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Microstructure generation with Kanapy

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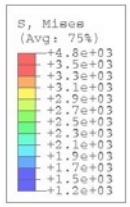
RUB

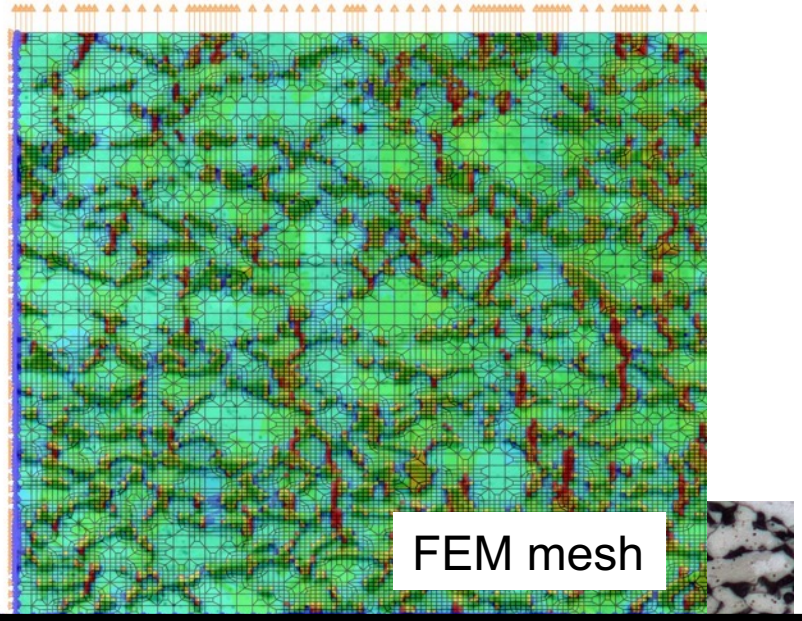
Outline

- 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

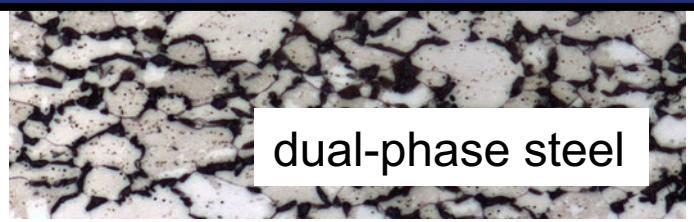
Micromechanical Modeling





FEM mesh

Micromechanical modeling requires many input parameters



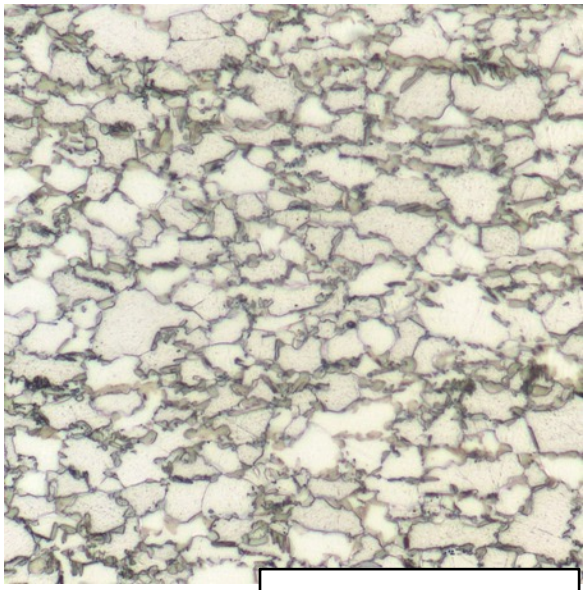
dual-phase steel

- 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

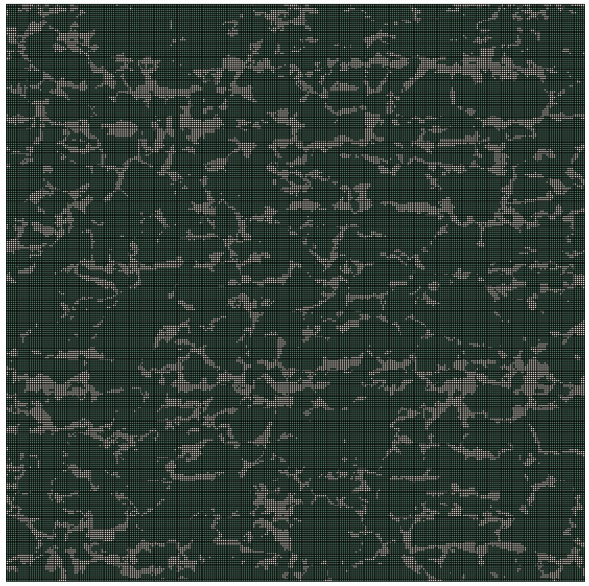
Micromechanical Modeling

- **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



100*100 µm²



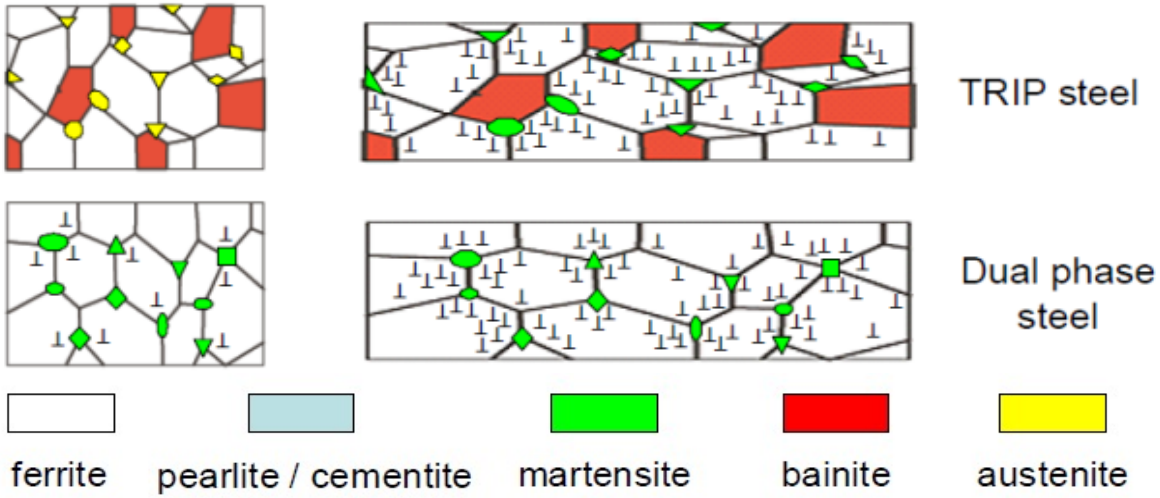
Vajragupta et al. Comp. Mat. Sci. 54 (2012)

