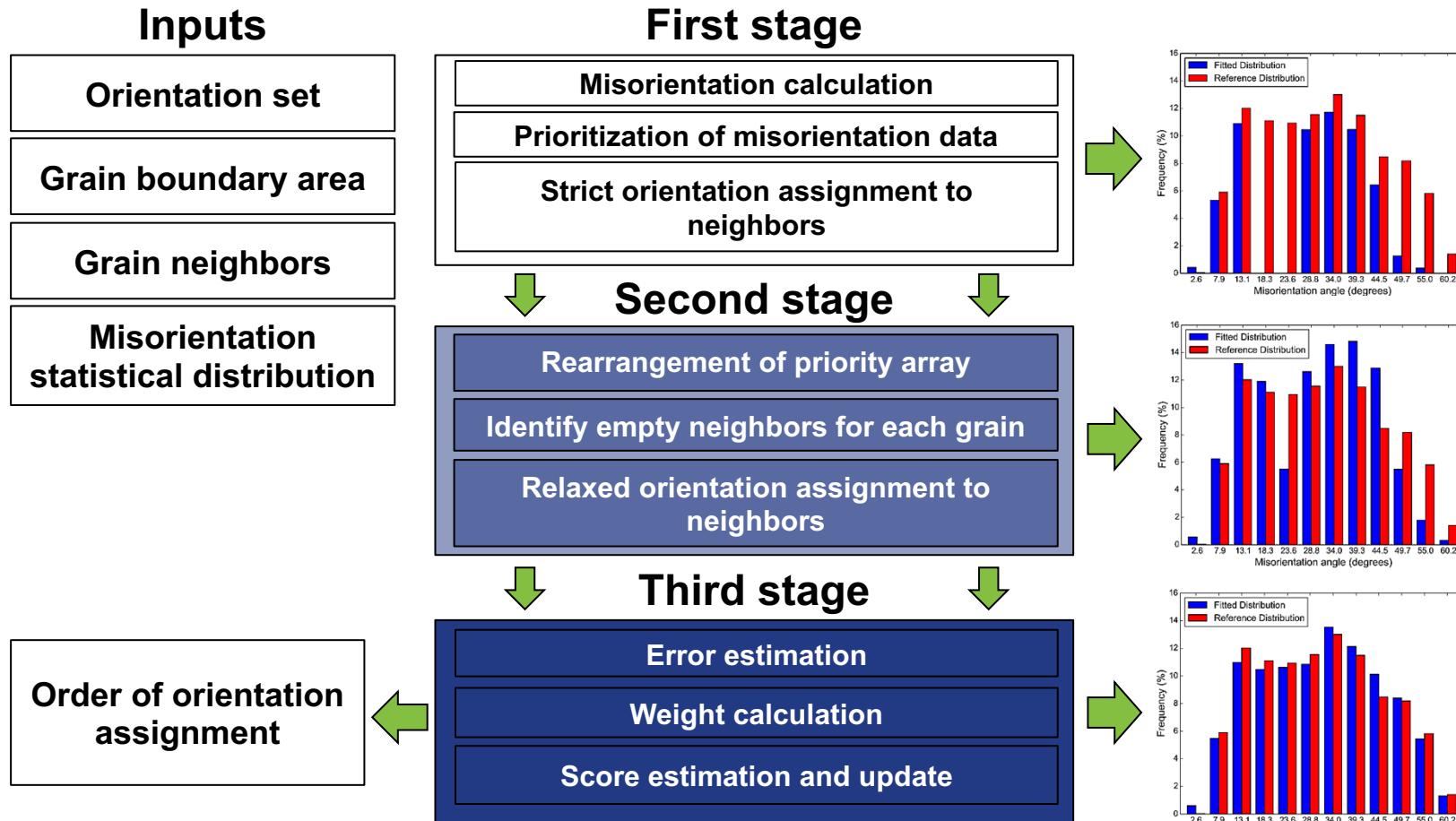


Stress distribution comparison



Kanapy: Synthetic microstructure generator

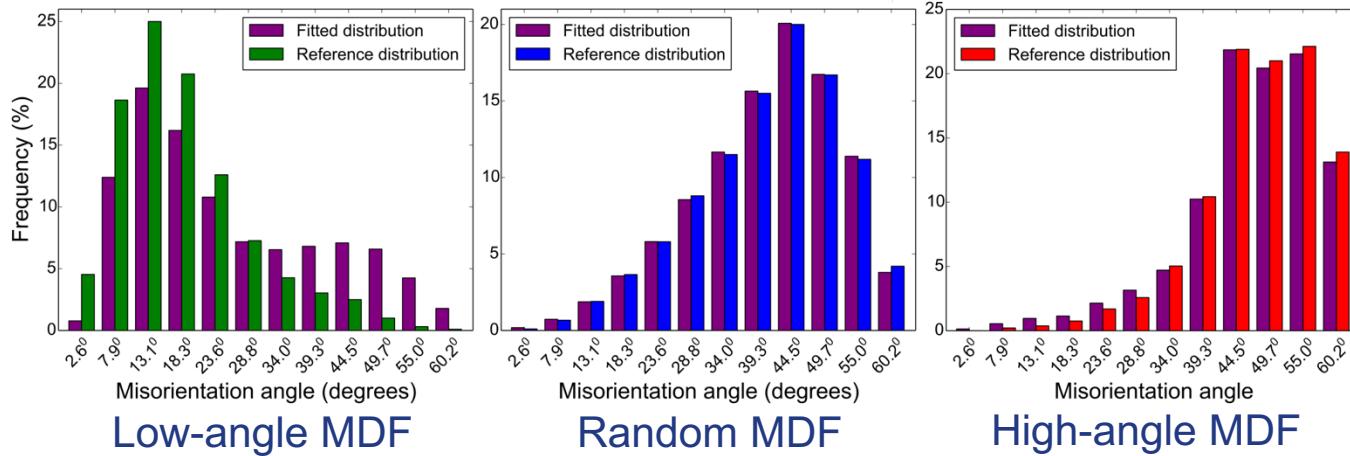
Kanapy orientations assignment module



