

Microstructure generation with Kanapy

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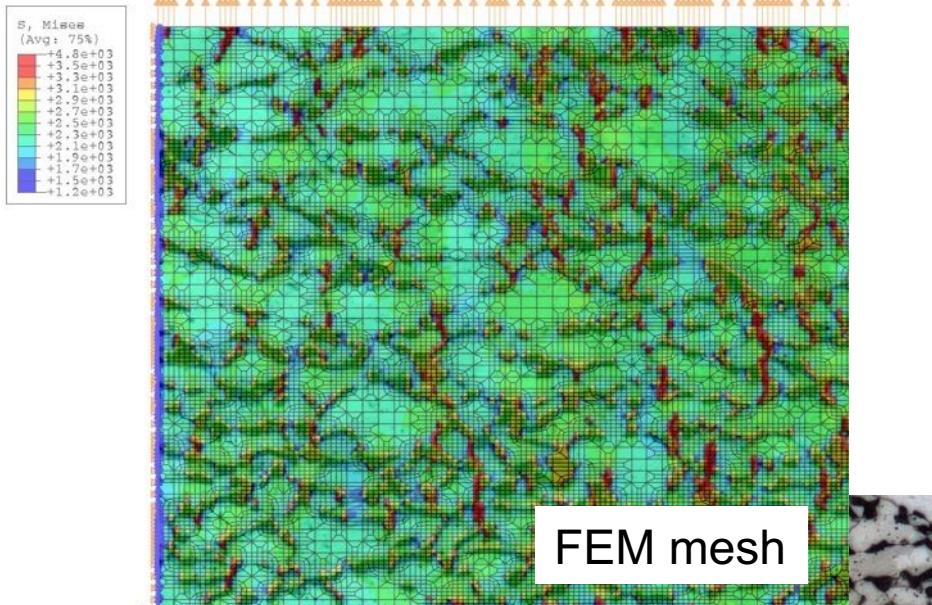
alexander.hartmaier@rub.de

Outline

- Micromechanical modeling with
 - experimental
 - simulated
 - synthetic microstructures
- Synthetic microstructures with Kanapy
- Influence of grain statistics
- Porous microstructures

- Demonstration 1: Two-phase microstructures
- Demonstration 2: Polycrystals and crystallographic texture

Micromechanical Modeling



Micromechanical modeling requires many input parameters



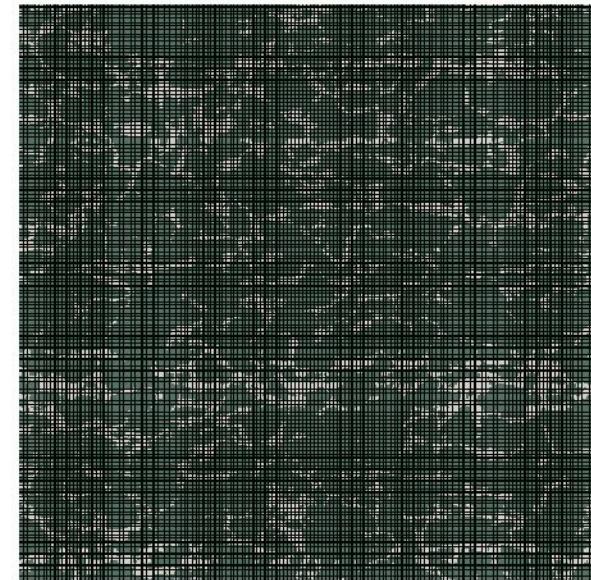
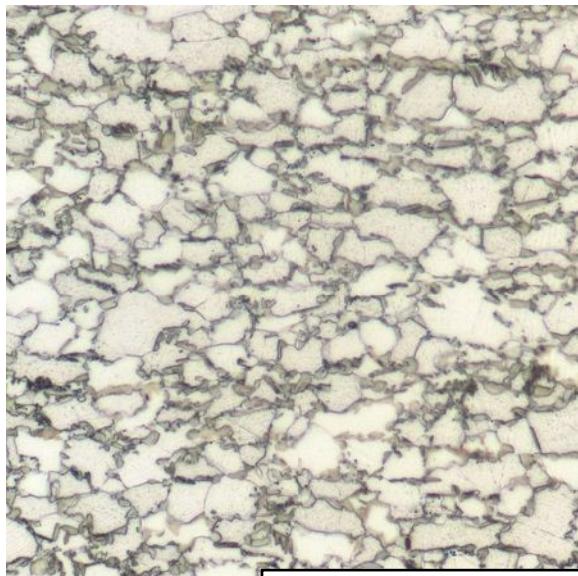
dual-phase steel

- Fully atomistic description of materials suffers from length and time scale dilemma
- Microstructure based prediction of mechanical properties of **multiphase materials**
- Consider multiphase materials as **composites**. Input is required on:
 - microstructure and microstructure evolution
 - local properties of individual phases
 - properties of interfaces
 - damage and failure initialization
 - interfacial sliding

Micromechanical Modeling

- **Representative Volume Elements** (RVE) from metallographic images
- Realistic microstructures can be considered, but
- inflexible and large effort for 3D

- Creation of **synthetic microstructures** representing statistical properties



Vajragupta et al. Comp. Mat. Sci. 54 (2012)

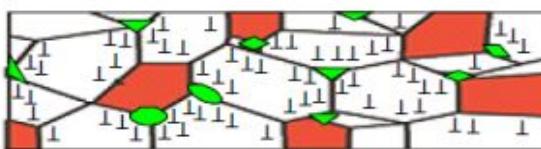
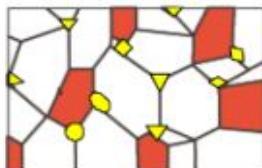
Micromechanical Modeling

Constitutive modelling

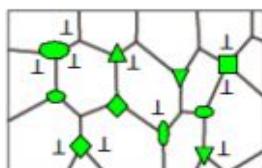
Empirical model for ferritic and martensitic phase
(Rodriguez, Mater. Sci. Forum 2003):

$$\sigma = \sigma_0 + \Delta\sigma + \alpha \cdot M \cdot \mu \cdot \sqrt{b} \cdot \sqrt{\frac{1 - \exp(-M \cdot k \cdot \varepsilon)}{k \cdot L}}$$

$$\sigma_0 = 77 + 80 \cdot (\%Mn) + 750 \cdot (\%P) + 60 \cdot (\%Si) + 80 \cdot (\%Cu) + 45 \cdot (\%Ni) \\ + 60 \cdot (\%Cr) + 11 \cdot (\%Mo) + 5000 \cdot N_{ss}$$



TRIP steel



Dual phase
steel



ferrite



pearlite / cementite



martensite

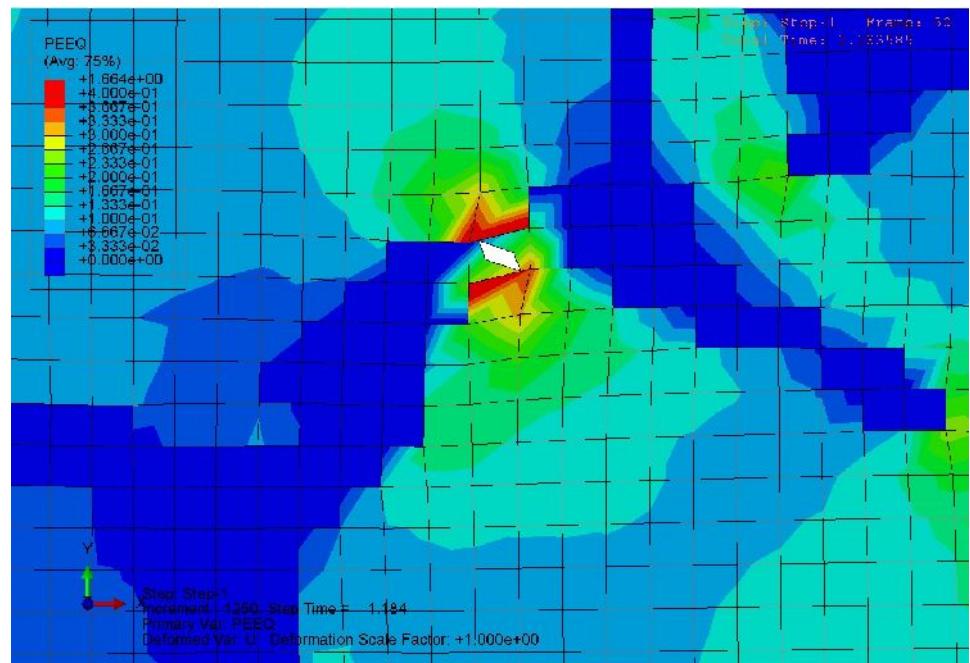
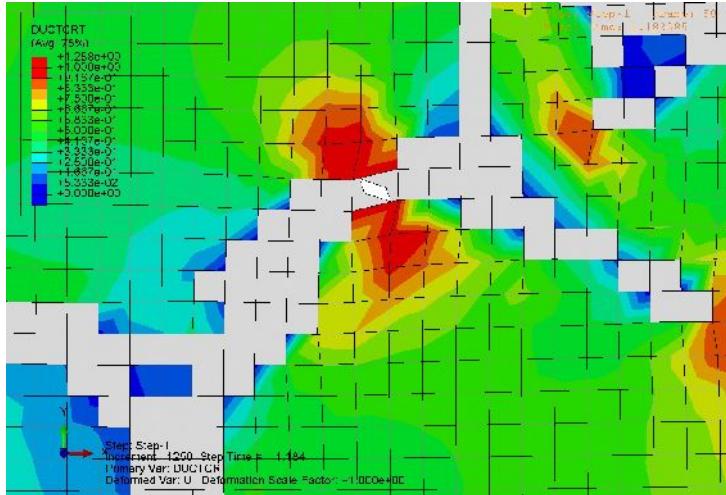


bainite



austenite

Micromechanical Modeling



Microcracks in martensite cause strain localization and failure in ferrite.

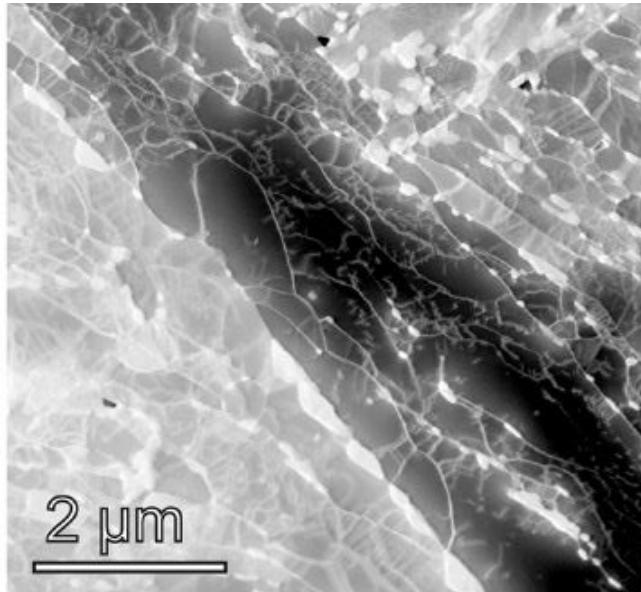


Vajragupta et al. Comp. Mat. Sci. 54 (2012)

ICAMS Demonstrator Project

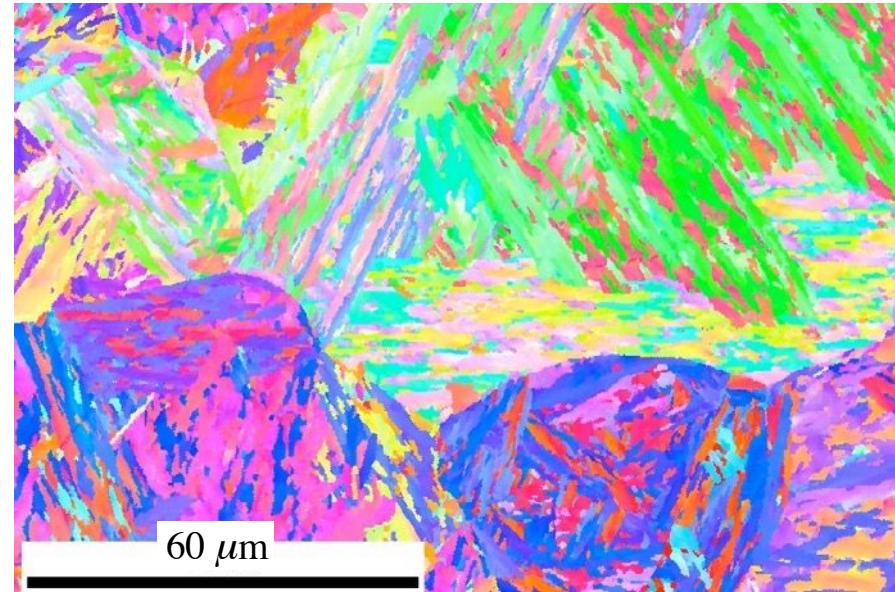
Alloy system: Fe – C (0.1/0.2/0.3 wt%) – Mn – Cr

Microstructure: tempered martensite, UTS 800 MPa – 1200 MPa



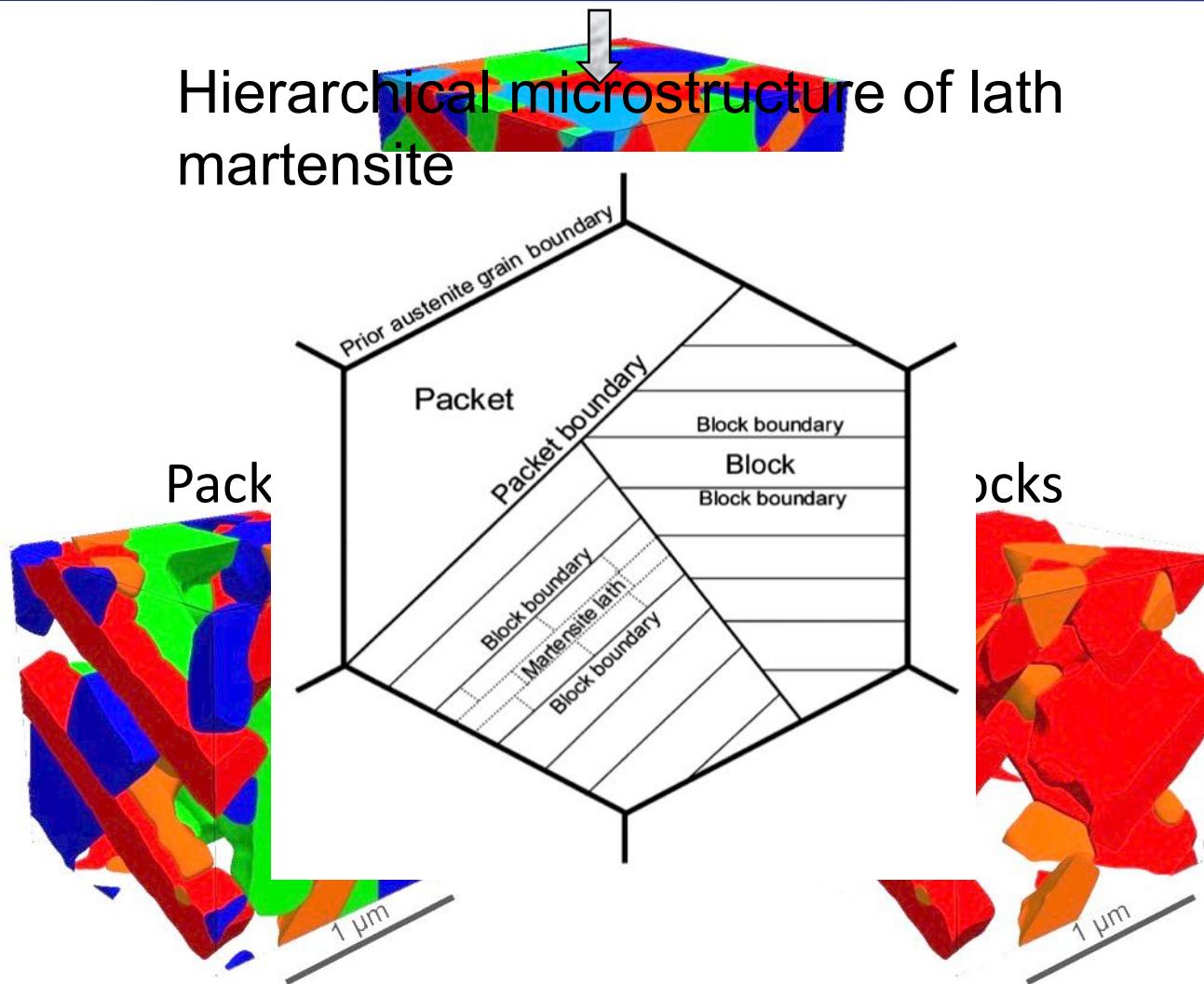
HAADF STEM micrograph
of dislocation structure after
long term ageing