Constitutive modelling

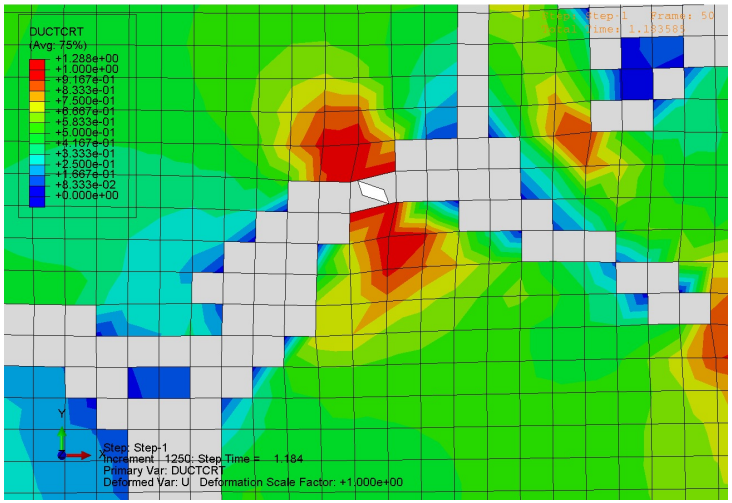
Empirical model for ferritic and martensitic phase (Rodriguez, Mater. Sci. Forum 2003):

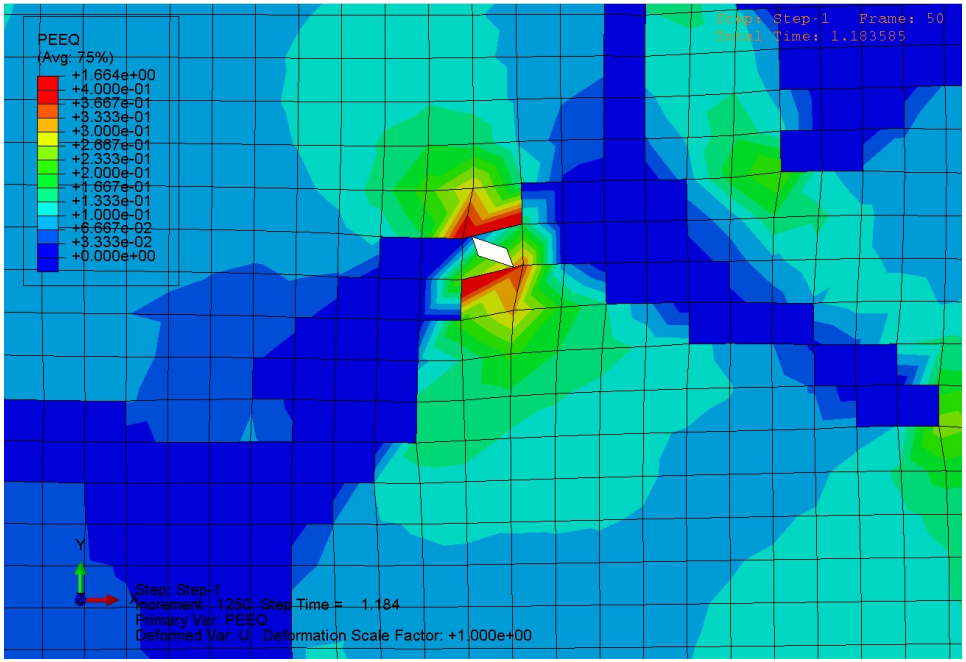
$$\sigma = \sigma_0 + \Delta\sigma + \alpha \cdot M \cdot \mu \cdot \sqrt{b} \cdot \sqrt{\frac{1 - \exp(-M \cdot k \cdot \varepsilon)}{k \cdot L}}$$

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



Micromechanical Modeling





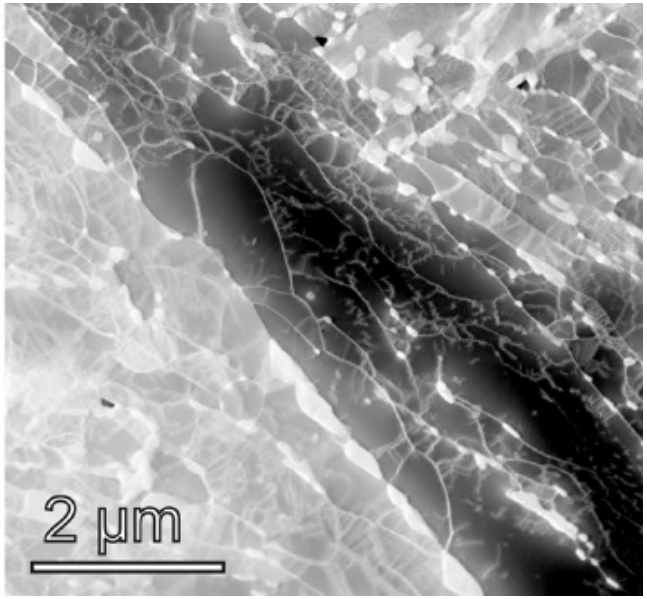
Microcracks in martensite cause strain localization and failure in ferrite.