A. Biswas et al. Adv. Eng. Mater. 2019



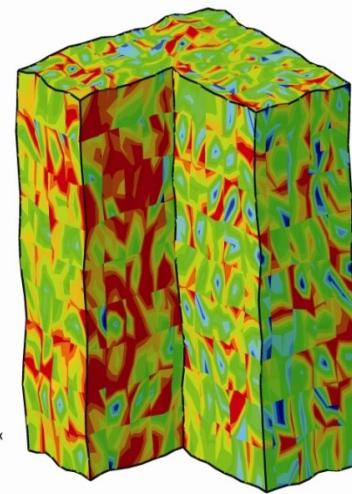
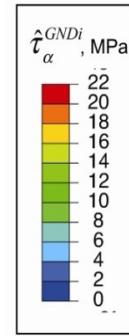
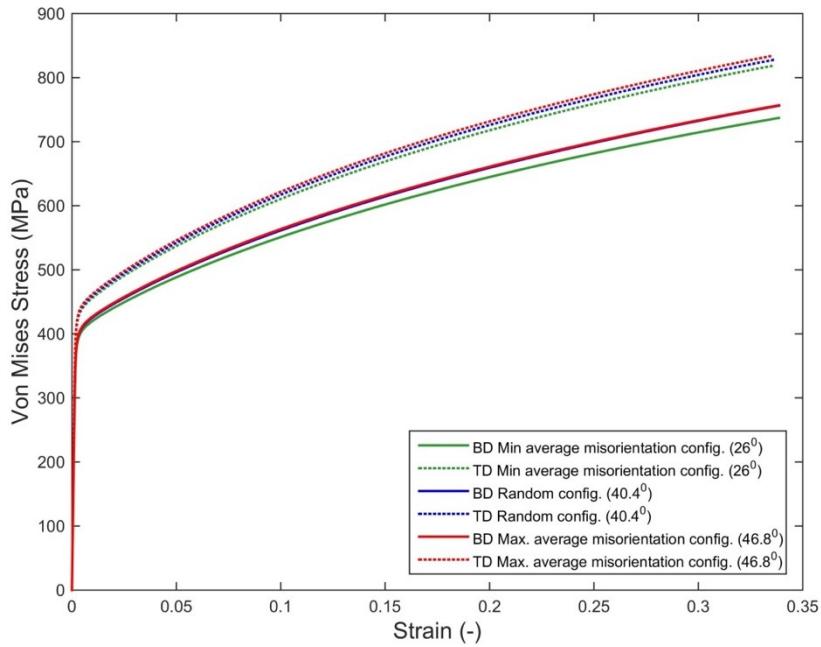
Influence of misorientation distribution (MDF)