Pesicka et al. Scripta Mater. 2010



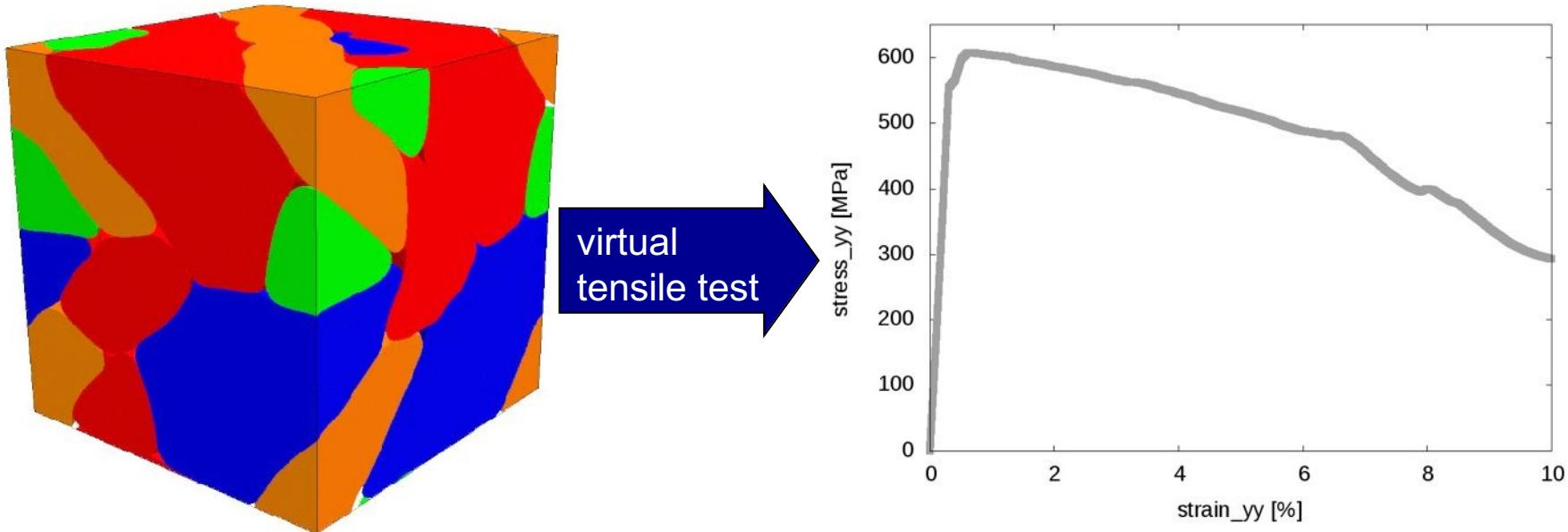
EBSD map of tempered martensite
(courtesy V. Yardley)

Simulation of martensitic microstructure



Phasefield simulations: STKS

Property prediction of simulated microstructures



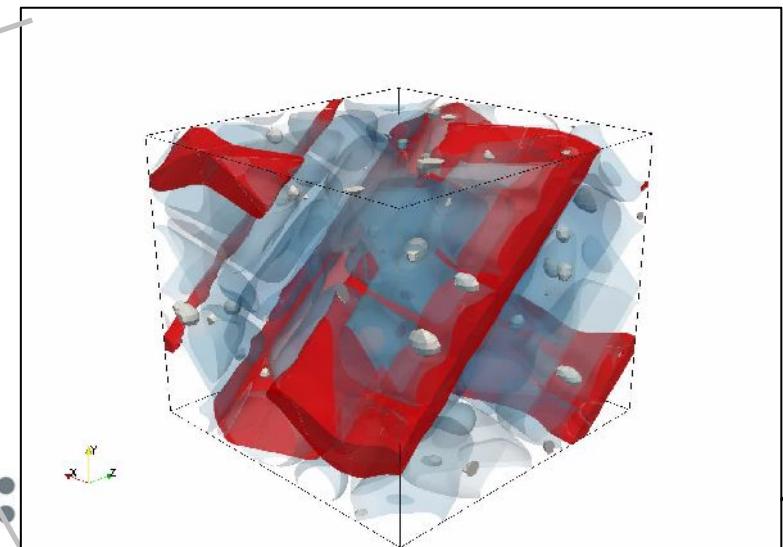
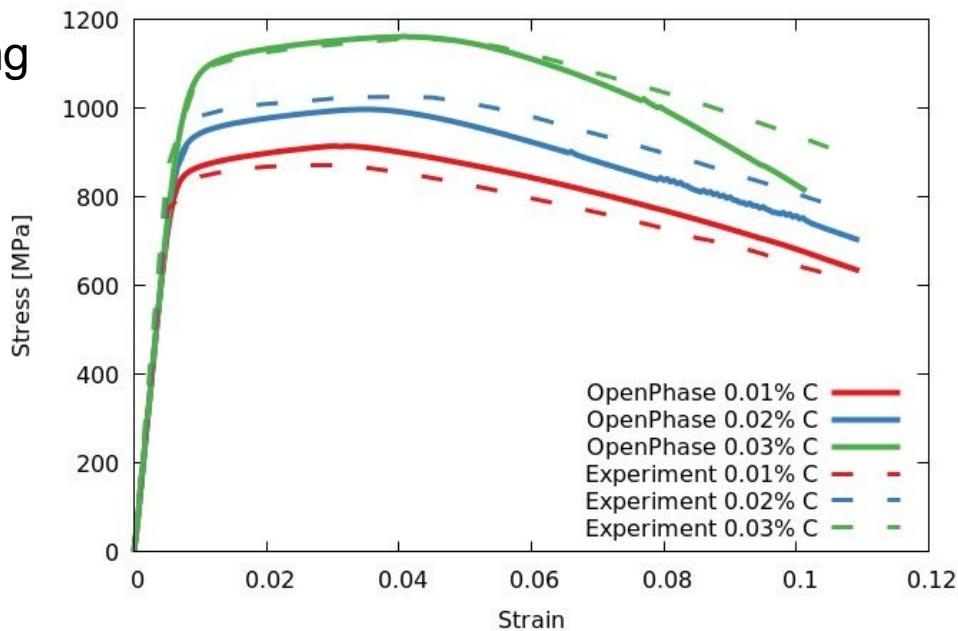
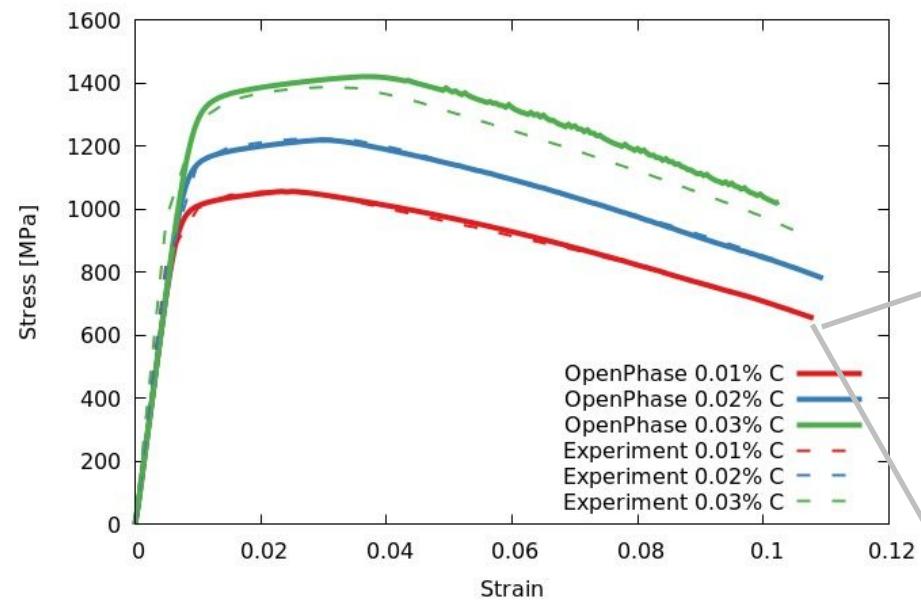
- Property prediction for microstructures from phasefield simulations
- Crystal plasticity and damage model → virtual tensile testing
- Direct modeling from processing to properties

Borukhovich, Du, Stratmann, Boeff, Shchyglo, Hartmaier, Steinbach, materials 9 (2016)

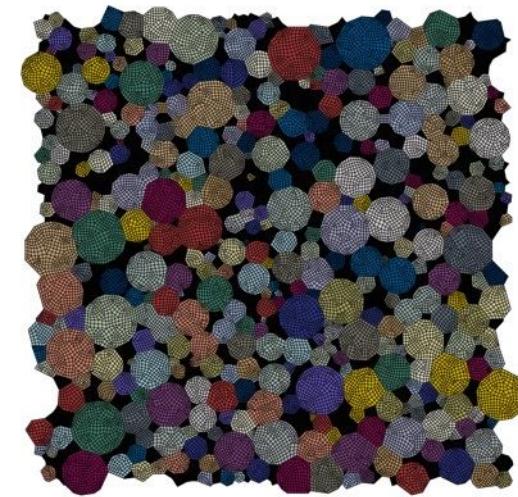
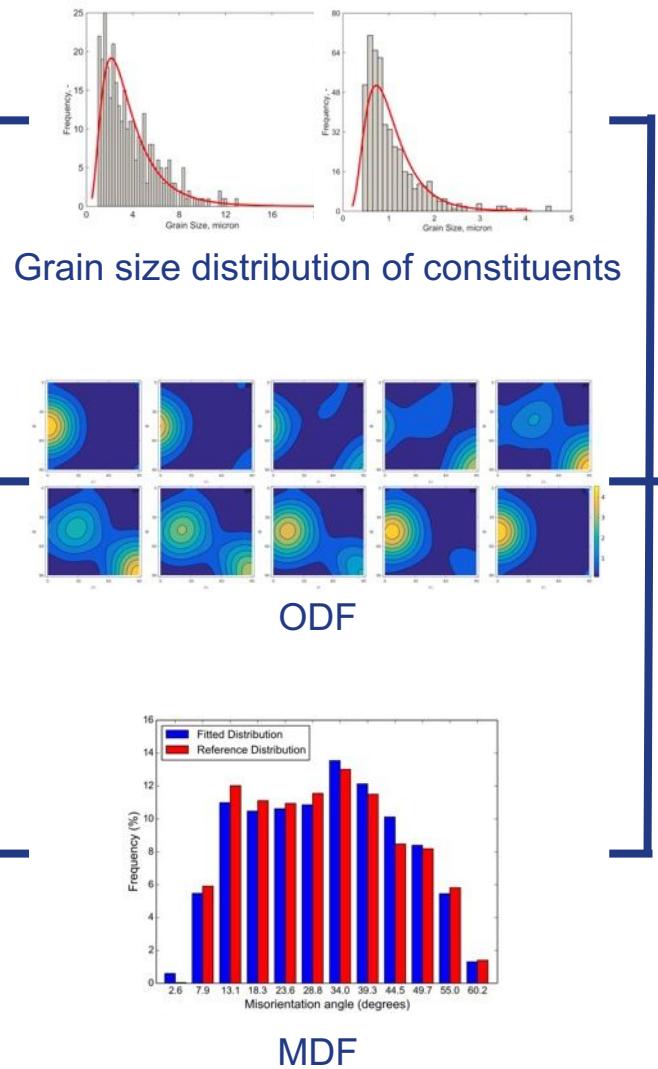
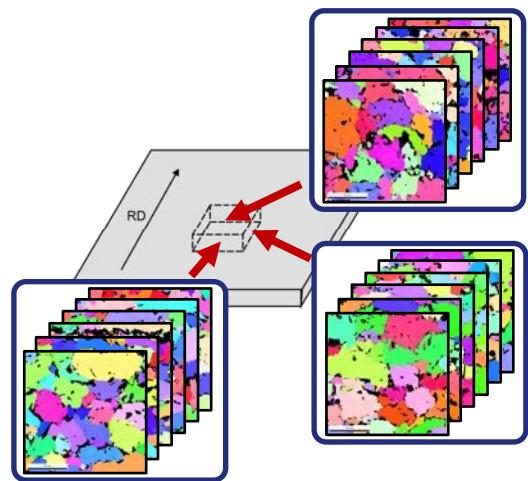
Virtual mechanical testing

100 min. tempering
(prediction)

5 min. tempering (fit)



Synthetic microstructure (RVE)



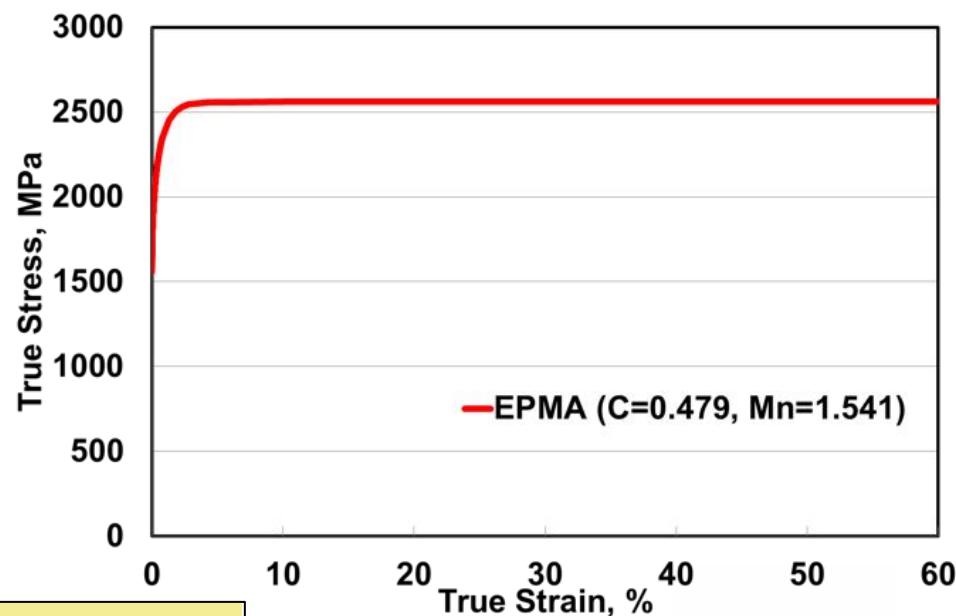
Synthetic microstructure (RVE)

- To describe the strain hardening behaviour of martensite, **empirical approach** is used.

$$\sigma = \sigma_0 + \Delta\sigma + \alpha \cdot M \cdot \mu \cdot \sqrt{b} \cdot \sqrt{\frac{1 - \exp(-M \cdot k \cdot \varepsilon)}{k \cdot L}}$$

$$\begin{aligned}\sigma_0 &= 77 + 80 \cdot (\%Mn) + 750 \cdot (\%P) + 60 \cdot (\%Si) + 80 \cdot (\%Cu) + 45 \cdot (\%Ni) \\ &+ 60 \cdot (\%Cr) + 11 \cdot (\%Mo) + 5000 \cdot N_{ss}\end{aligned}$$

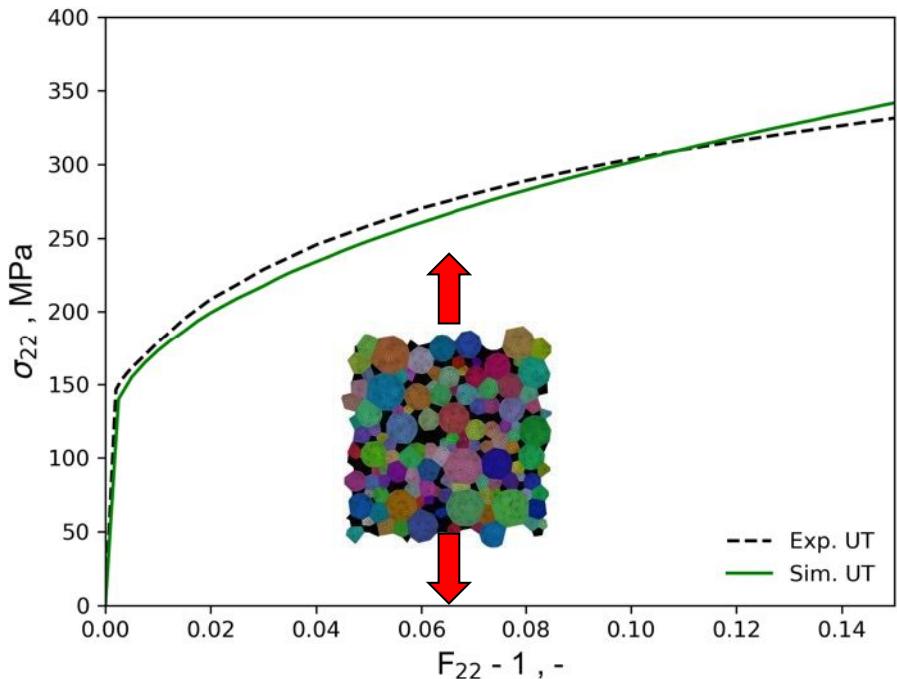
$$\Delta\sigma = 3065 \cdot (\%C_{ss}^f) - 161$$