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

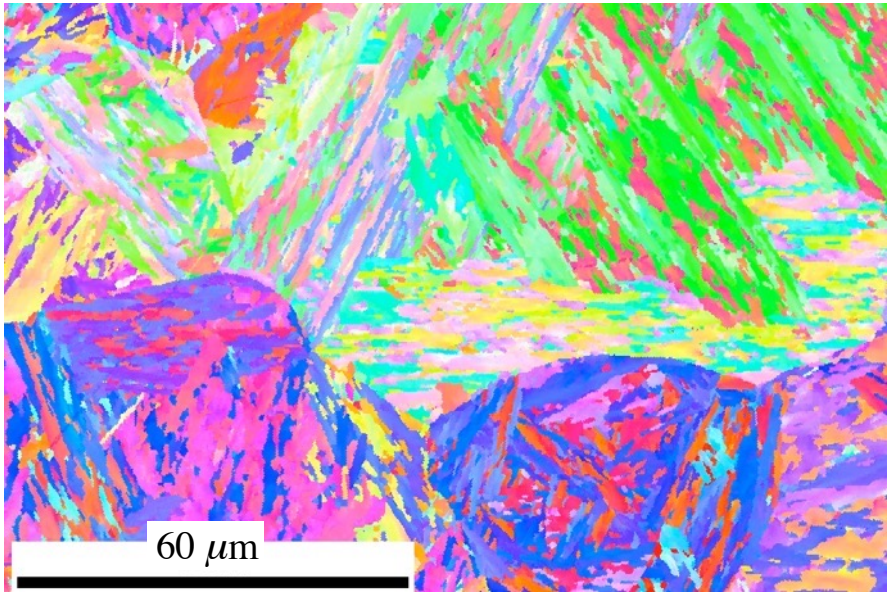
ICAMS Demonstrator Project

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

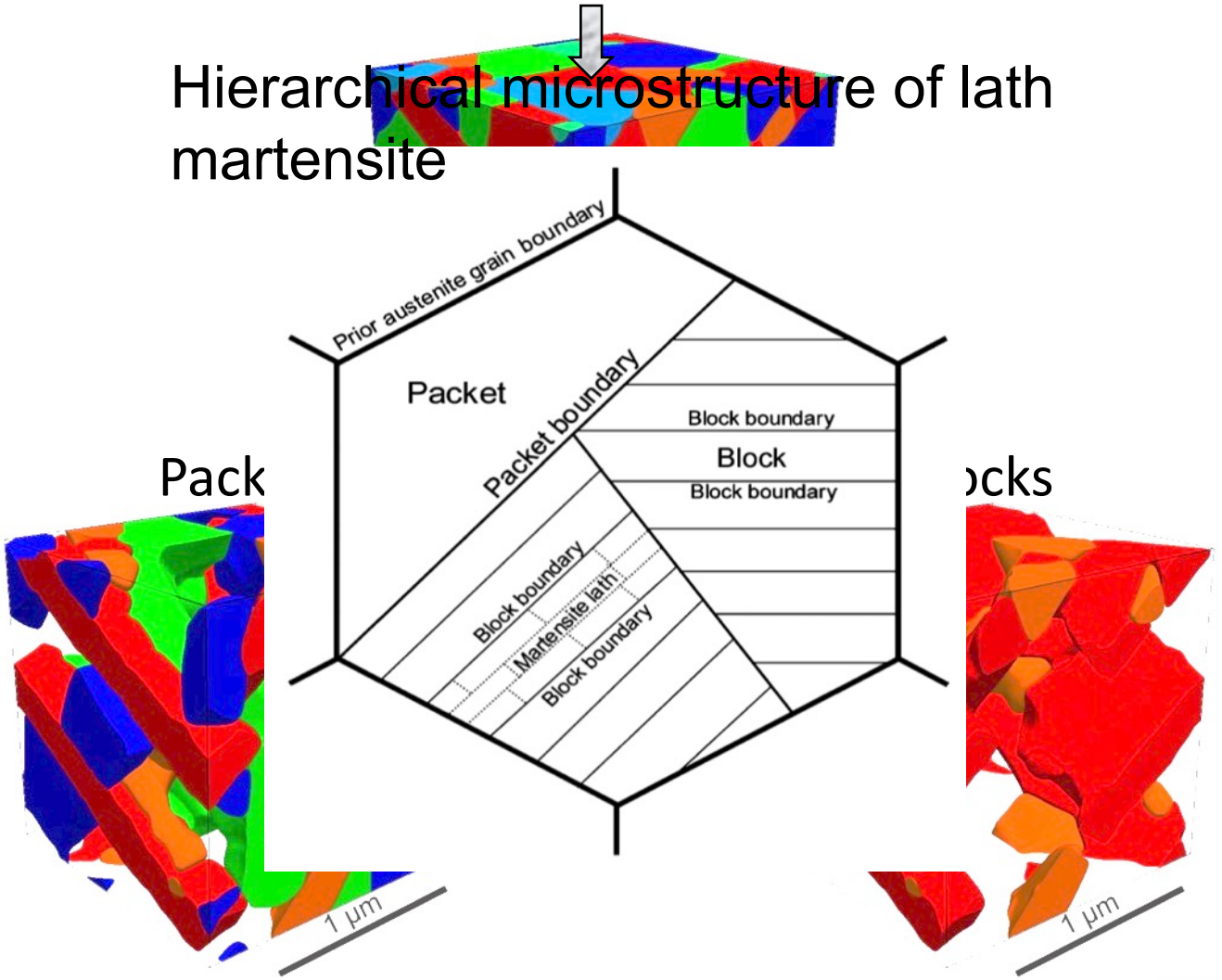


EBSD map of tempered martensite (courtesy V. Yardley)

Pesicka et al. Scripta Mater. 2010

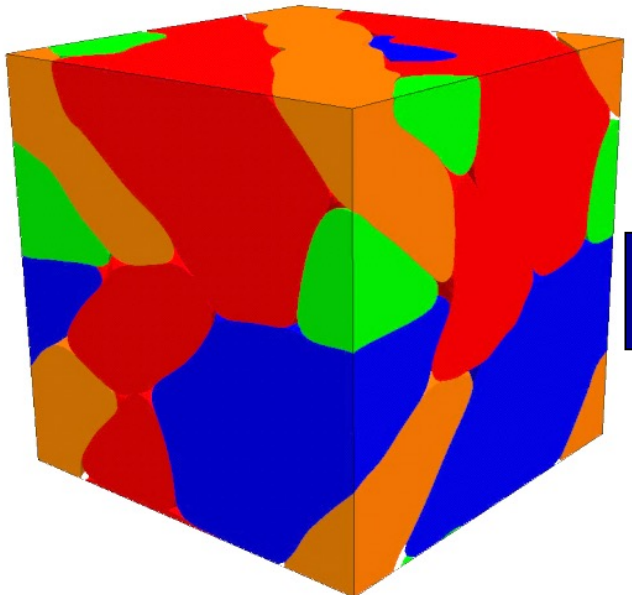
Simulation of martensitic microstructure