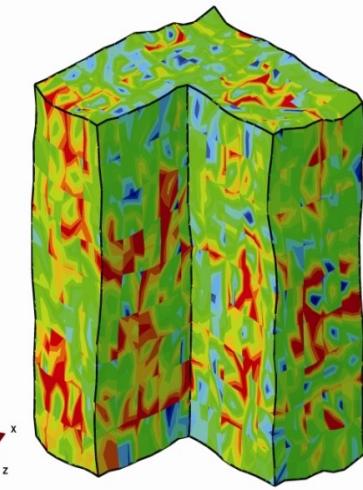
Low-angle MDF

Random MDF

High-angle MDF



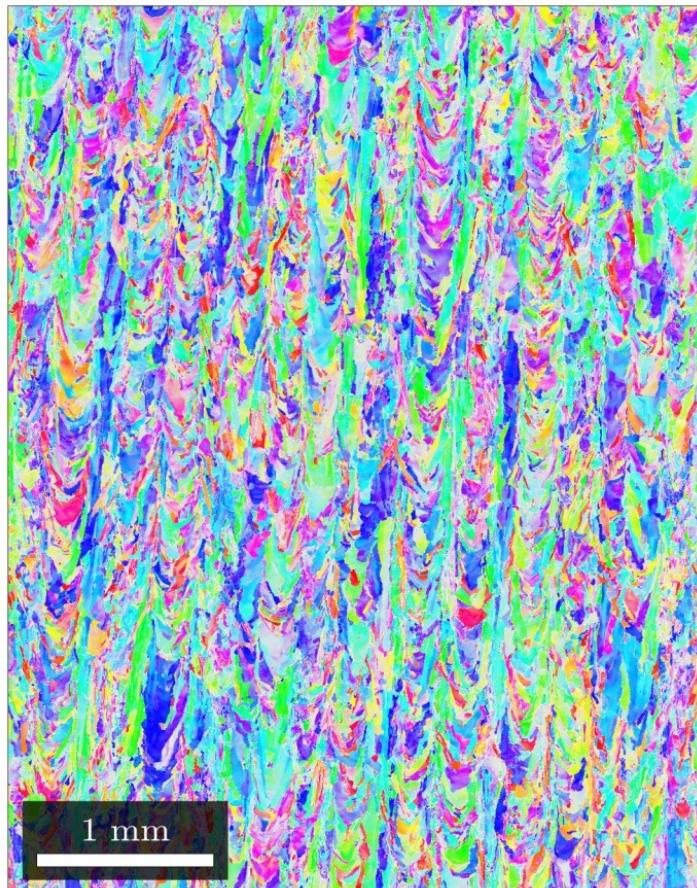
High-angle MDF



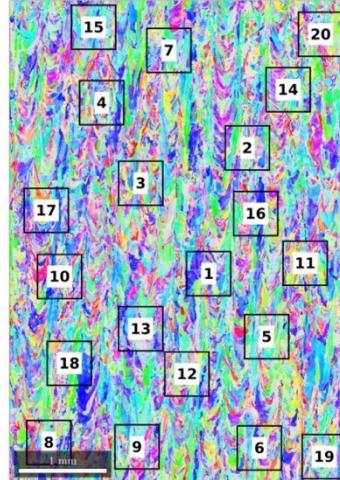
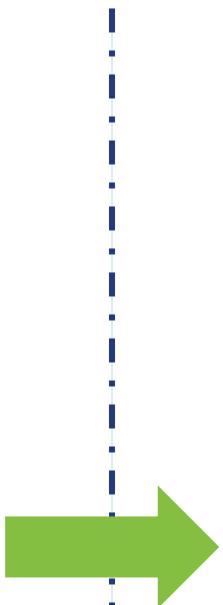
Low-angle MDF



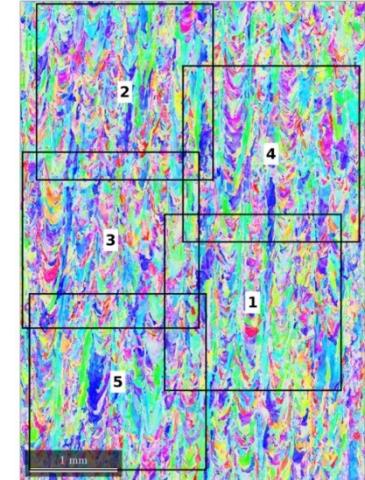
Effect of grain statistics on micromechanical modeling