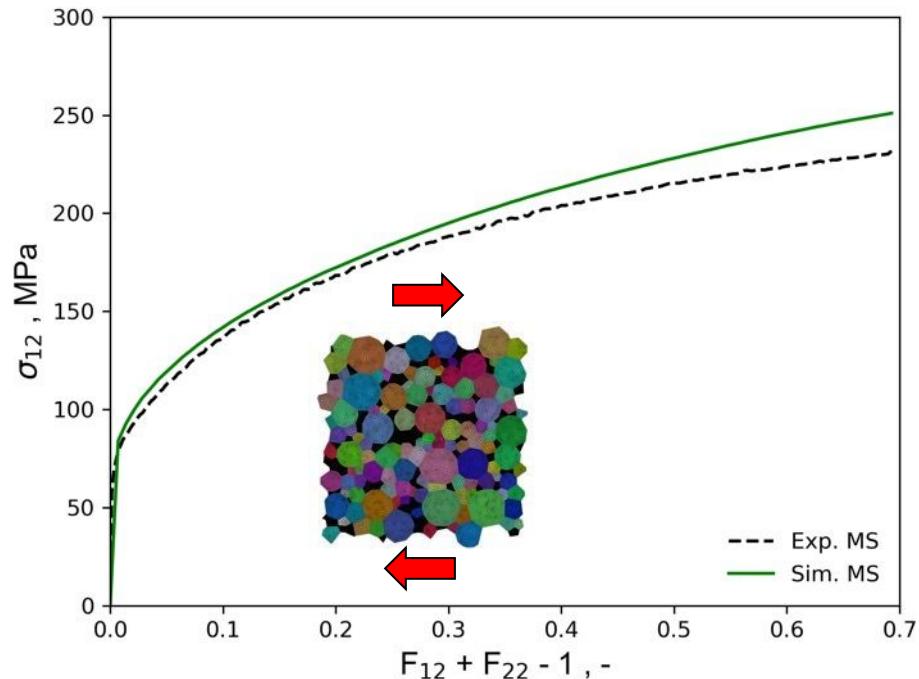
Vajragupta et al. Comp. Mat. Sci. 94 (2014)

Parameterization of nonlocal crystal plasticity model

Parameter fitting



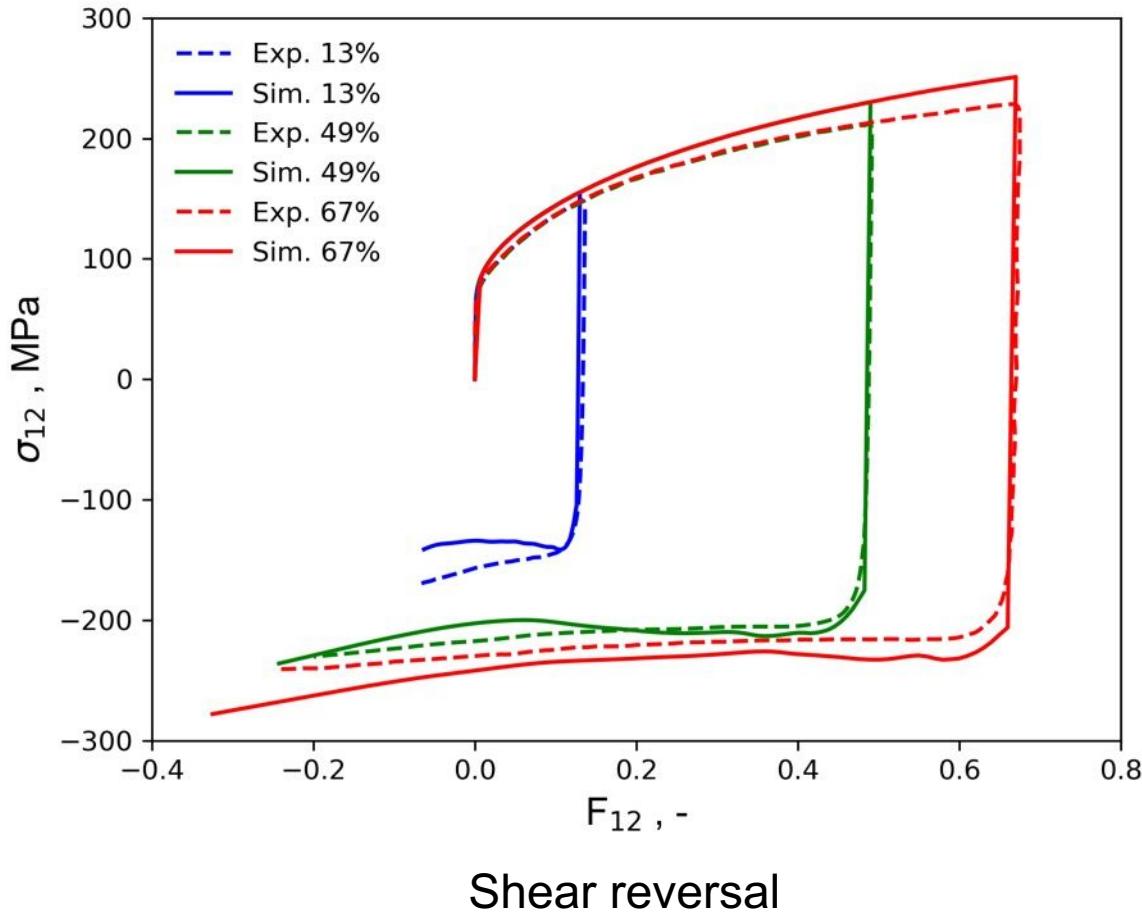
Uniaxial tension



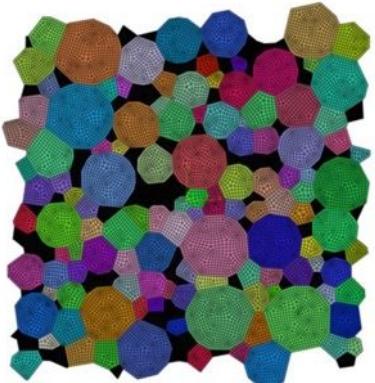
Monotonic shear

Parameterization of nonlocal crystal plasticity model

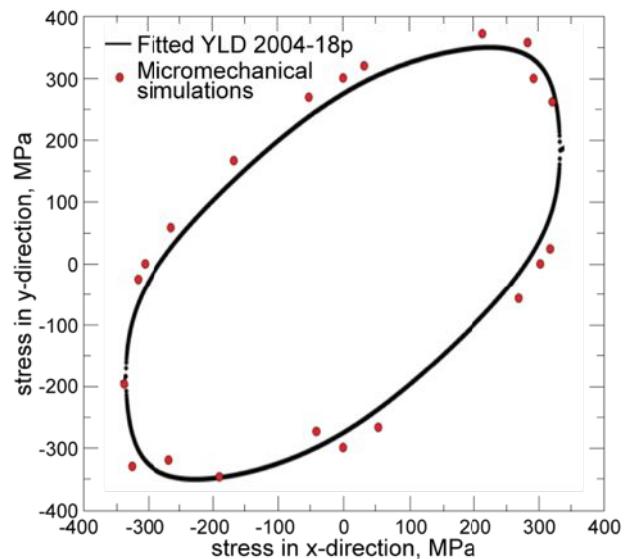
Parameter validation



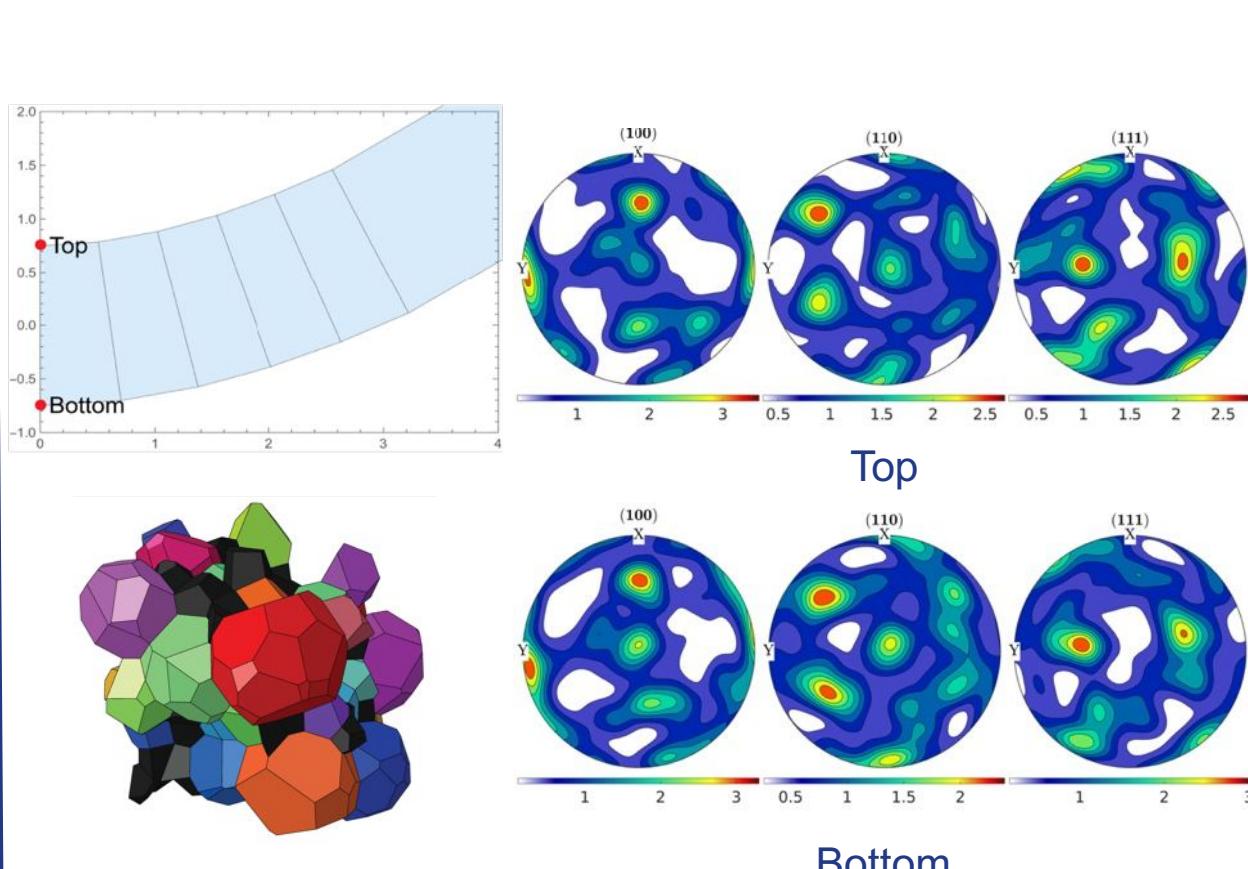
Micromechanical modeling of DP600 steel



DP600 microstructure



Parameterization of Barlat YLD2004-18p



Texture evolution during air bending process



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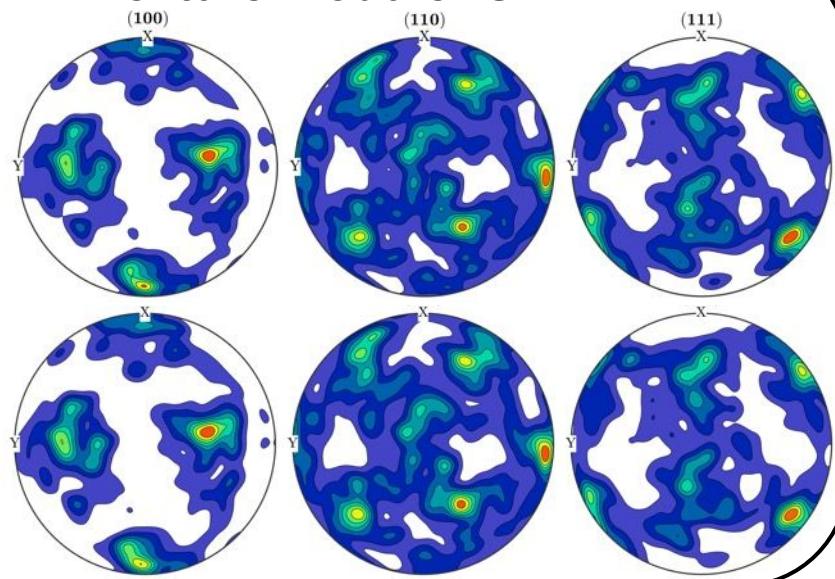
Kanapy: Work flow

EBSD



Texture module: ODF

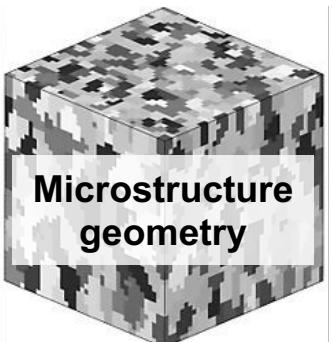
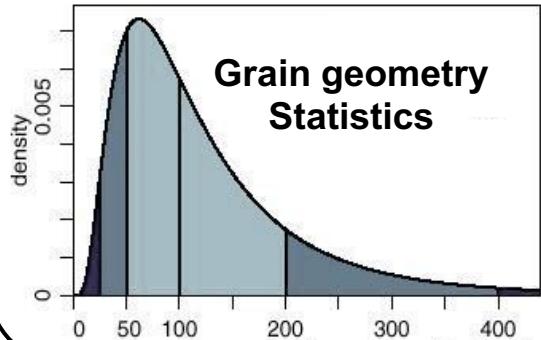
EBSD
ODF