Hierarchical microstructure of lath martensite

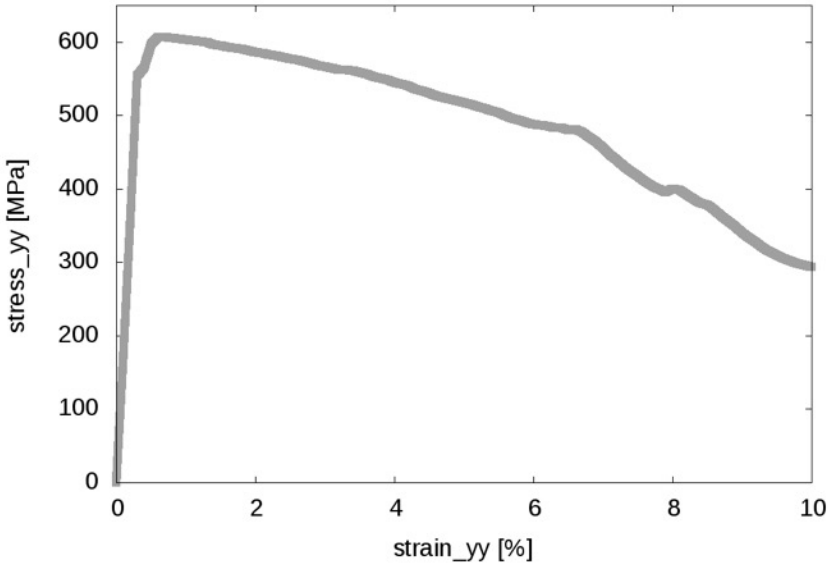


Phasefield simulations: STKS

Property prediction of simulated microstructures



virtual
tensile test

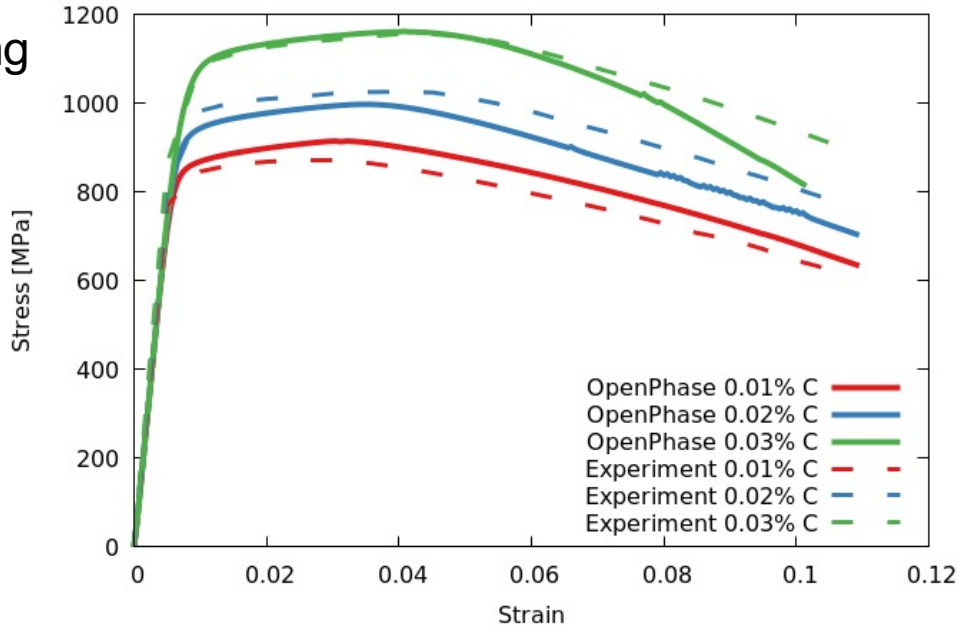


- Property prediction for microstructures from phasefield simulations
- Crystal plasticity and damage model → virtual tensile testing
- Direct modeling from processing to properties

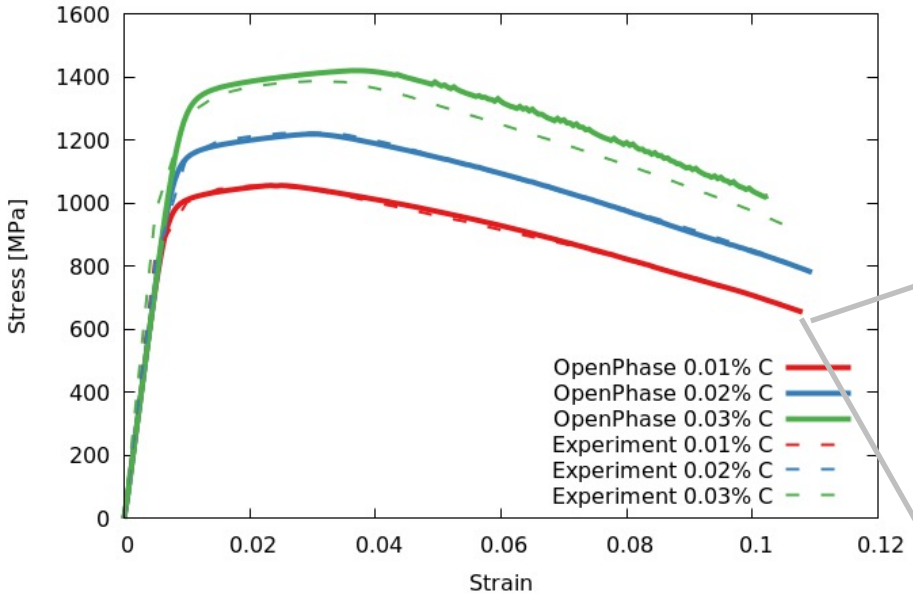
Borukhovich, Du, Stratmann,Boeff, Shchyglo, Hartmaier, Steinbach, materials 9 (2016)

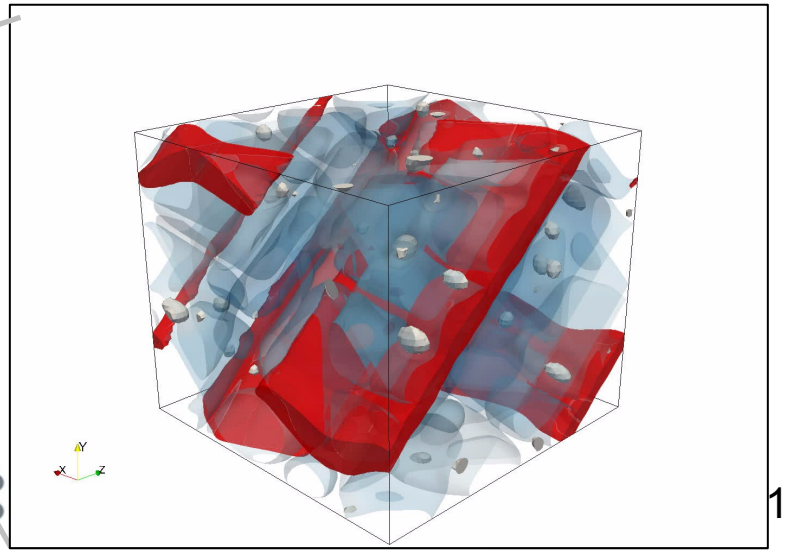
Virtual mechanical testing

100 min. tempering (prediction)