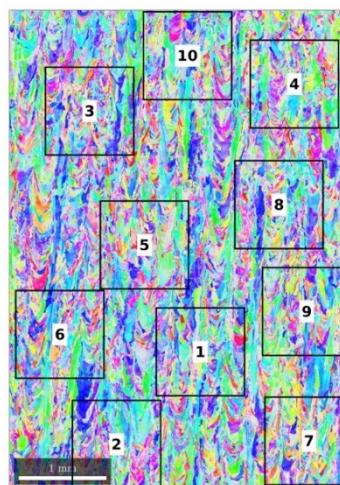
$4 \times 5 \text{ mm}^2$ EBSD



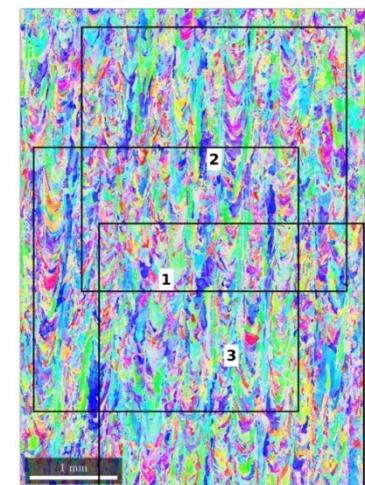
$0.5 \times 0.5 \text{ mm}^2$



$2 \times 2 \text{ mm}^2$



$1 \times 1 \text{ mm}^2$

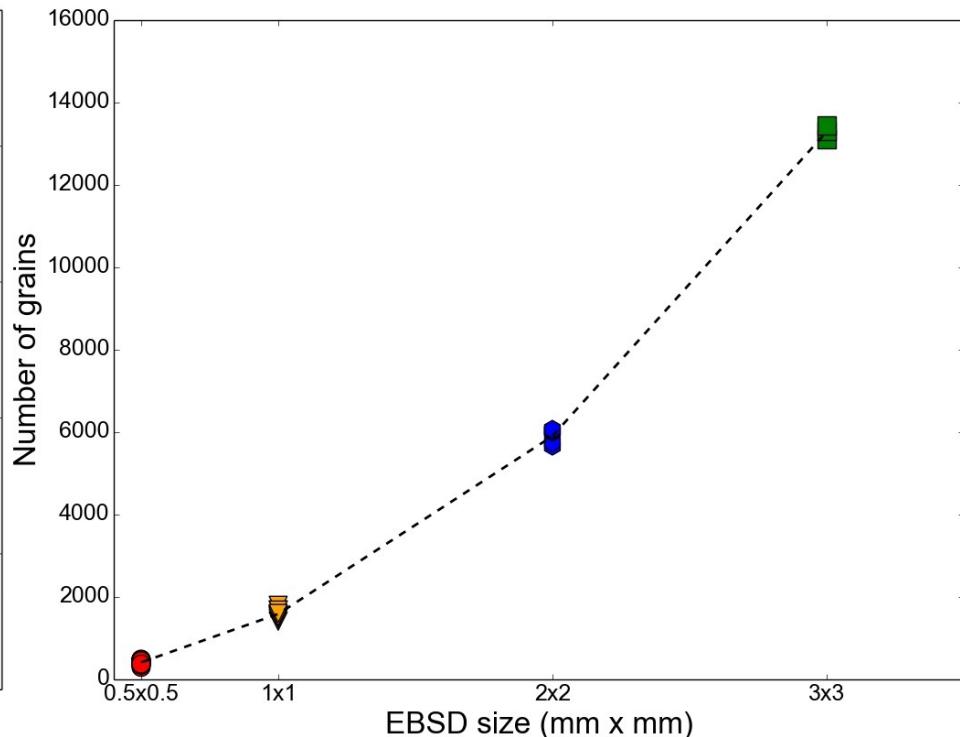
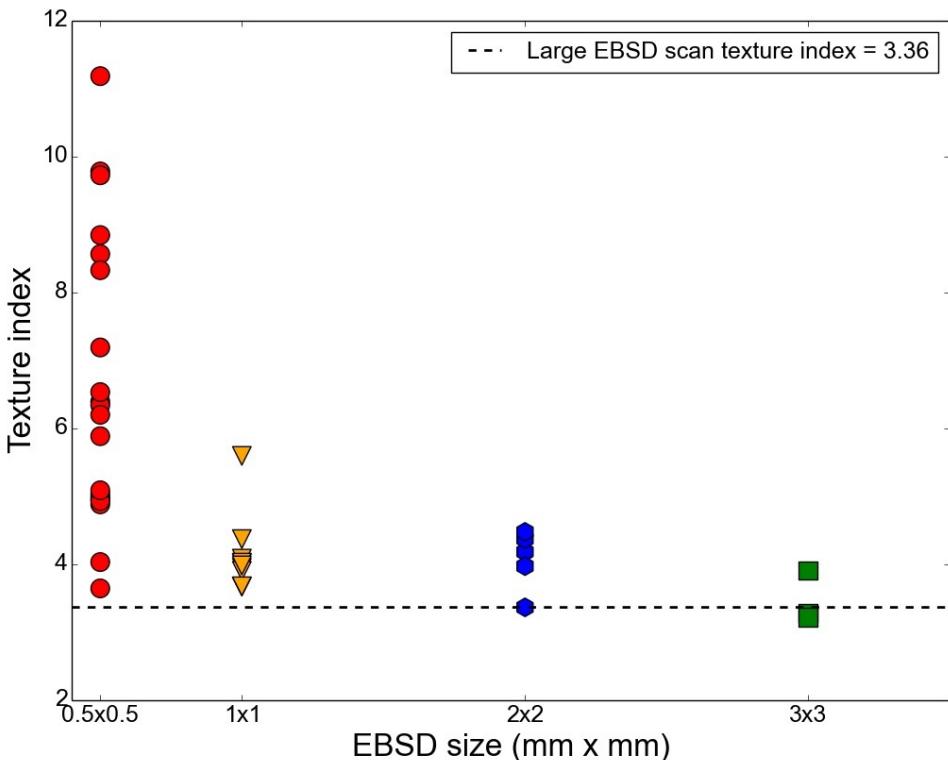