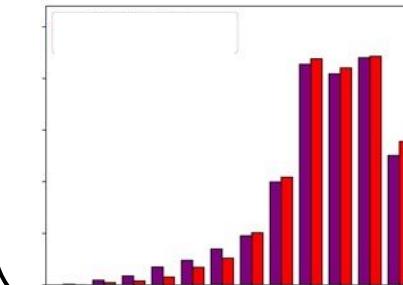
Reduced
ODF

Geometry module

Grain geometry
Statistics



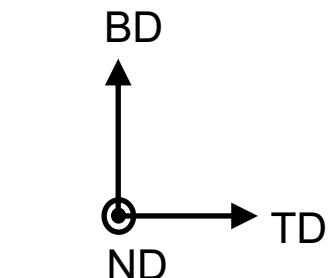
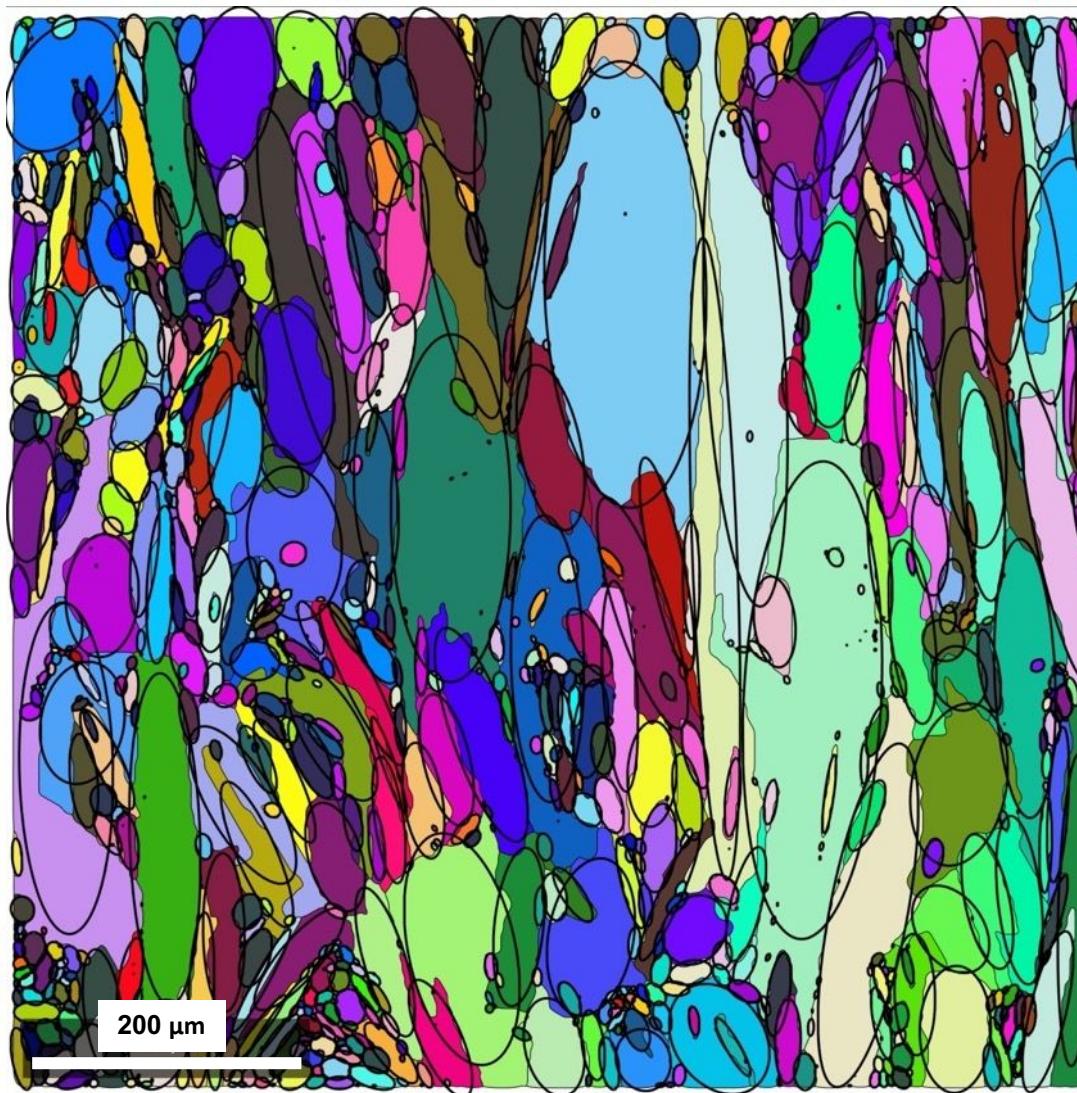
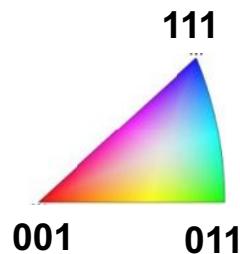
Texture module:
MDF



Synthetic
Microstructure



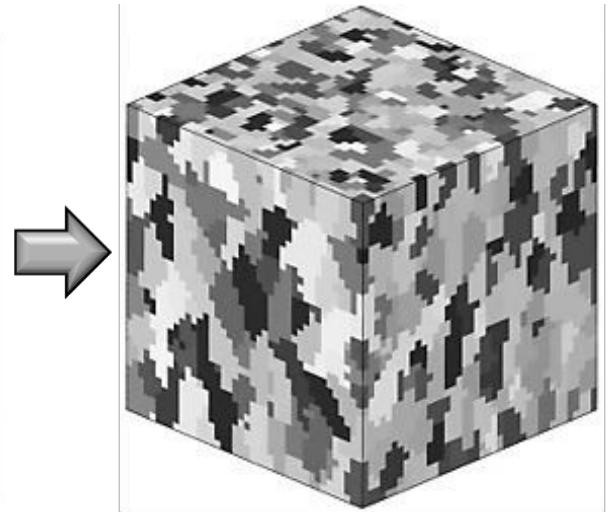
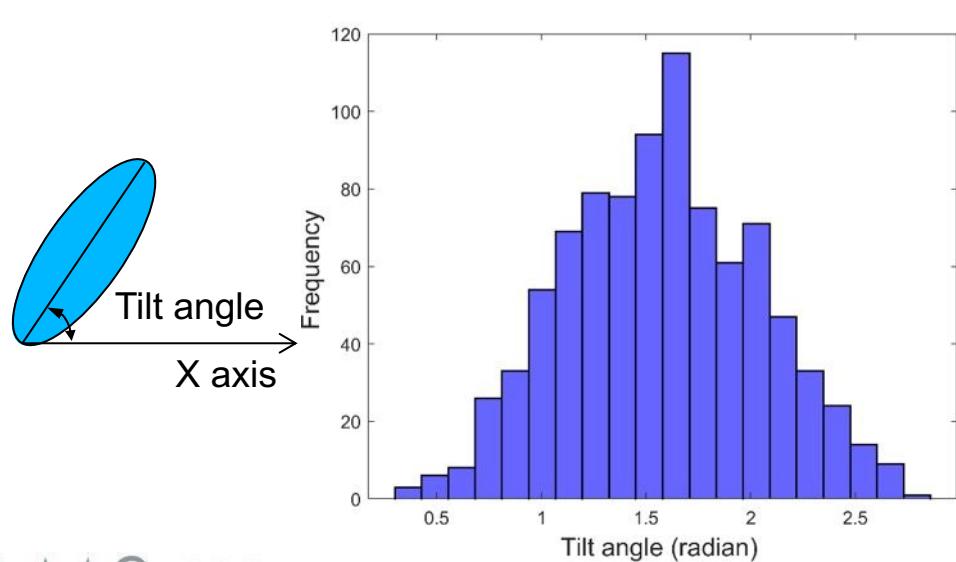
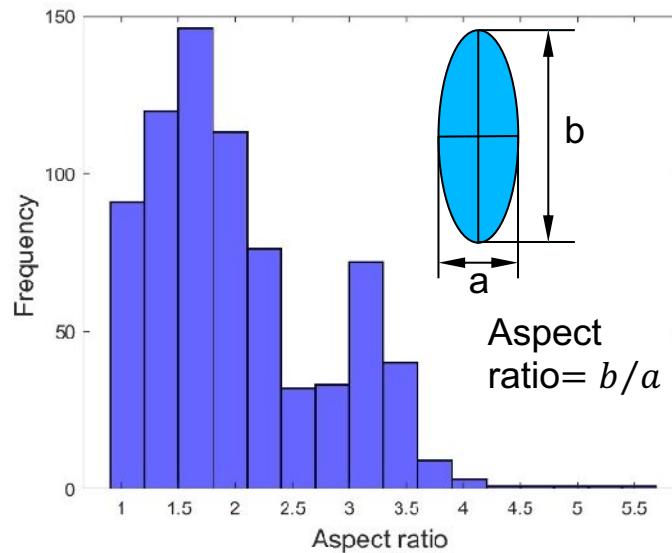
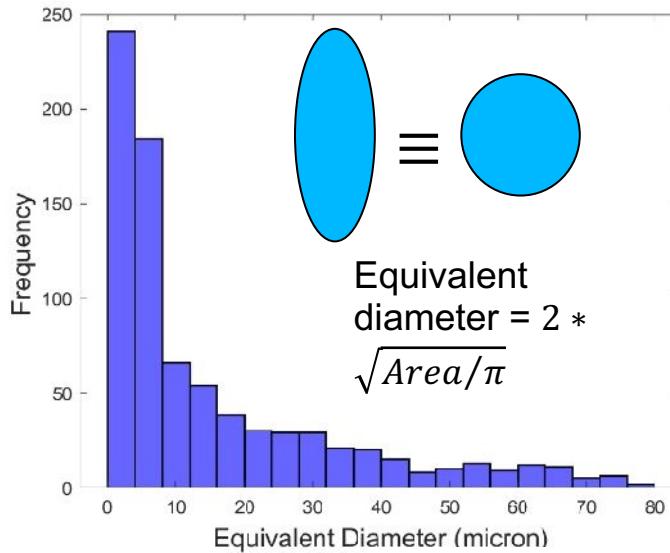
Elements of microstructure : Grains



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

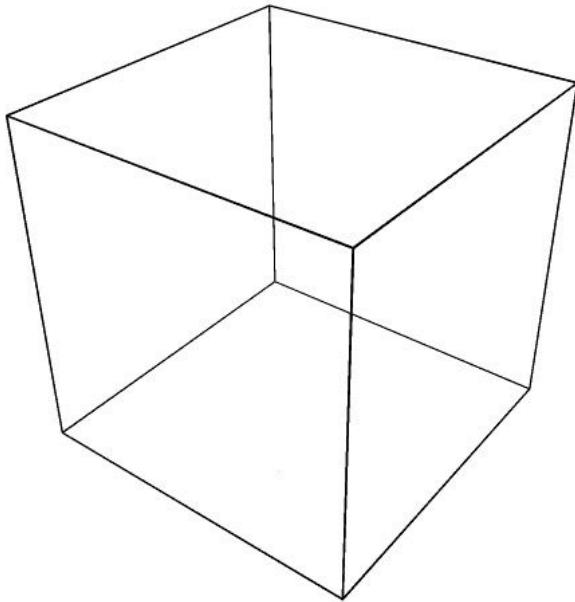
MTEX documentation
<https://mtex-toolbox.github.io/Documentation.html>

Elements of microstructure : Grain statistics

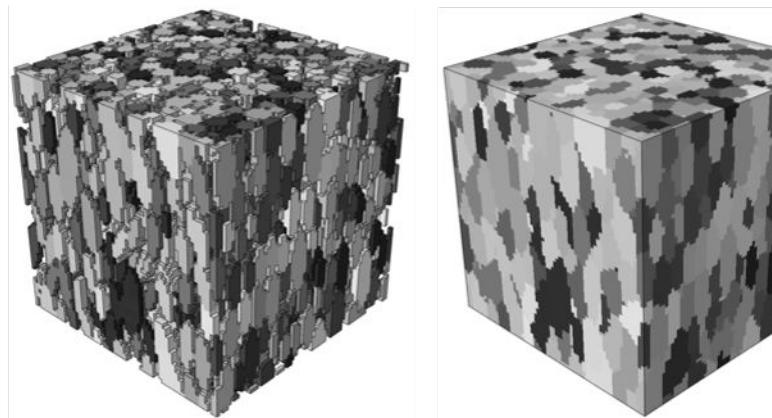


Kanapy: Synthetic microstructure generator

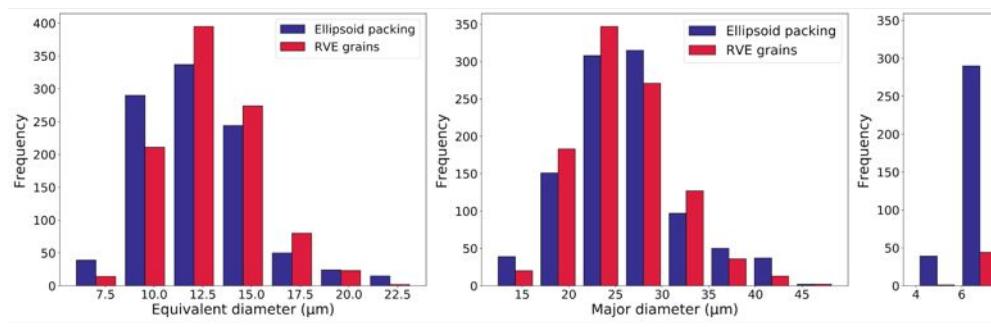
Kanapy geometry module



Time-driven particles
packing method
(advantages over RSA)