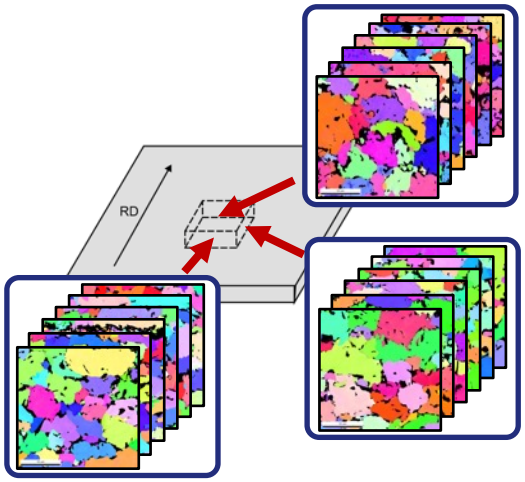


5 min. tempering (fit)

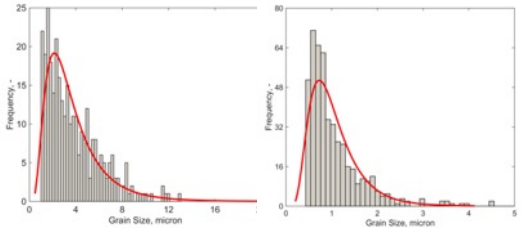




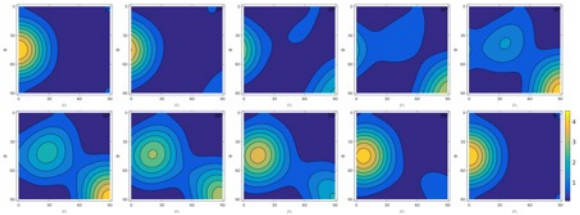
Synthetic microstructure (RVE)



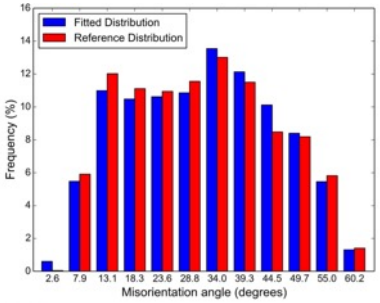
Microstructure characterization



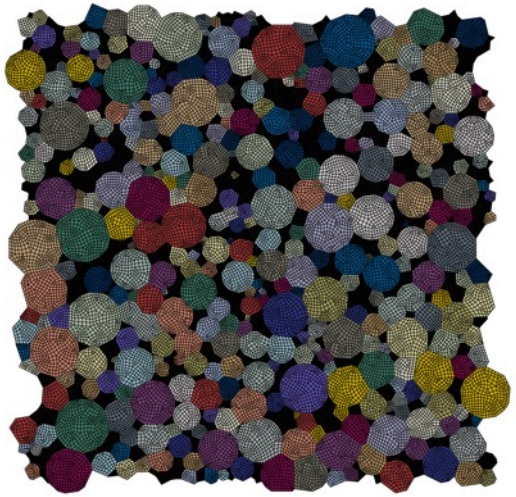
Grain size distribution of constituents



ODF



MDF



Microstructure model

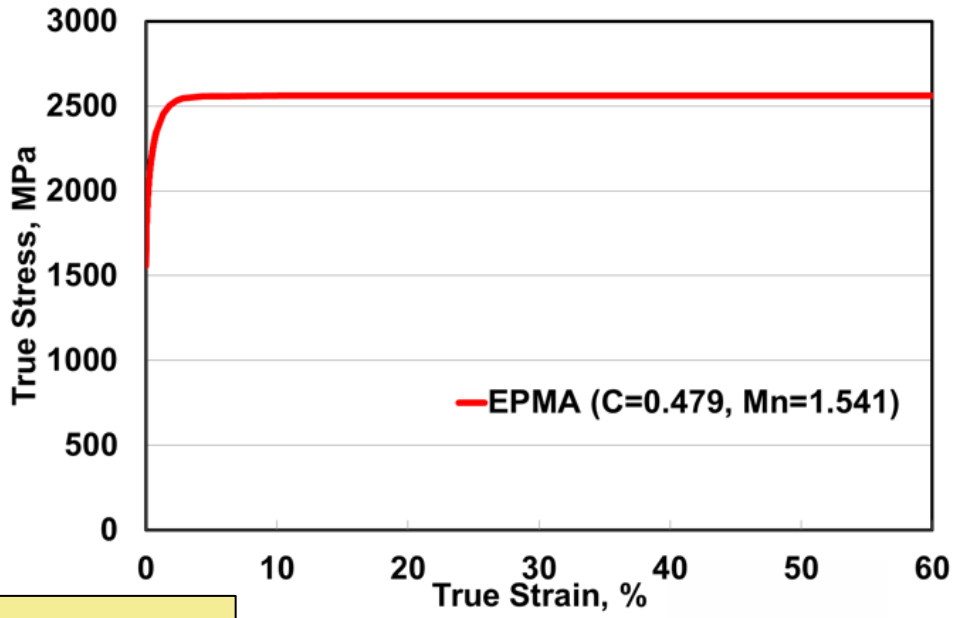
Synthetic microstructure (RVE)

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

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

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

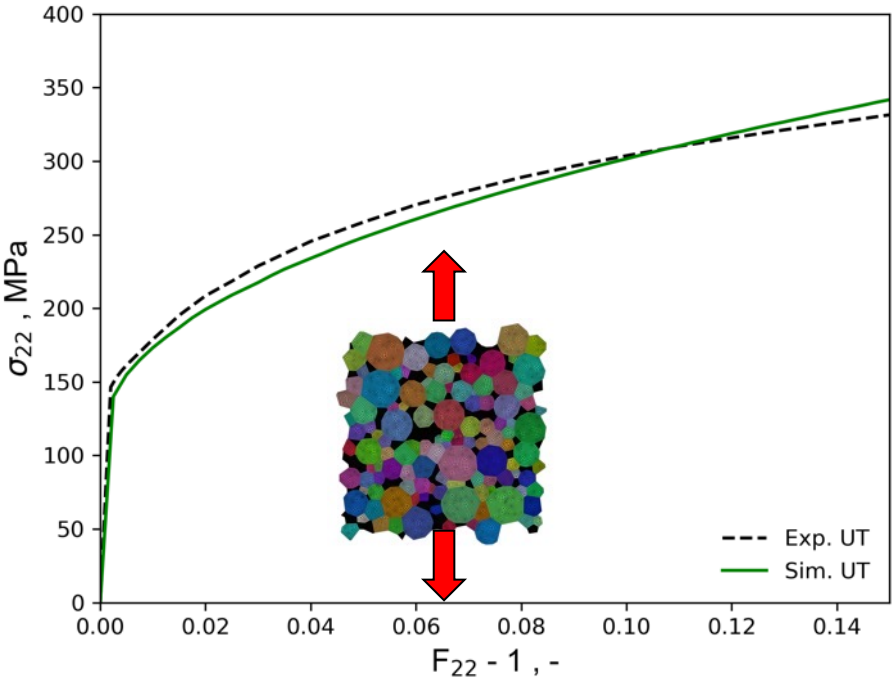
$$\Delta\sigma = 3065 \cdot \left(\%C_{ss}^{f}\right) - 161$$