$3 \times 3 \text{ mm}^2$



Source: Biswas et al., Adv. Eng. Mater. 2020

Effect of grain statistics on micromechanical modeling



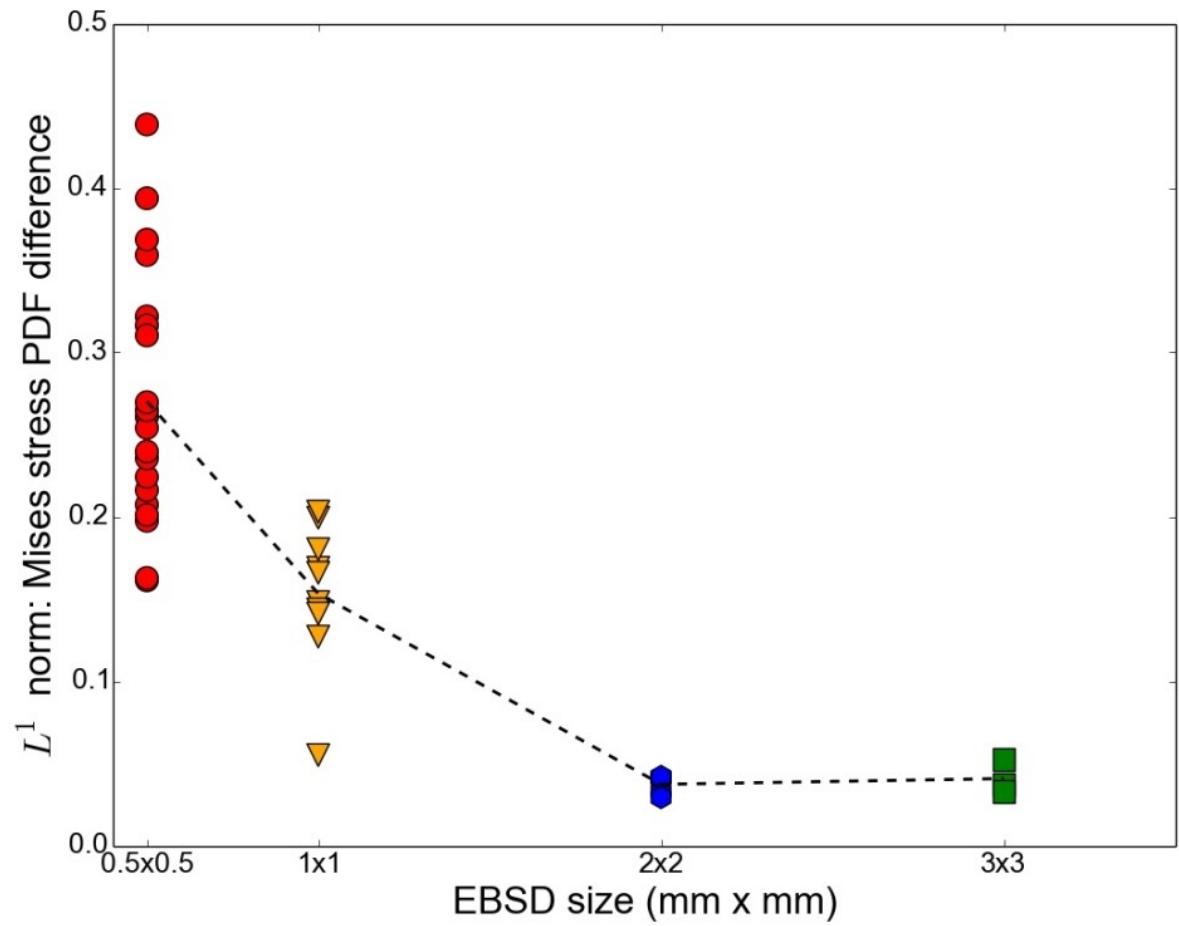
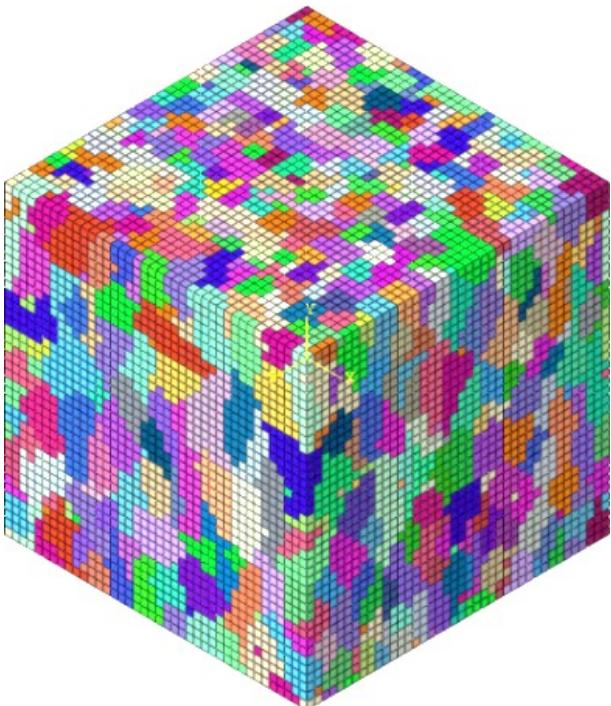
\bar{f} : ODF estimated from cropped EBSD

f : ODF estimated from large EBSD scan



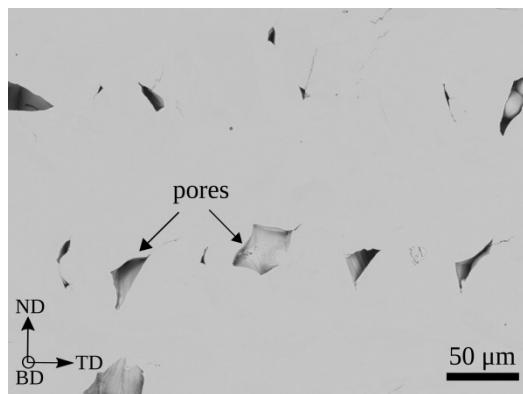
Source: Biswas et al., Adv. Eng. Mater. 2020