Voxelization



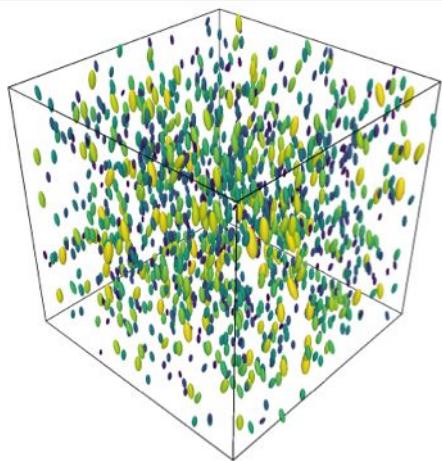
Equivalent diameter

Major diameter

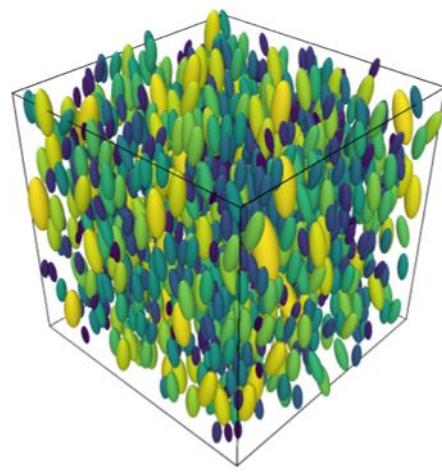
Statistical comparison of grain geom

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

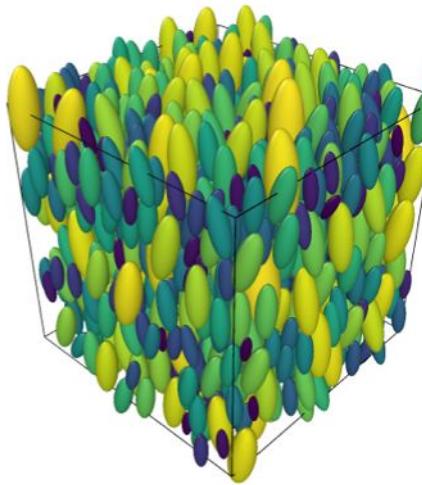
Geometry Module: Particle simulation



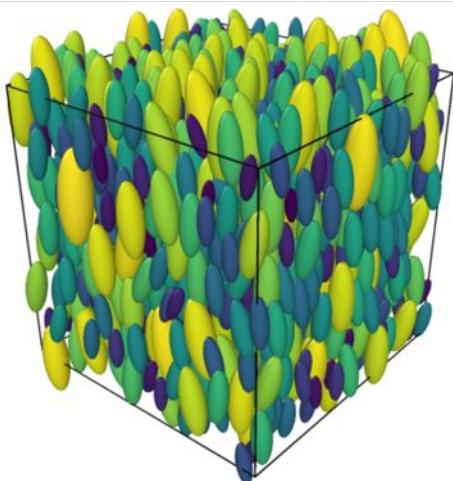
Time step : 250



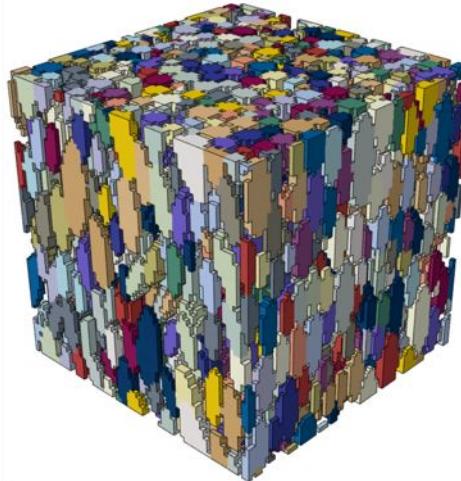
Time step : 550



Time step : 850



Ellipsoid packing

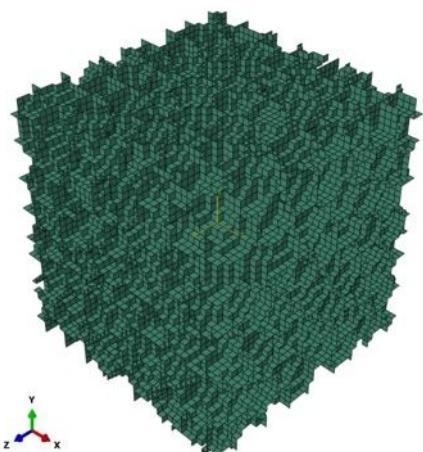


Voxelization - Hexahedral meshing

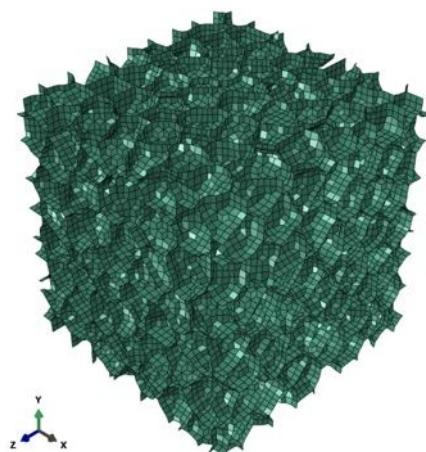


Kanapy: Synthetic microstructure generator

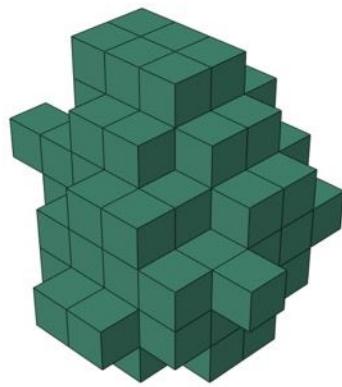
Kanapy geometry module



Voxelated grain
boundaries



Smoothed grain
boundaries



Voxelated grain



Smoothed

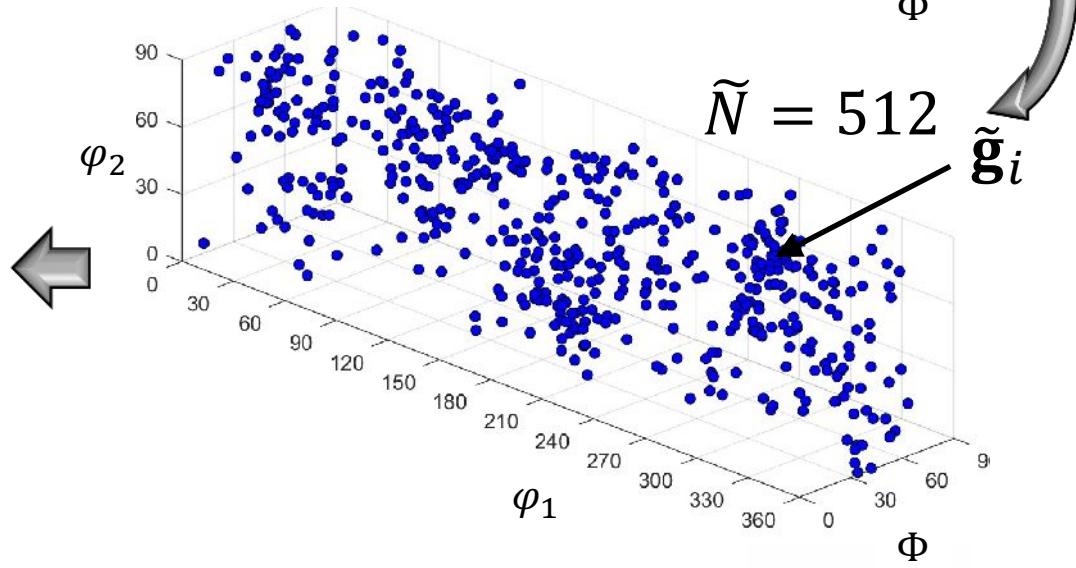
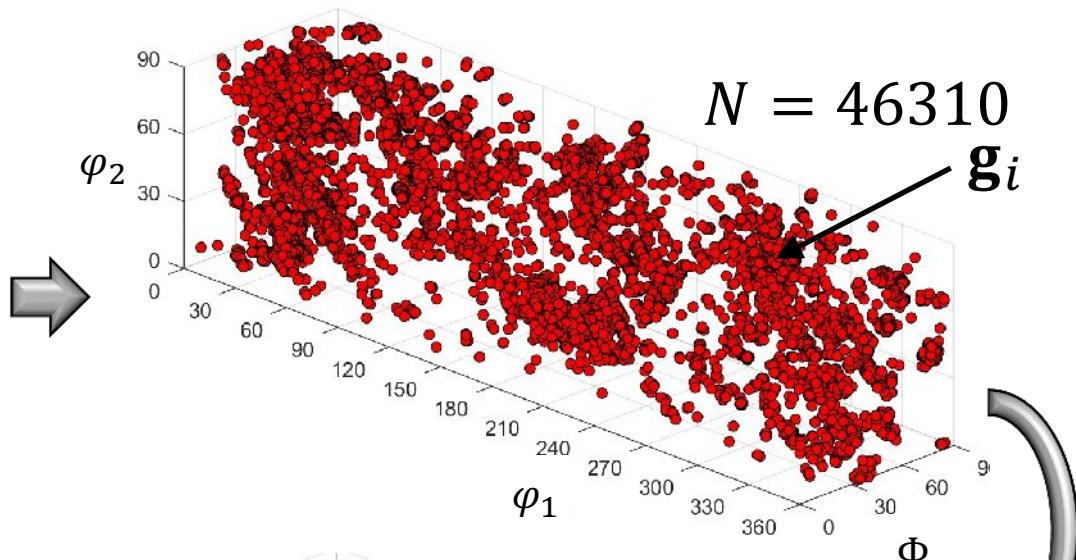
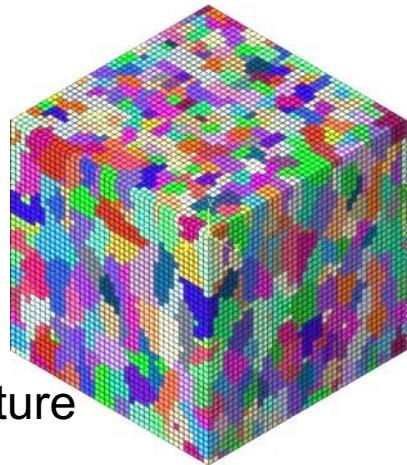
Source: <https://github.com/ICAMS/Kanapy>

Orientation distribution reconstruction



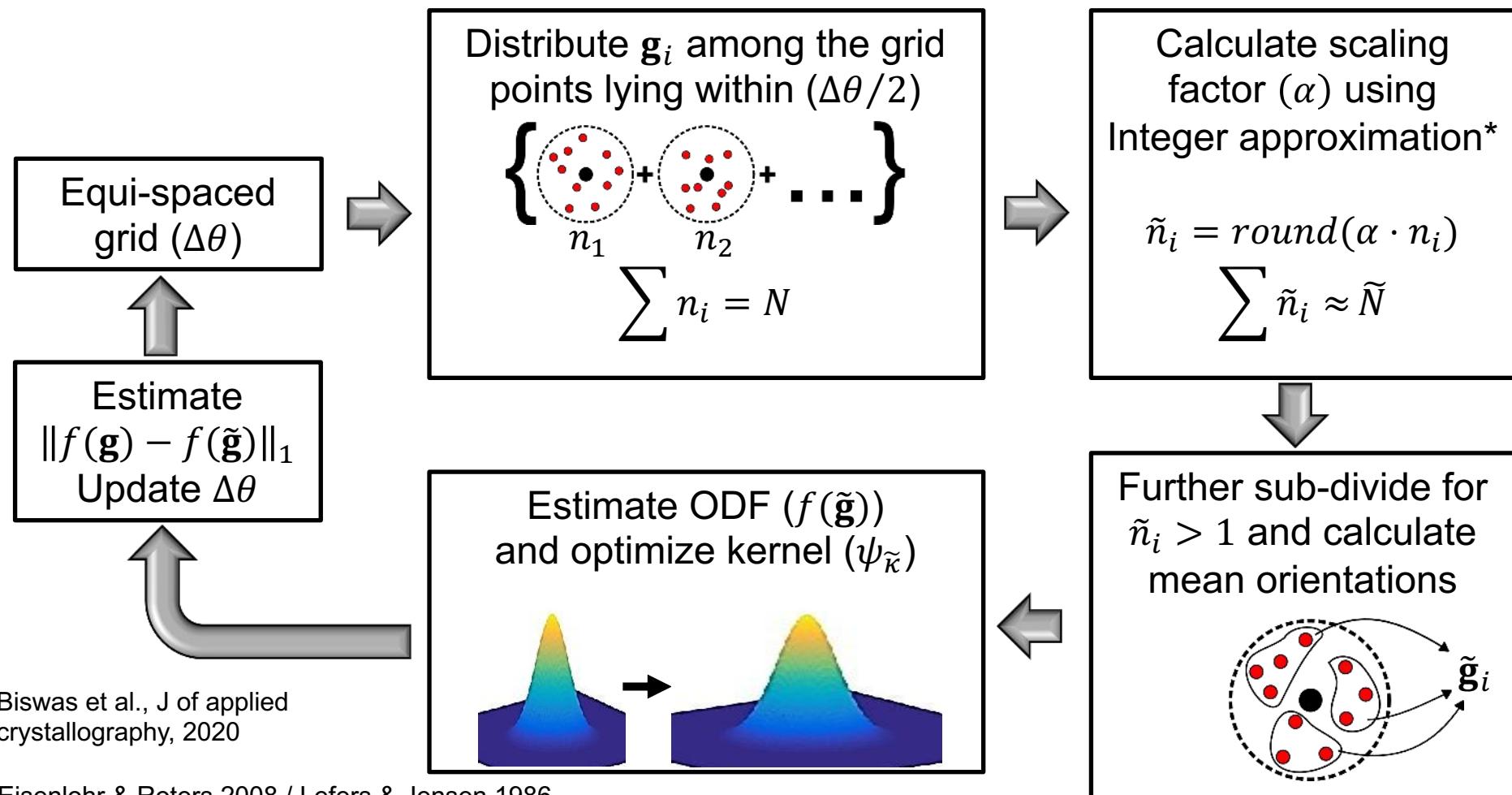
EBSD

Virtual
microstructure

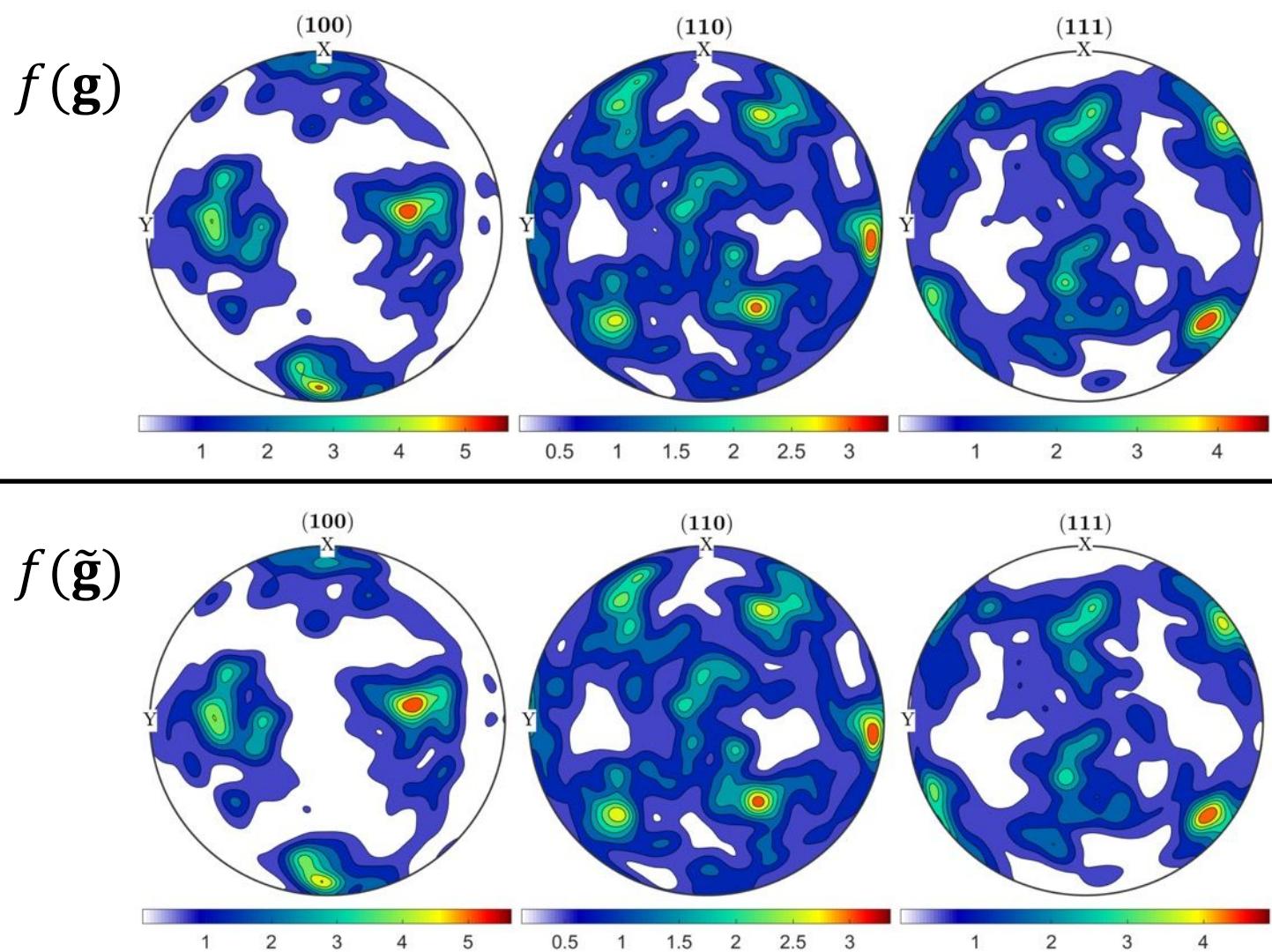


Orientation distribution reconstruction

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

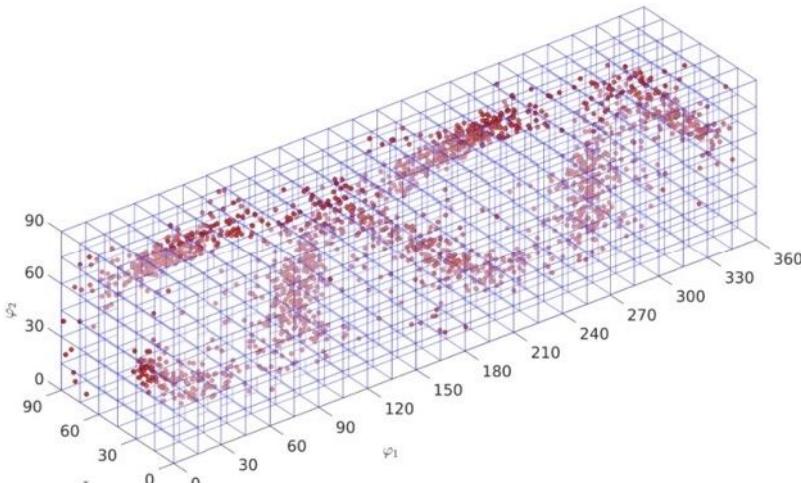


Orientation distribution reconstruction

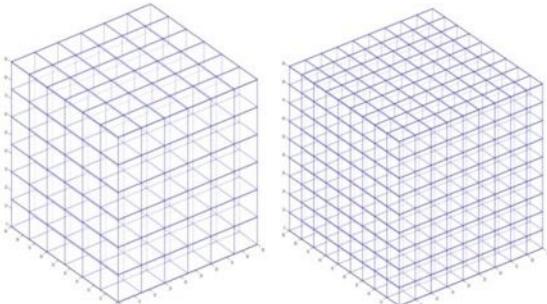


Kanapy: Synthetic microstructure generator

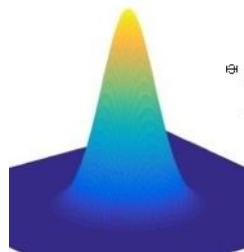
Kanapy ODF reconstruction module



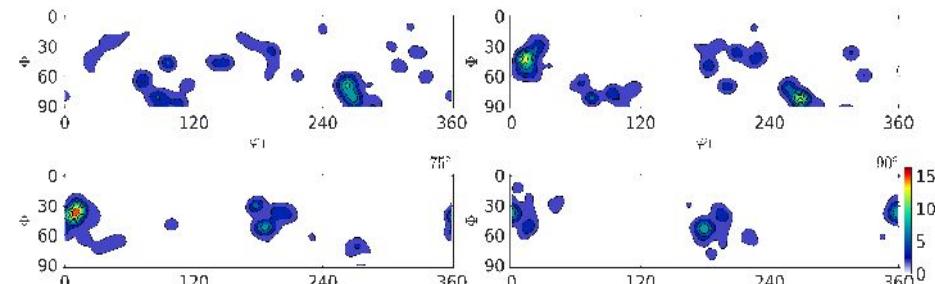
Integer Approximation (IA)



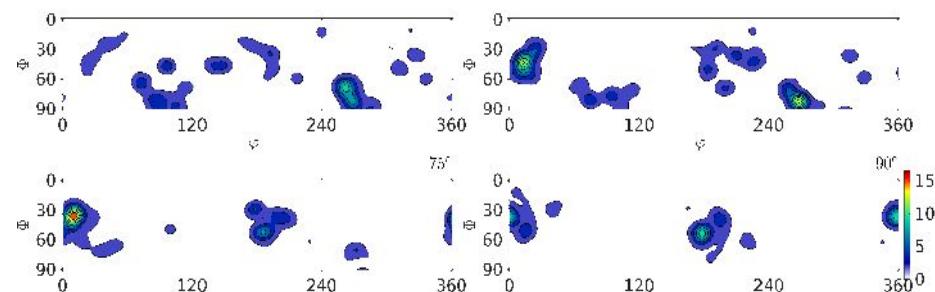
Grid spacing $\Delta\theta$ optimization