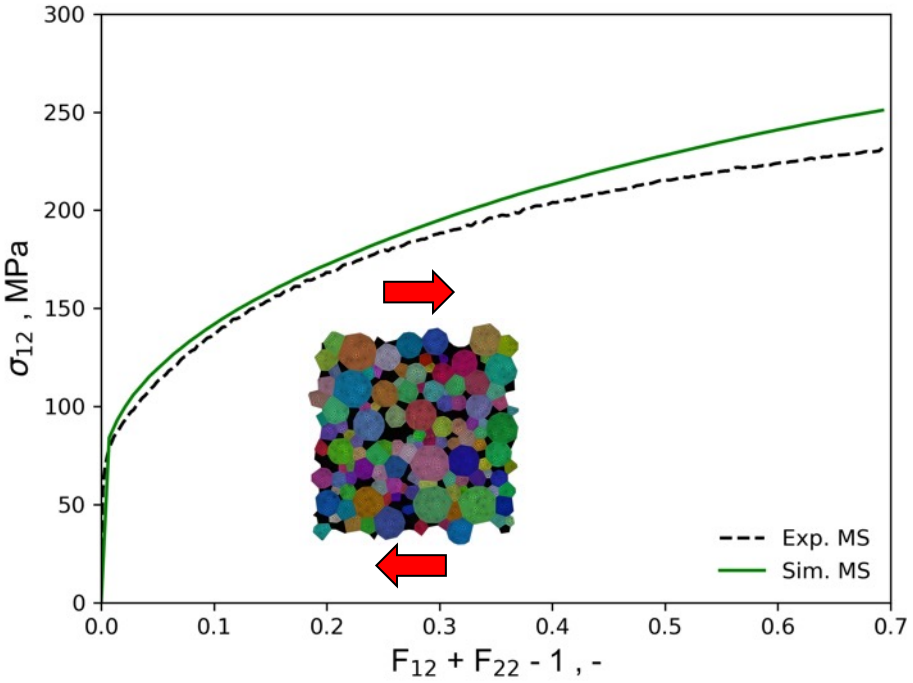
Vajragupta et al. Comp. Mat. Sci. 94 (2014)