Effect of grain statistics on micromechanical modeling

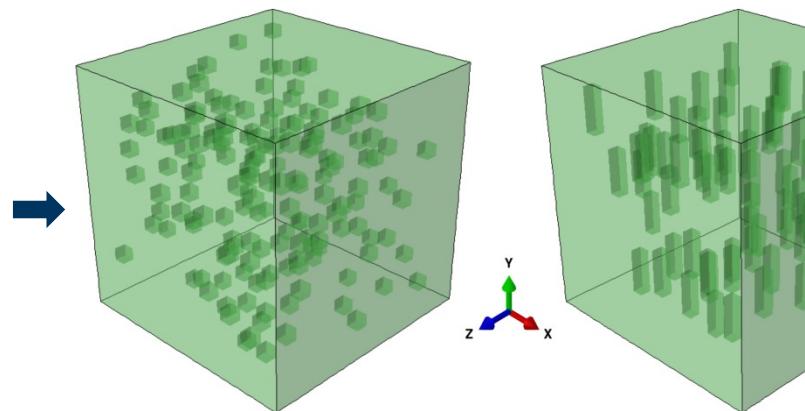


Source: Biswas et al., Adv. Eng. Mater. 2020

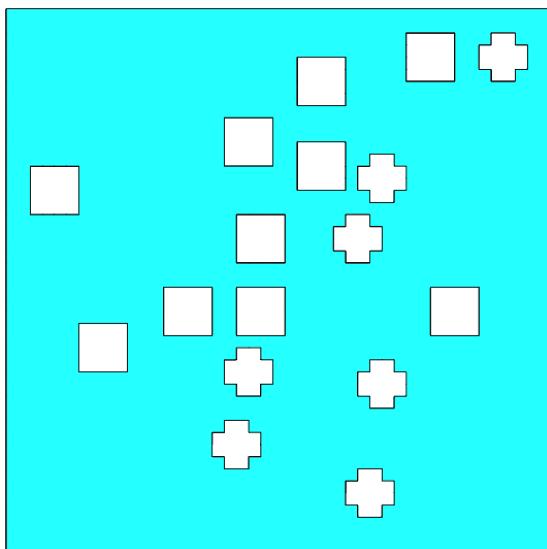
Micromechanical modeling – Modeling pores and Damage



Pores

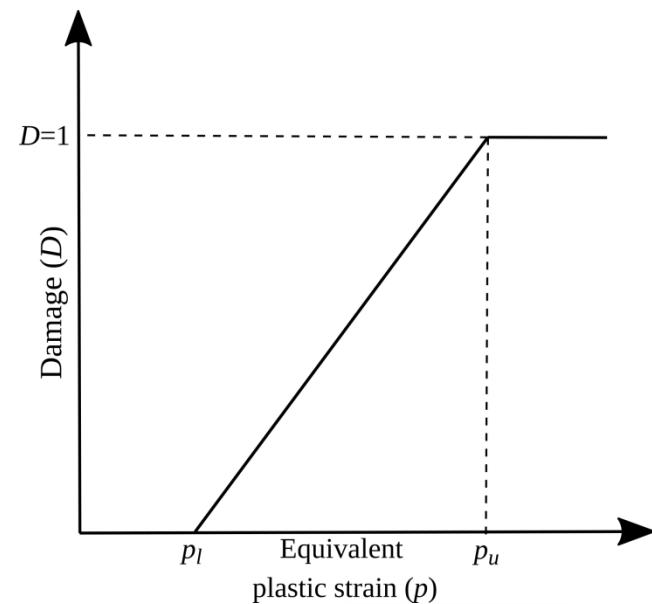


RVEs containing equiaxed and elongated pores



$$D = \frac{p - p_l}{p_u - p_l}$$

$$\dot{p} = \sqrt{\frac{2}{3}} \|\dot{E}_p\|$$



Micromechanical modeling – Nonlocal CP model

Flow rule

$$\dot{\gamma}_\alpha = \dot{\gamma}_0 \left| \frac{\tau_\alpha + \tau_\alpha^{GNDk}}{\hat{\tau}_\alpha + \hat{\tau}_\alpha^{GNDi}} \right|^{p_1} sgn(\tau_\alpha + \tau_\alpha^{GNDk})$$

Resolved shear stress

$$\tau_\alpha = \tilde{\mathbf{S}}_\alpha : \mathbf{M}_\alpha$$

Slip resistance

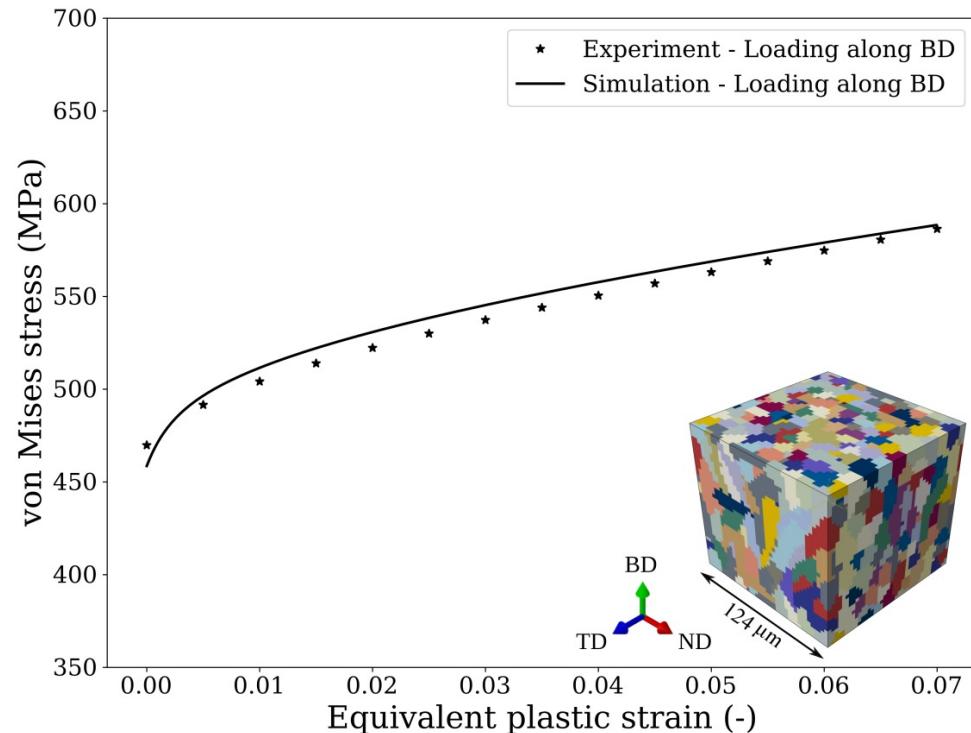
$$\dot{\tau}_\alpha = \sum_{\beta=1}^N h_0 \chi_{\alpha\beta} \left(1 - \frac{\hat{\tau}_\alpha}{\hat{\tau}_{sat}}\right)^{p_2} |\dot{\gamma}_\beta|$$