Kernel optimization



Experimental ODF

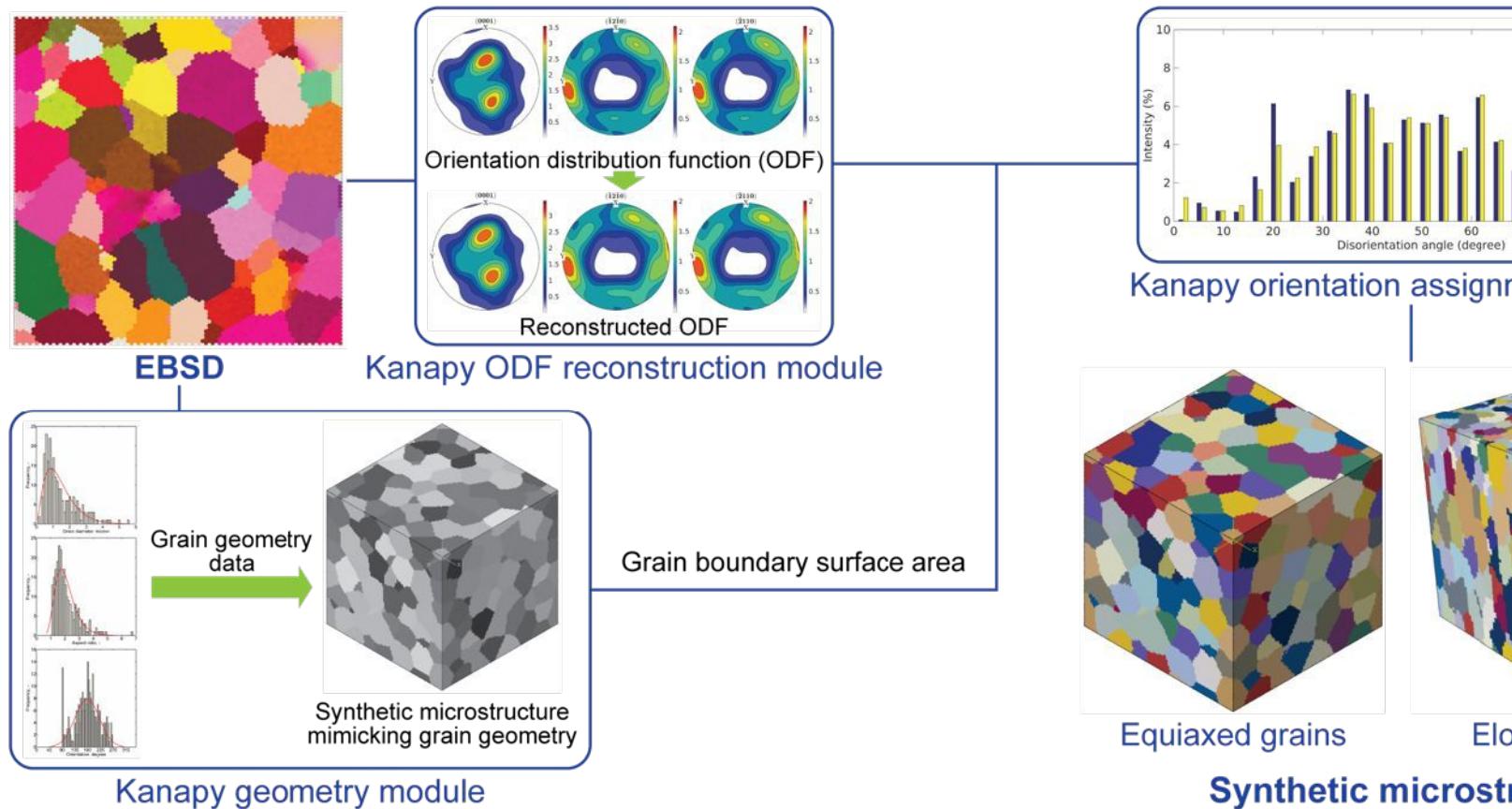


Discretized ODF



Source: Biswas et al. J. Appl. Crystallogr. 2020

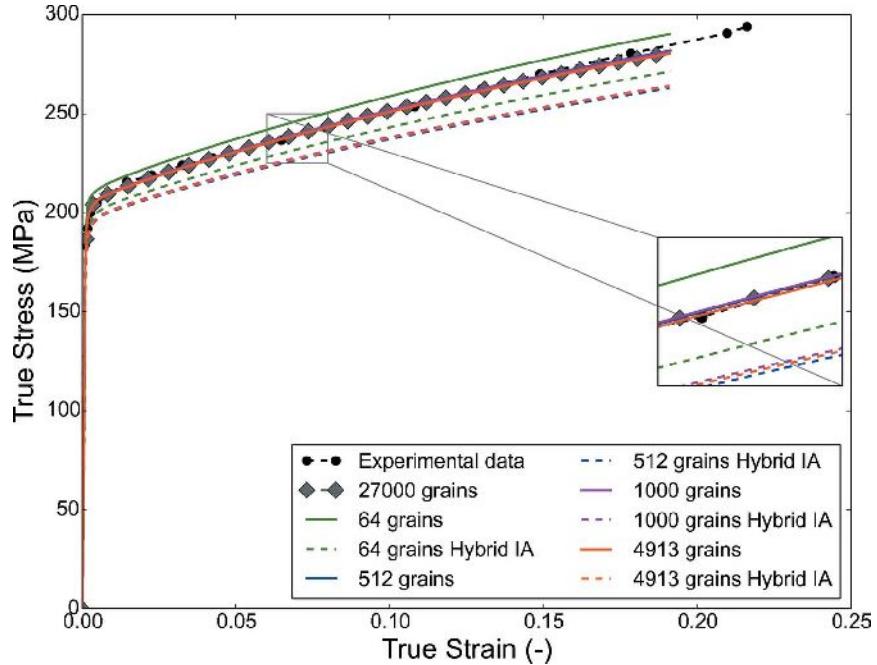
Kanapy: Synthetic microstructure generator



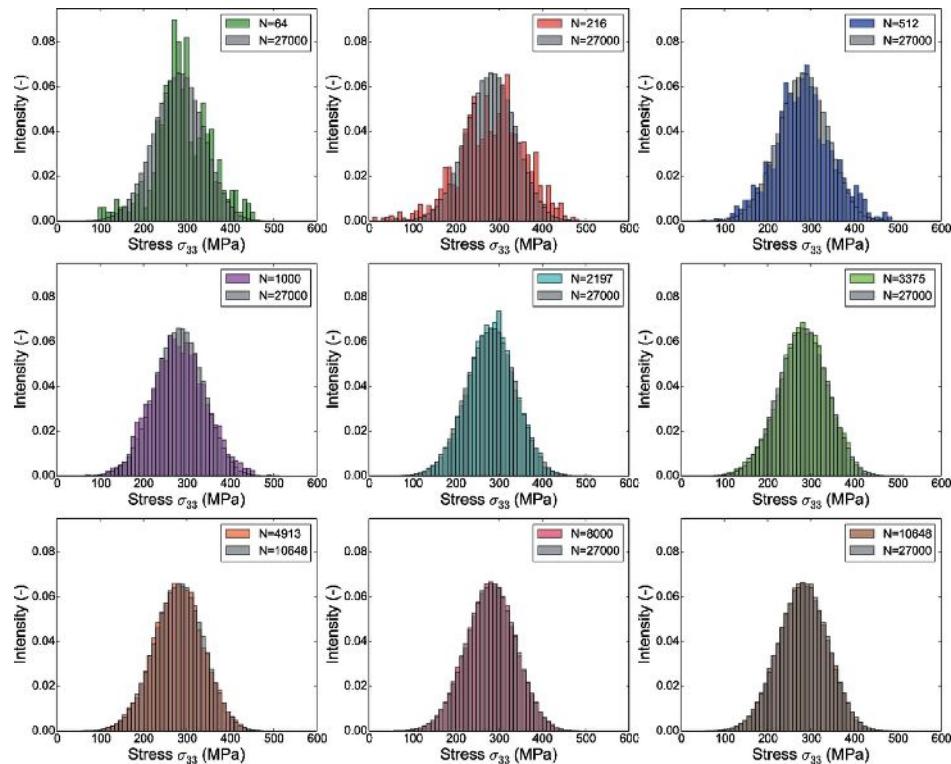
Source: <https://github.com/ICAMS/Kanapy>

Kanapy: Synthetic microstructure generator

Kanapy ODF reconstruction module



Flow curves comparison



Stress distribution comparison

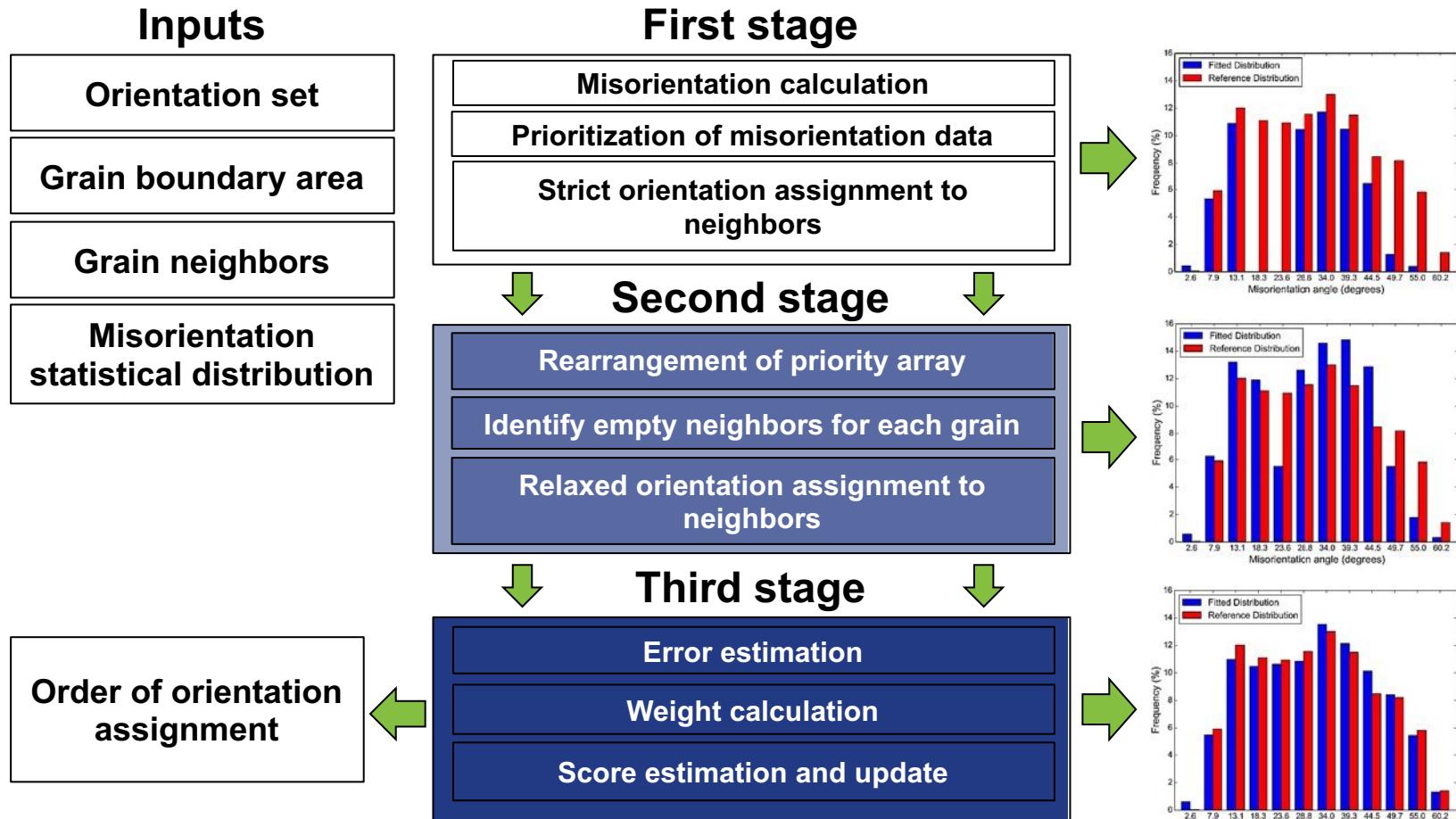


Source: Biswas et al. J. Appl. Crystallogr. 2020



Kanapy: Synthetic microstructure generator

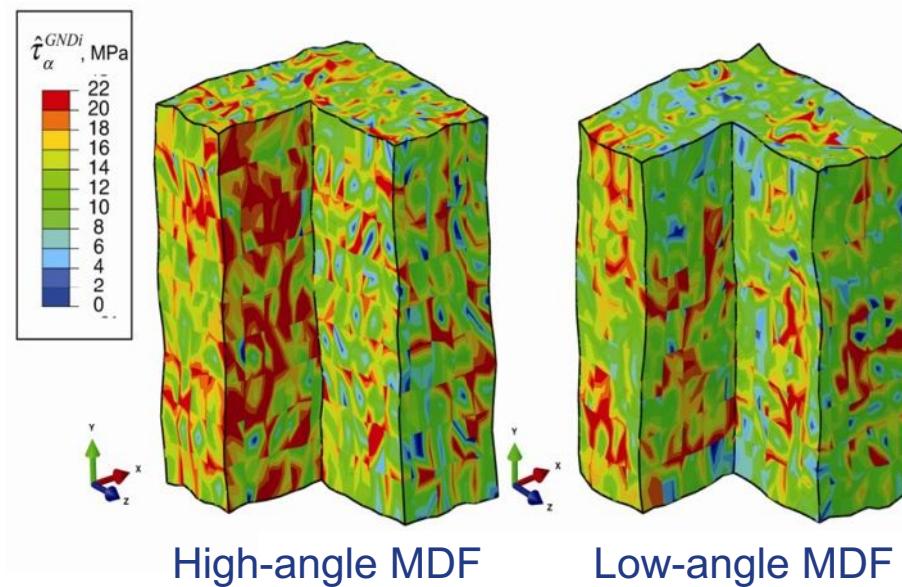
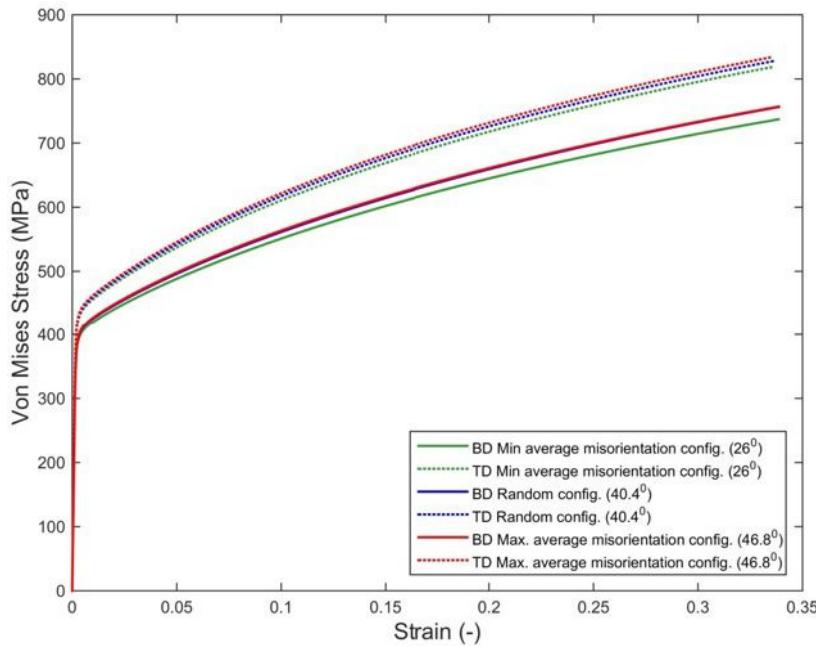
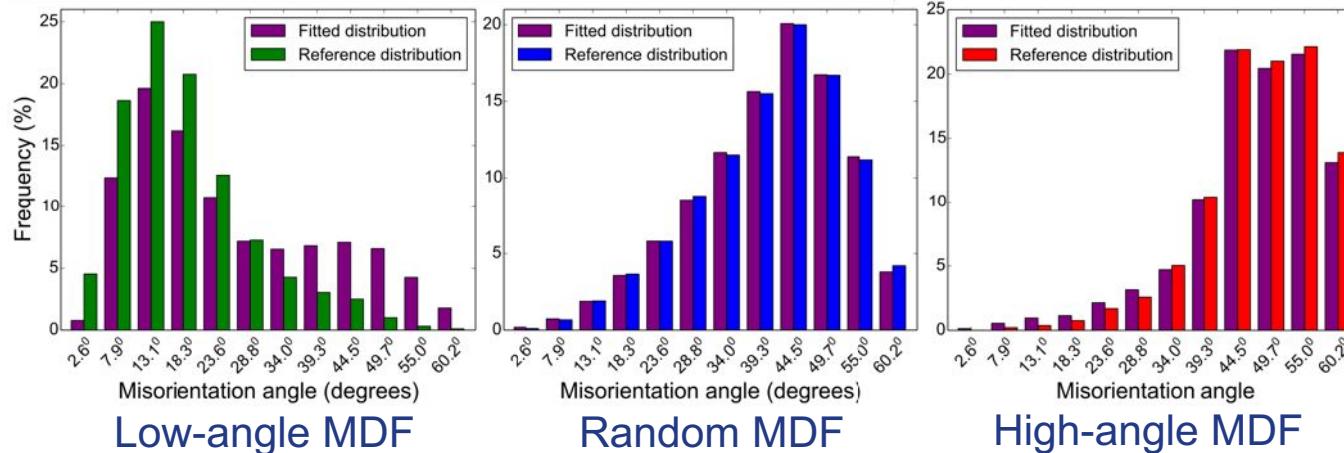
Kanapy orientations assignment module