Parameterization of nonlocal crystal plasticity model

Parameter fitting



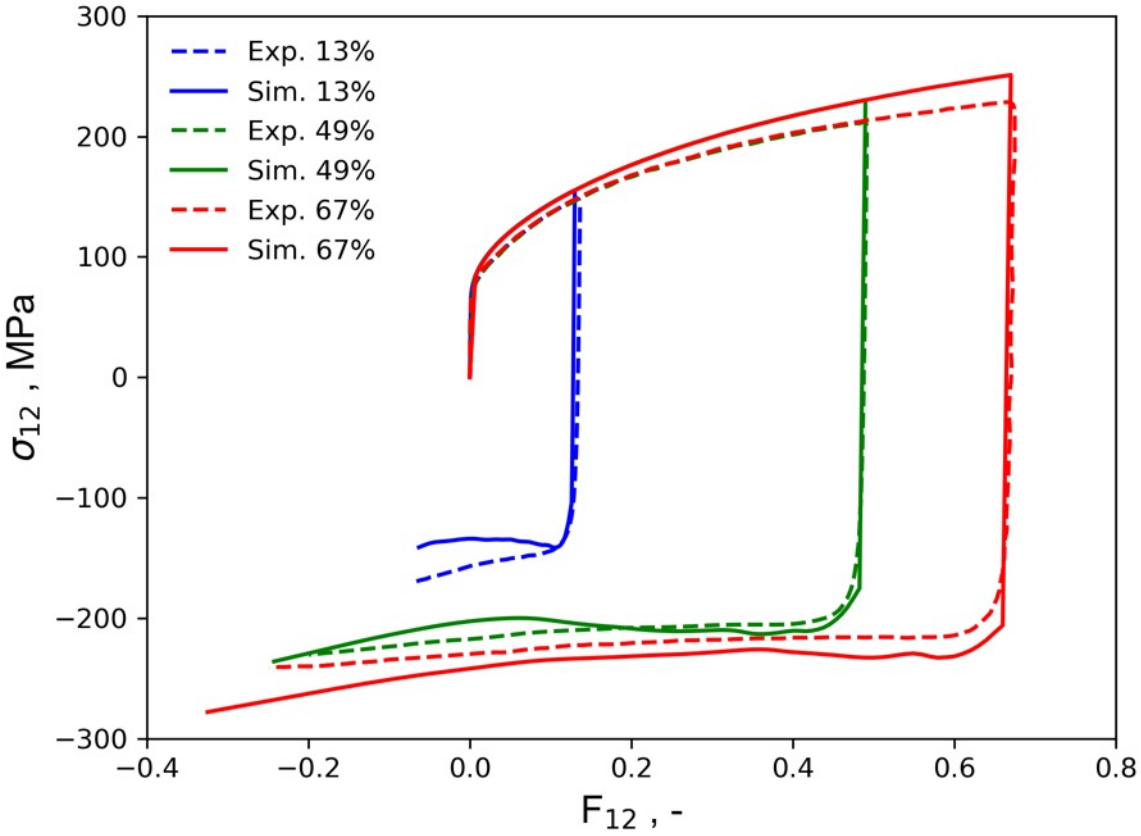
Uniaxial tension



Monotonic shear

Parameterization of nonlocal crystal plasticity model

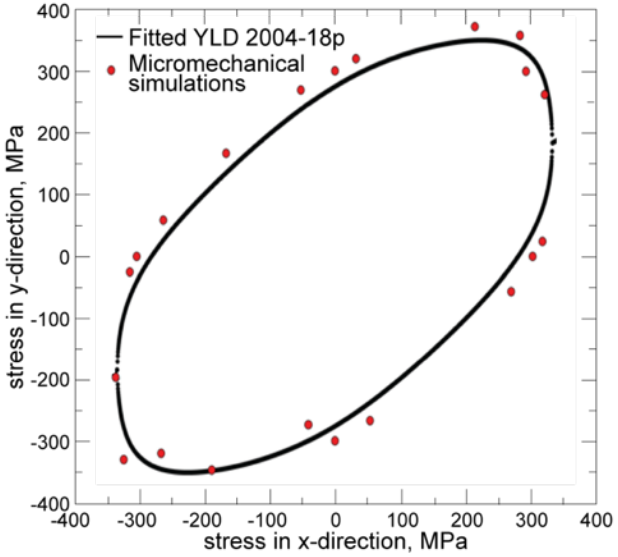
Parameter validation



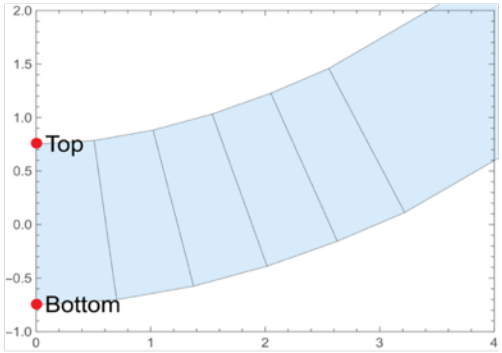
Shear reversal

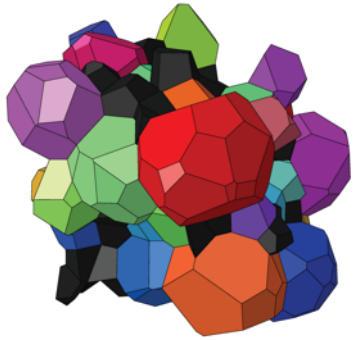
Micromechanical modeling of DP600 steel

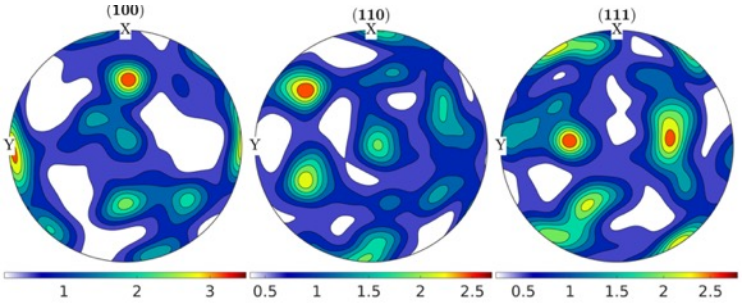
DP600 microstructure



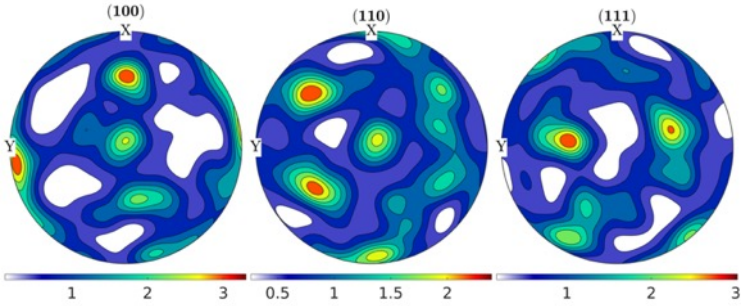
Parameterization of Barlat YLD2004-18p







Top



Bottom

Texture evolution during air bending process

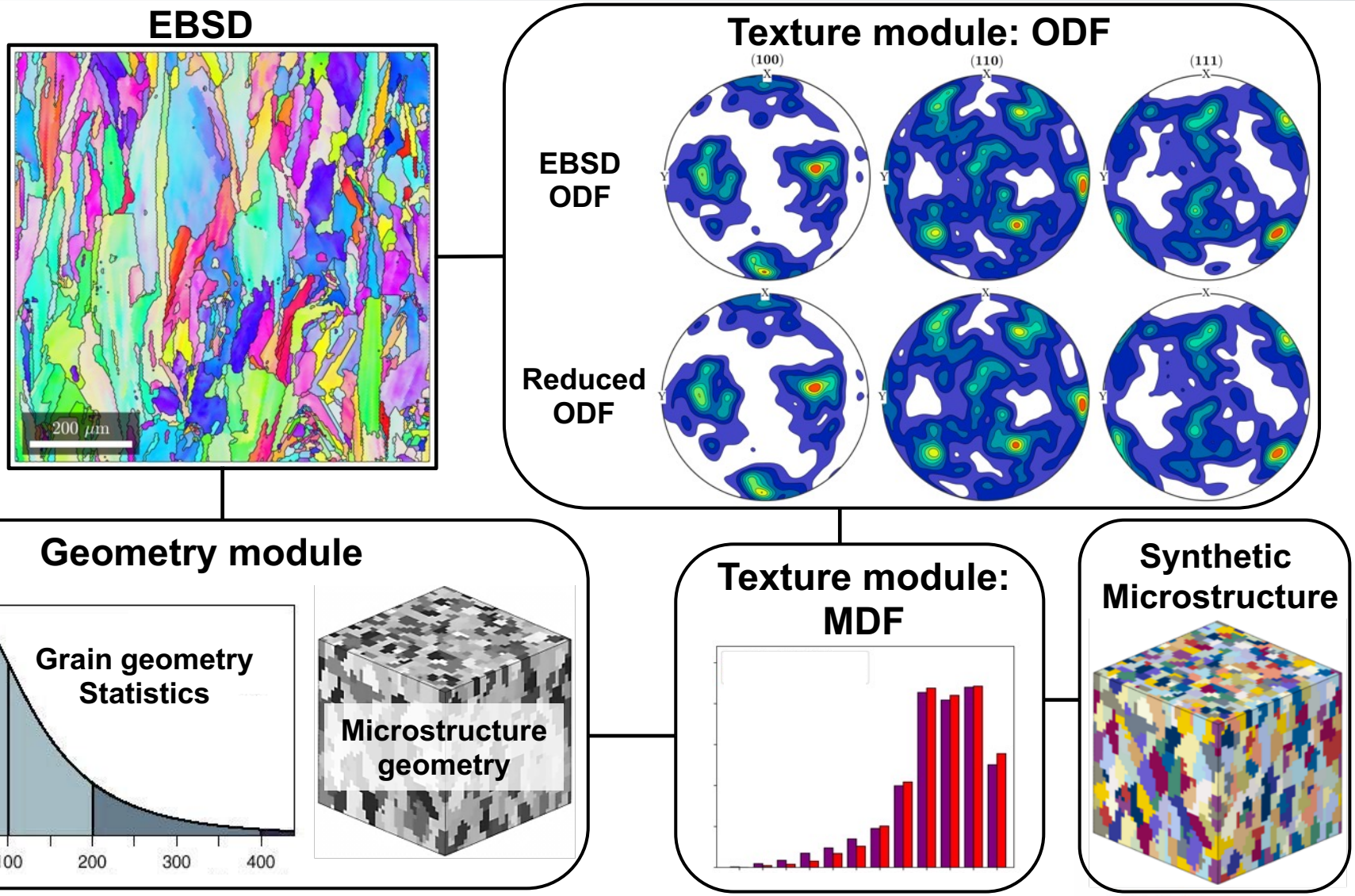
Source: Vajragupta et al., Procedia Manufacturing 2020