Kinematic hardening

$$\tau_\alpha^{GNDk} = \tilde{\mathbf{S}}^{GND} : \mathbf{M}_\alpha$$

Isotropic hardening

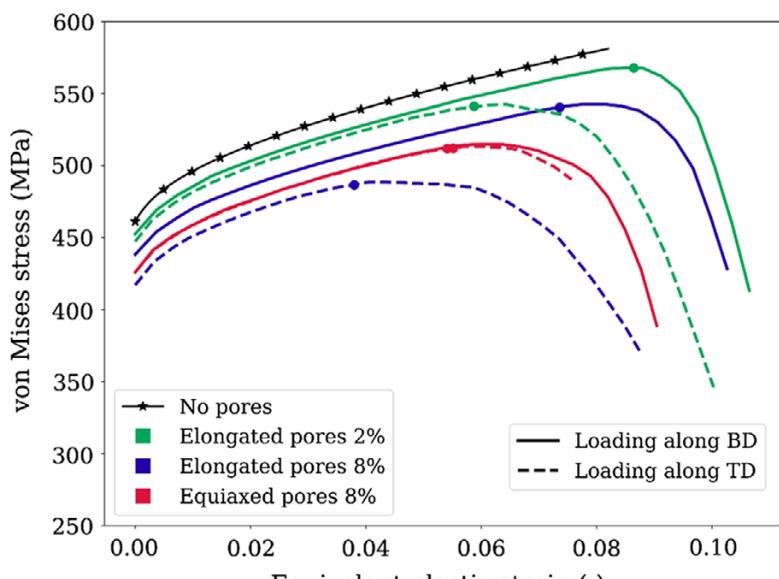
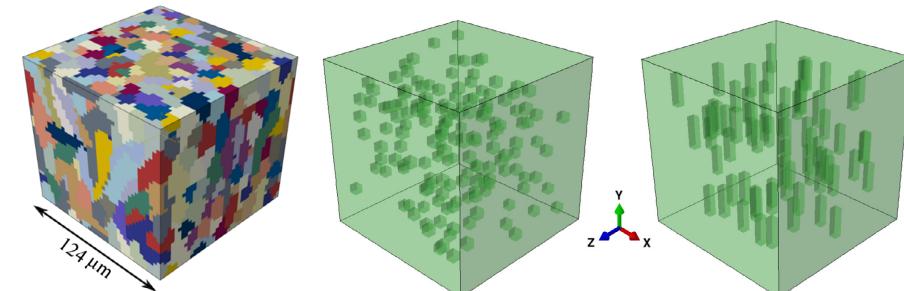
$$\hat{\tau}_\alpha^{GNDi} = c_1 \mu b \sqrt{\sum_{\beta=1}^9 \chi_{\alpha\beta}^{GND} |\bar{\rho}_\beta|}$$



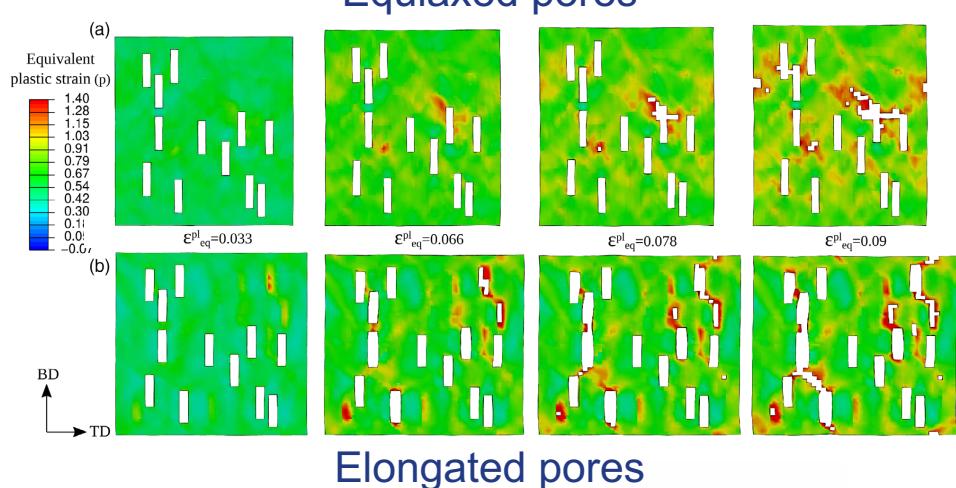
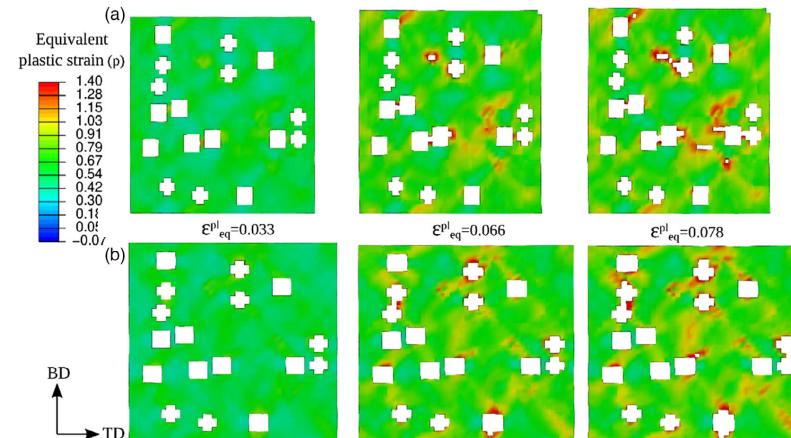
Ma & Hartmaier.
Phil Mag (2014)