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



Influence of misorientation distribution (MDF)



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

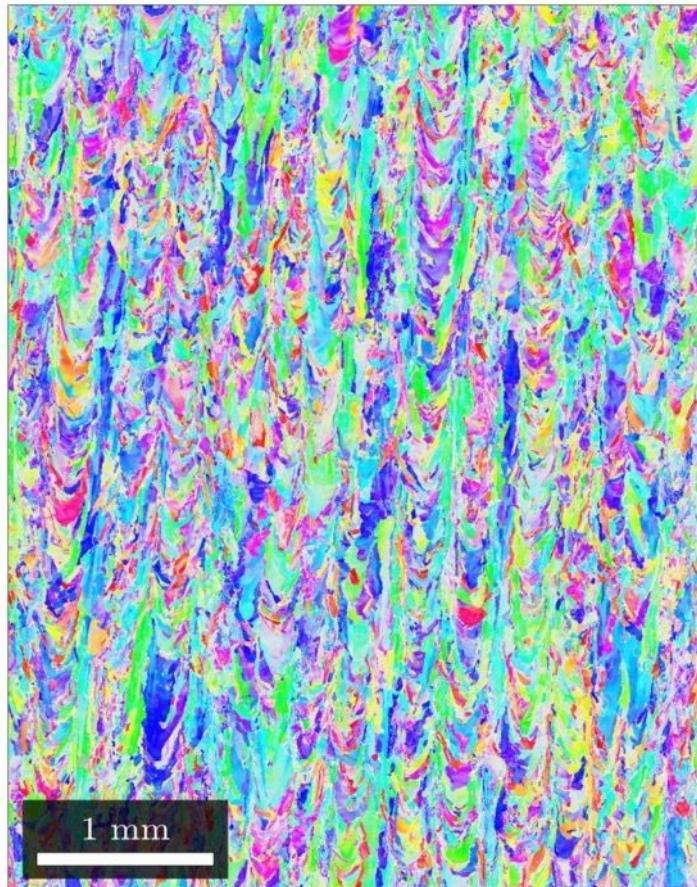


Outline

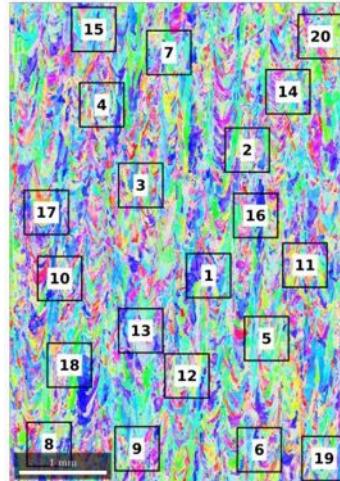
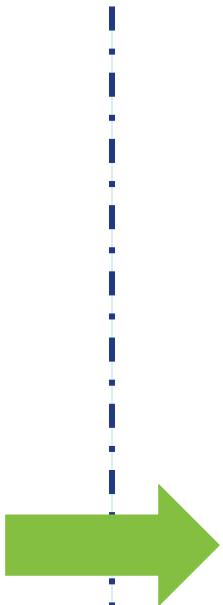
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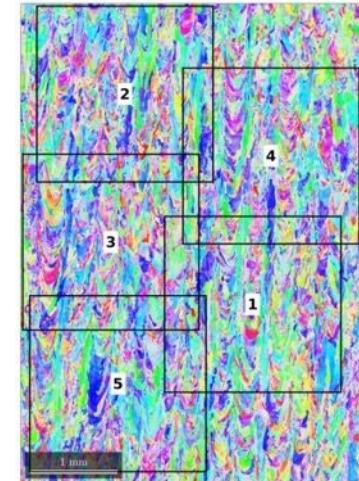
Effect of grain statistics on micromechanical modeling



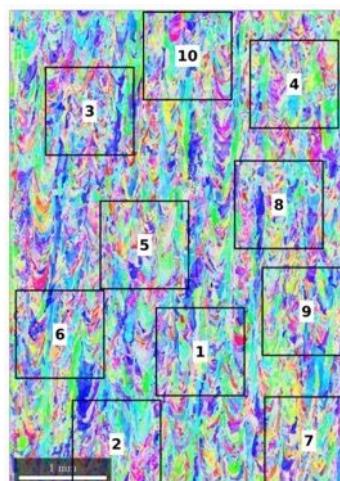
4x5 mm² EBSD



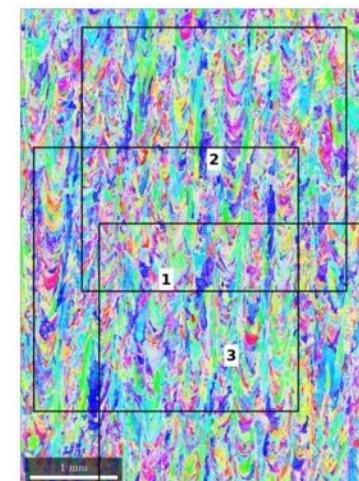
0.5x0.5 mm²



2x2 mm²



1x1 mm²

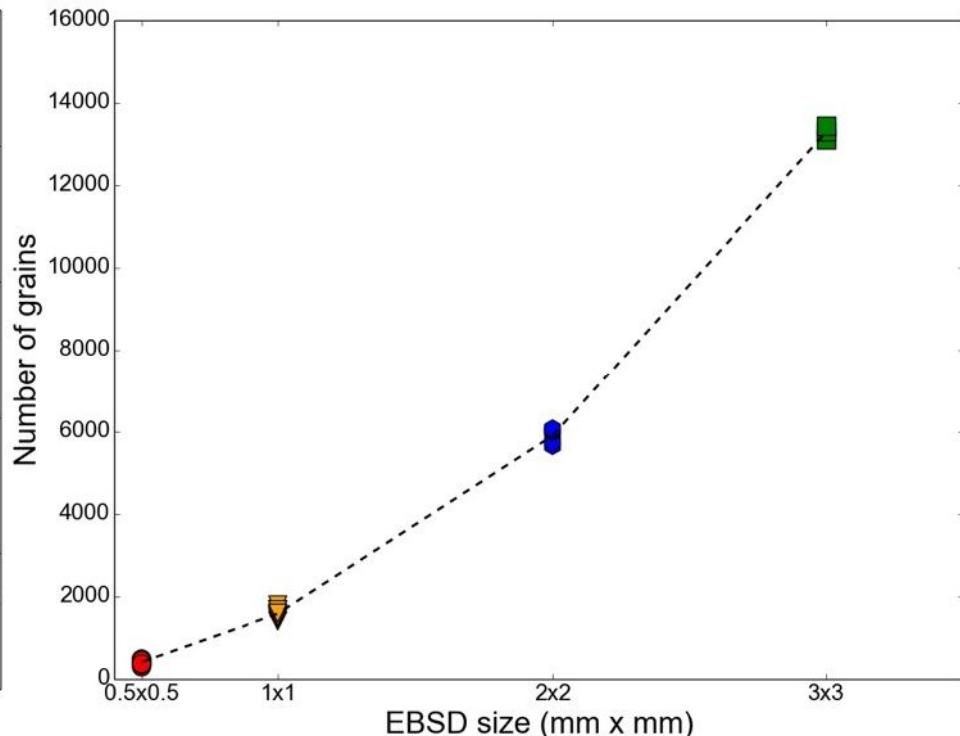
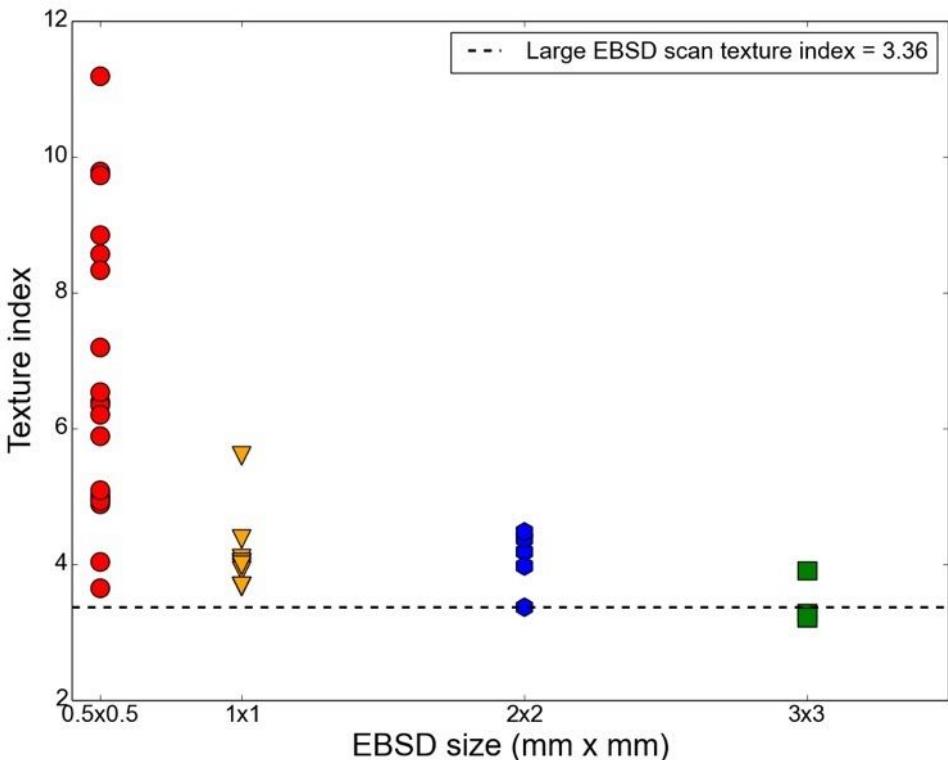


3x3 mm²



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

Effect of grain statistics on micromechanical modeling



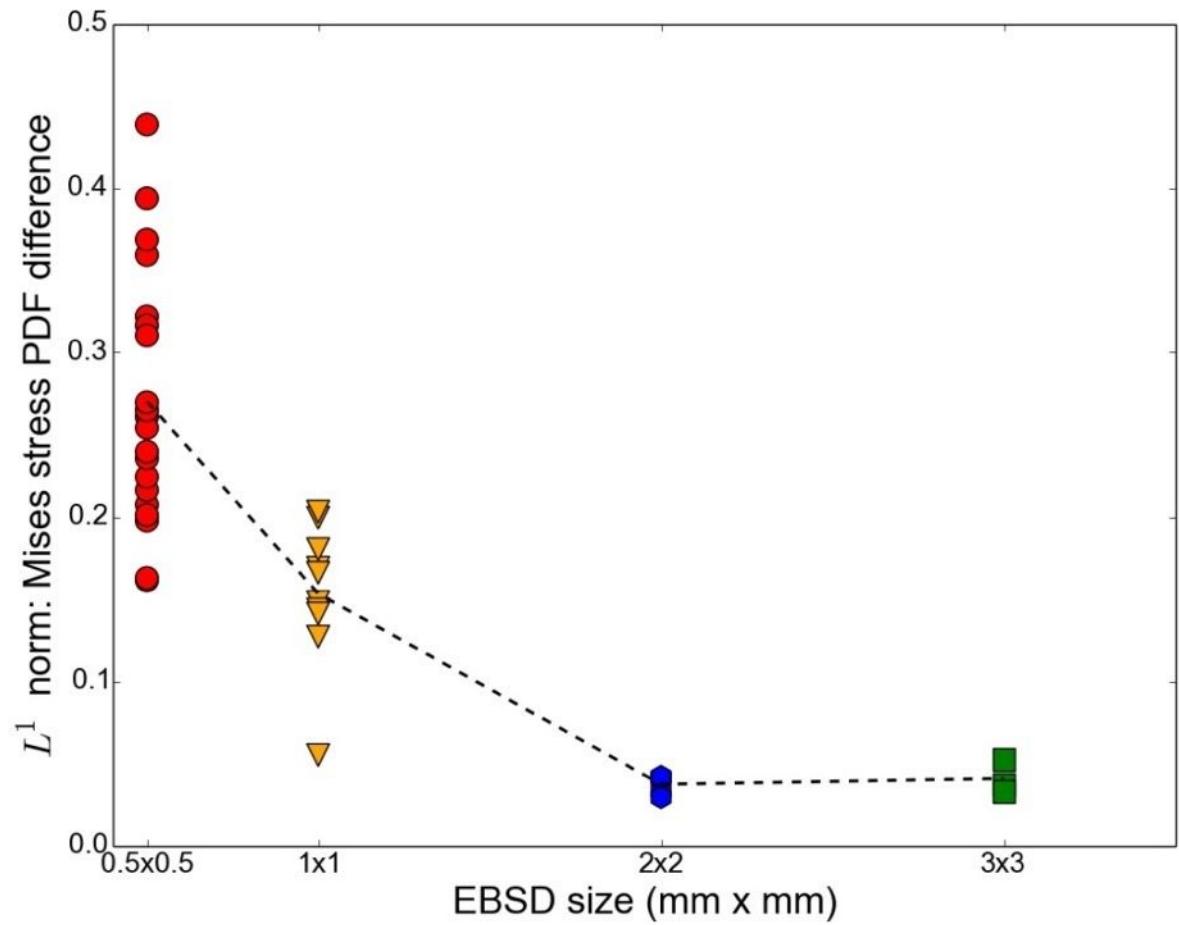
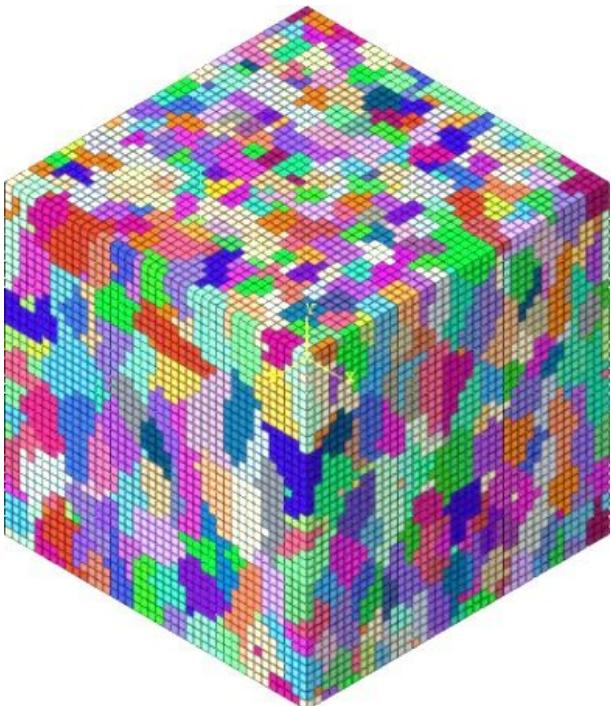
\bar{f} : ODF estimated from cropped EBSD

f : ODF estimated from large EBSD scan



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

Effect of grain statistics on micromechanical modeling



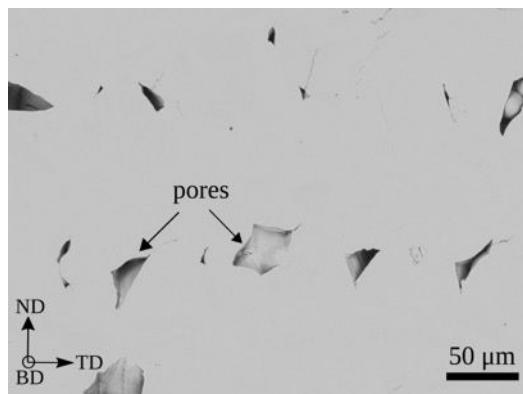
Source: Biswas et al., Adv. Eng. Mater. 2020

Outline

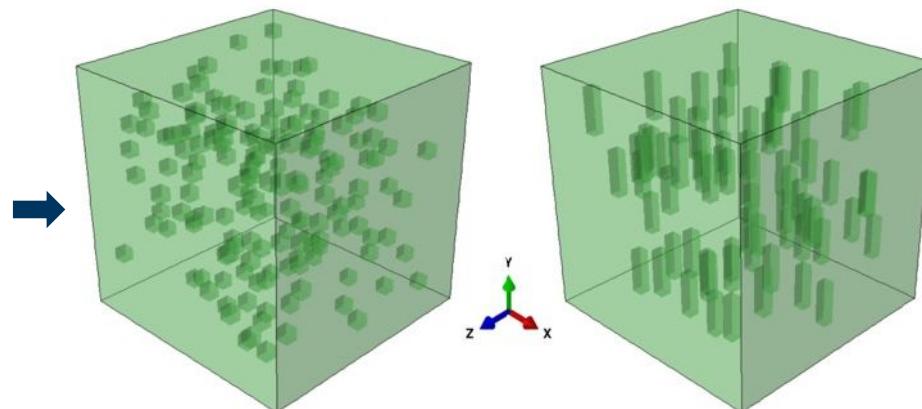
- Micromechanical modeling with
 - experimental
 - simulated
 - synthetic microstructures
- Synthetic microstructures with Kanapy
- Influence of grain statistics
- Porous microstructures

- Demonstration 1: Two-phase microstructures
- Demonstration 2: Polycrystals and crystallographic texture

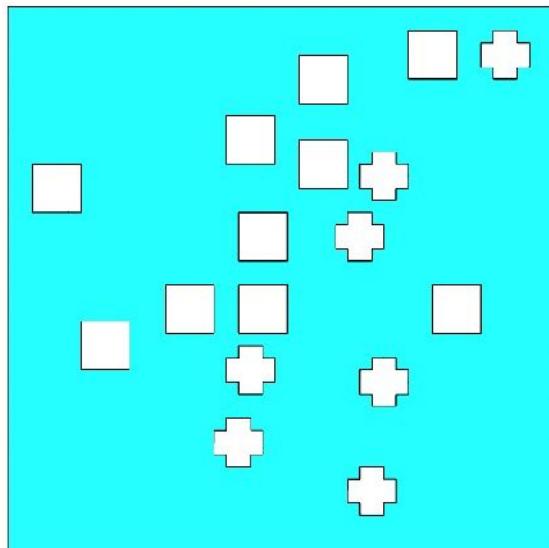
Micromechanical modeling – Modeling pores and Damage



Pores

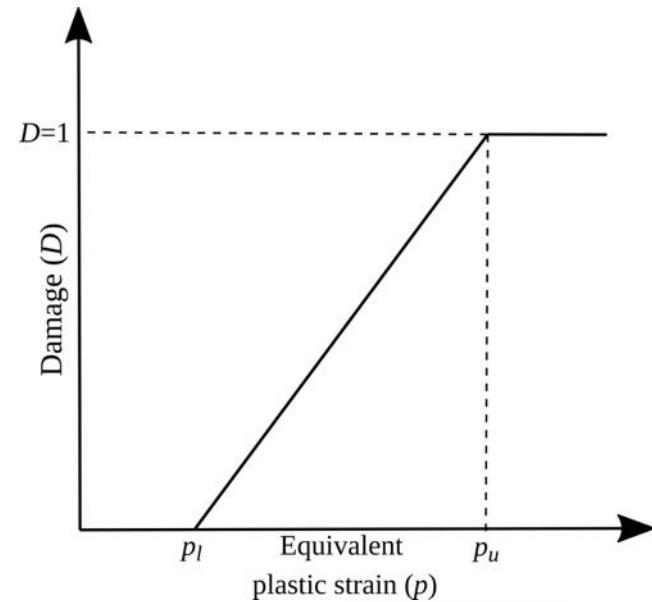


RVEs containing equiaxed and elongated pores



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

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



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

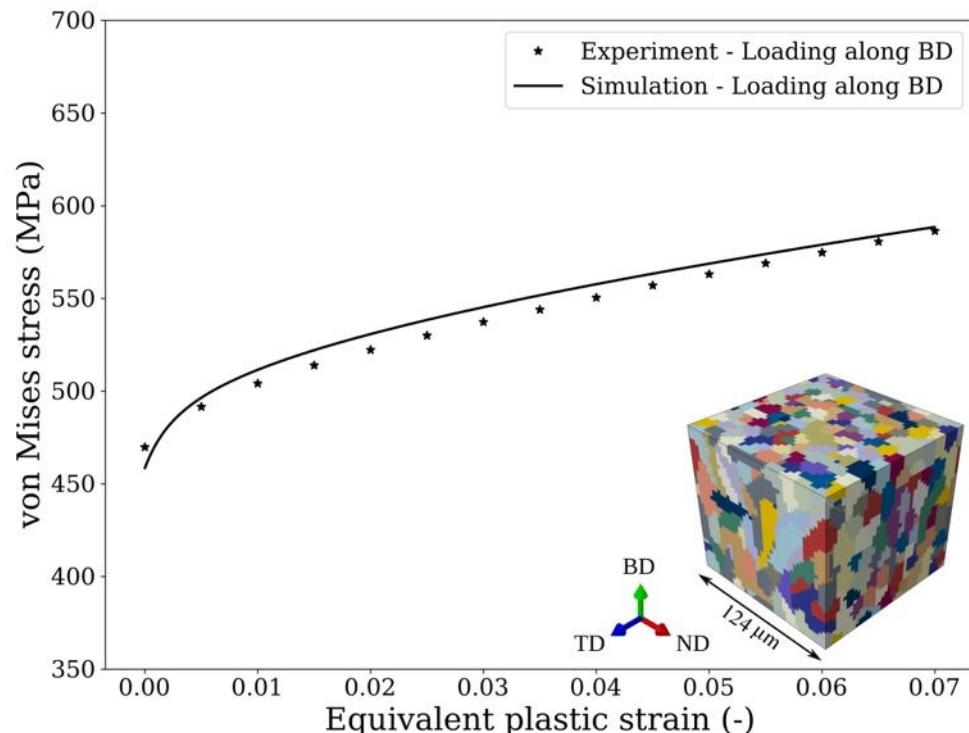
$$\dot{\hat{\tau}}_\alpha = \sum_{\beta=1}^N h_0 \chi_{\alpha\beta} \left(1 - \frac{\hat{\tau}_\alpha}{\hat{\tau}_{sat}}\right)^{p_2} |\dot{\gamma}_\beta|$$

Kinematic hardening

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

Isotropic hardening

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

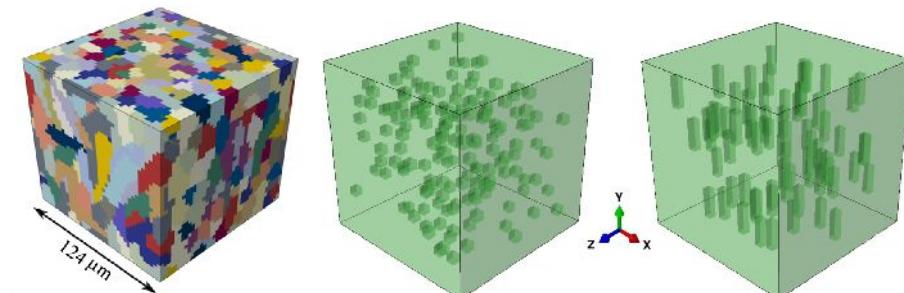


Parameter	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	\hat{t}_0 (MPa)	\hat{t}_{sat} (MPa)	p_1	p_2	h_0 (MPa)	c_1
Value	247	106	71	147	250	20	2.25	160	0.03

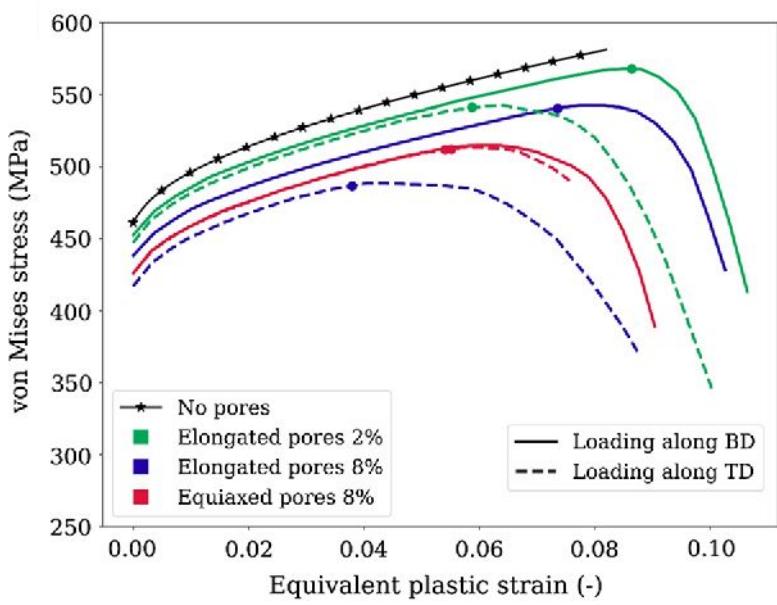
Ma & Hartmaier.
Phil Mag (2014)



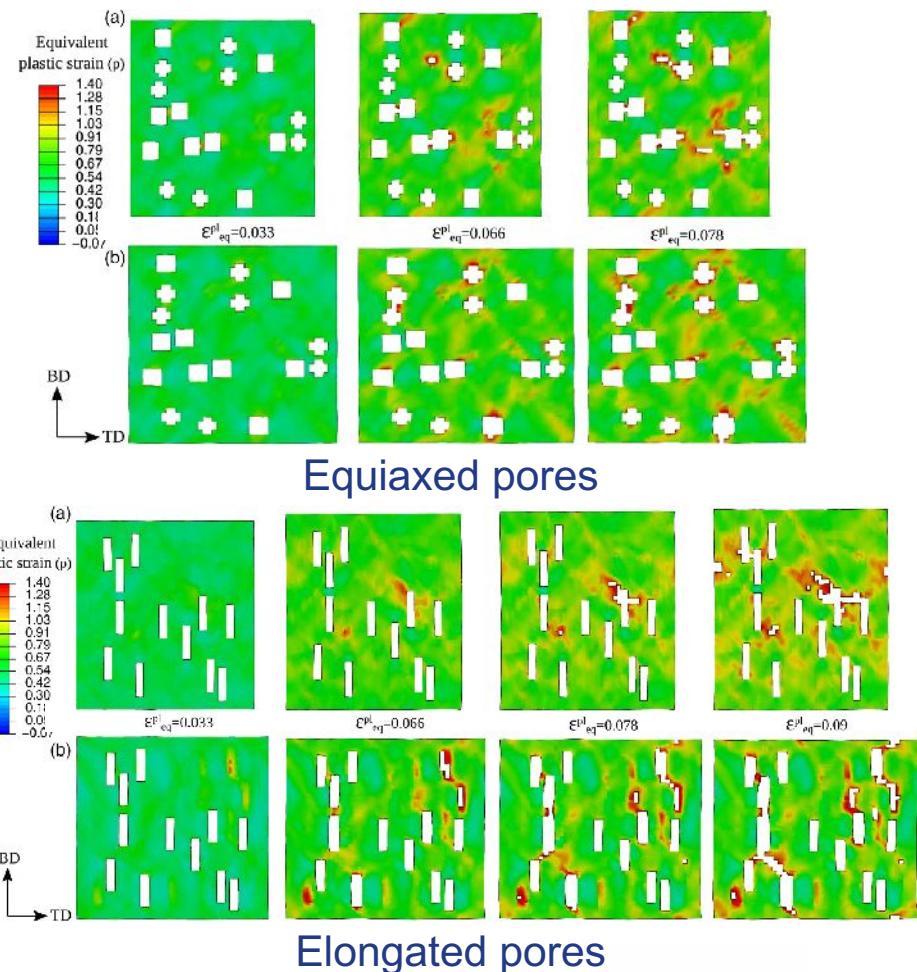
Influence of pore shape on anisotropy



Synthetic
microstructure Equiaxed
pores Elongated
pores

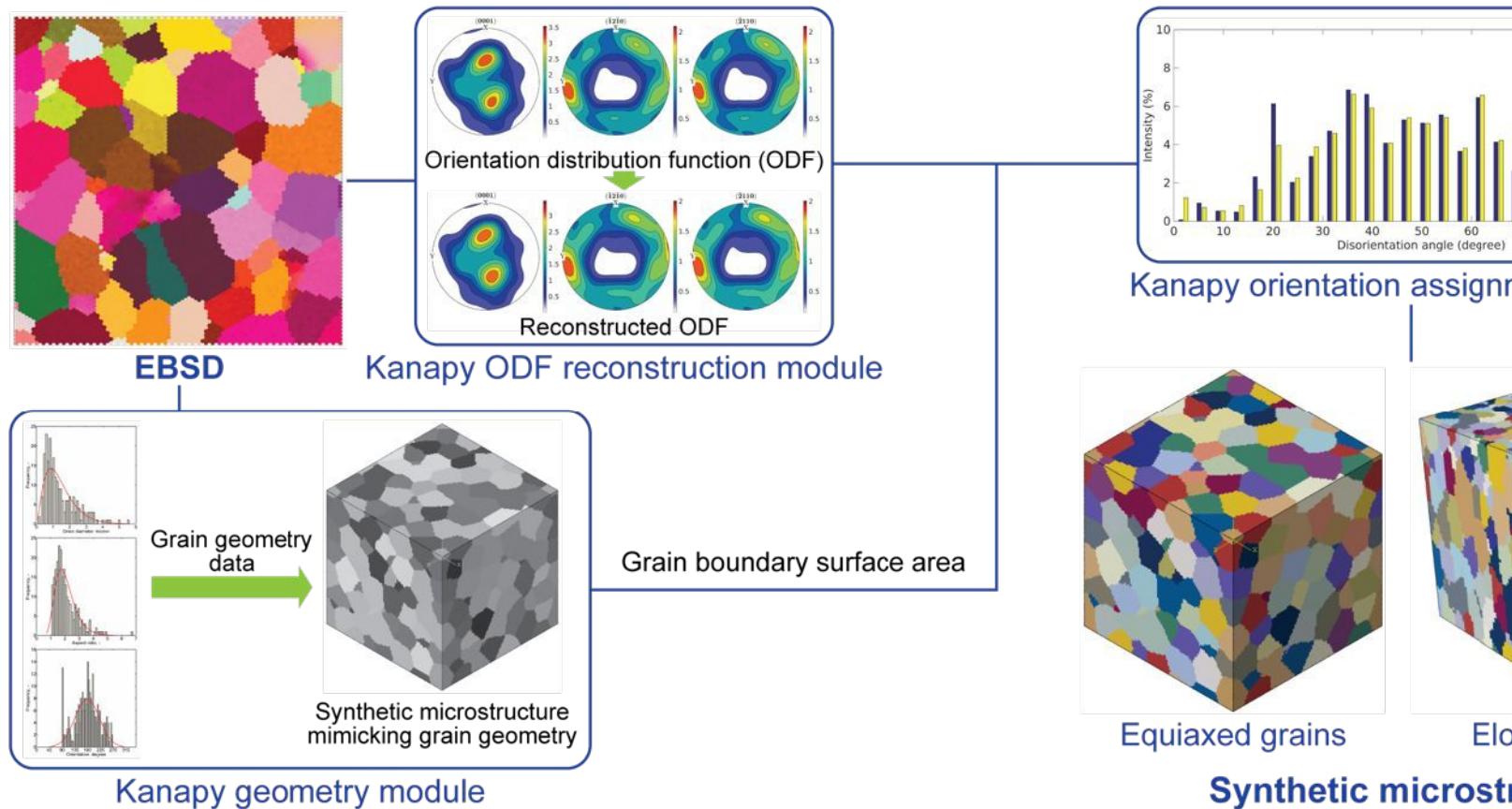


Flow curves



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

Summary



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

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