Parameter	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	$\hat{\tau}_0$ (MPa)	$\hat{\tau}_{sat}$ (MPa)	p_1	p_2	h_0 (MPa)	c_1
Value	247	106	71	147	250	20	2.25	160	0.03

Influence of pore shape on anisotropy



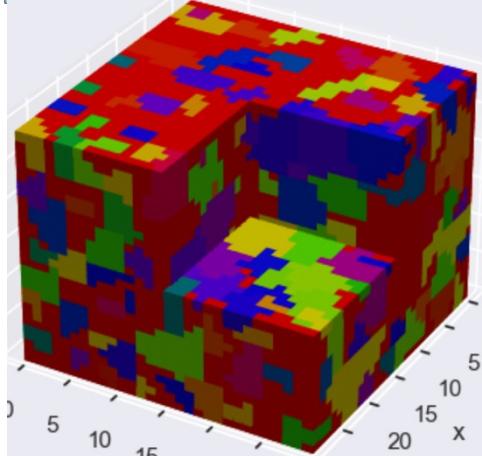
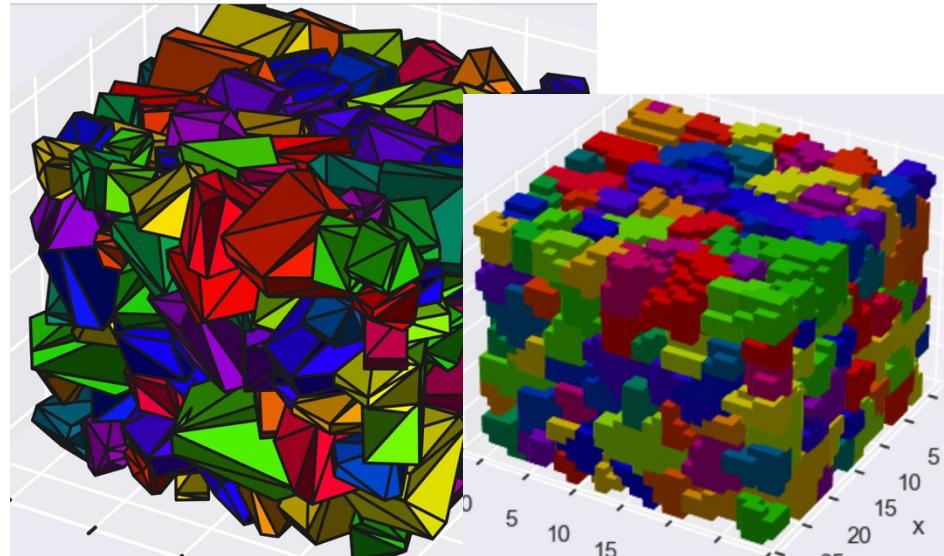
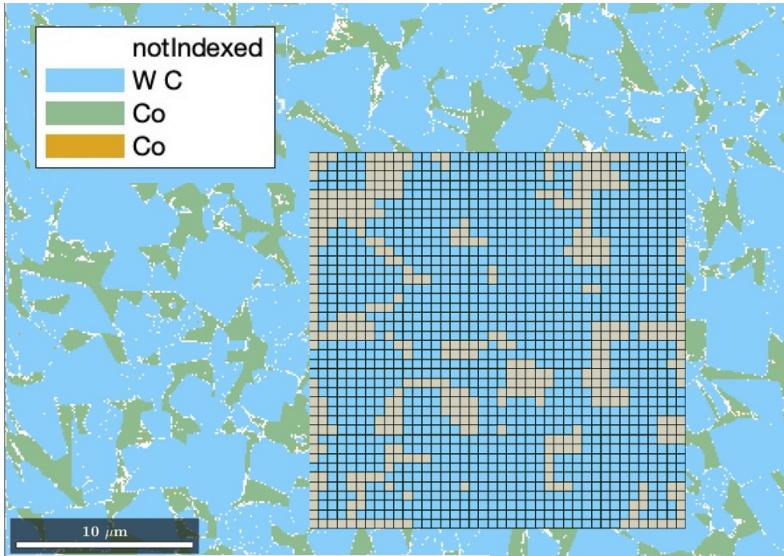
Flow curves



Source: Prasad et al., Adv. Eng. Mater. 2020

Dual phase microstructures

Application of Kanapy workflow to cemented carbide



Automated detection of volume fractions and shape statistics of phases (WC particles in Co matrix).

Capped triangles are inscribed into ellipsoidal particles.

Summary

- Kanapy: Open-source python tool for automated microstructure analysis and generation of 3D representative volume elements (RVE)
- Based on statistical descriptors for microstructures (obtained from EBSD maps or voxelized 3D microstructures)
- Calculation of polyhedral hulls of grains or phases and output as finite element models.