Outline

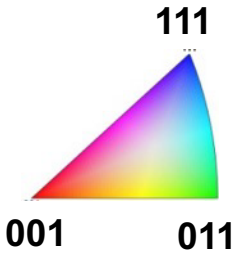
- Micromechanical modeling with
  - experimental
  - simulated
  - synthetic microstructures
- Synthetic microstructures with Kanapy
- Influence of grain statistics
- Porous microstructures

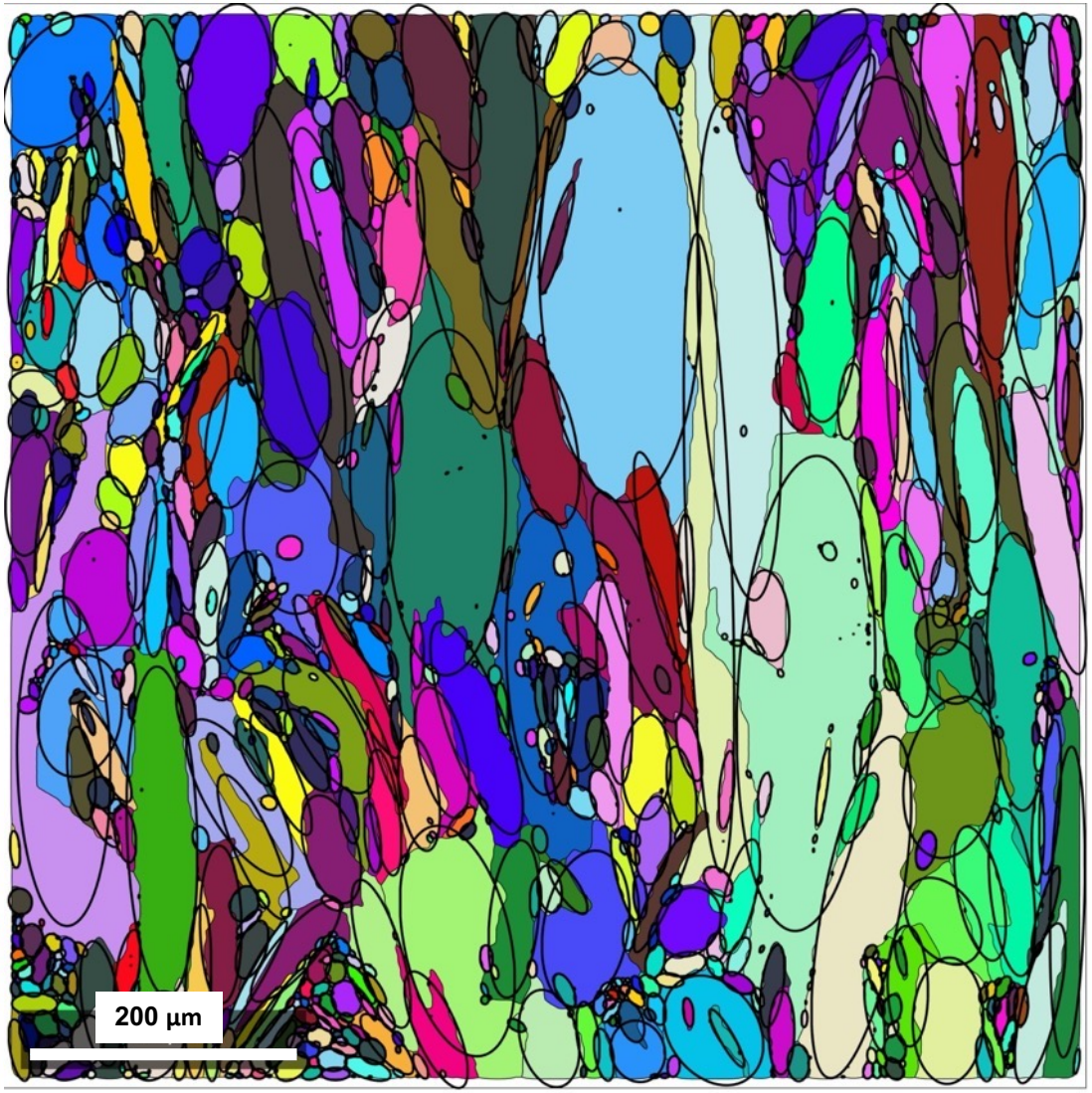
- Demonstration 1: Two-phase microstructures
- Demonstration 2: Polycrystals and crystallographic texture

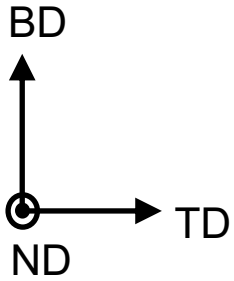
Kanapy: Work flow



Elements of microstructure : Grains



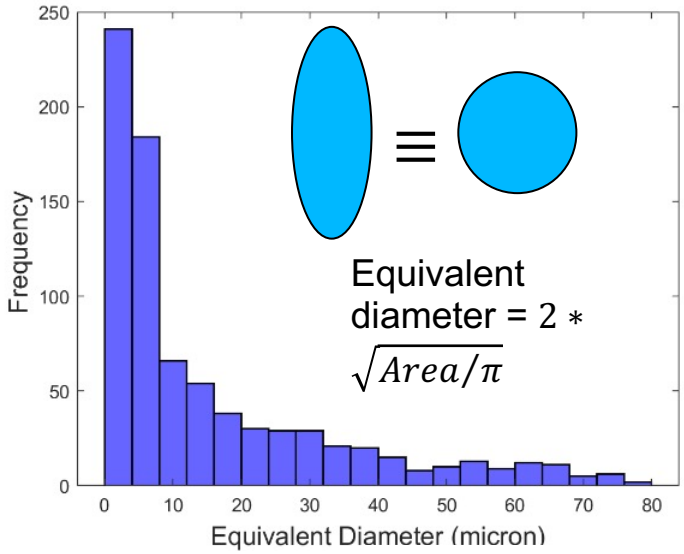


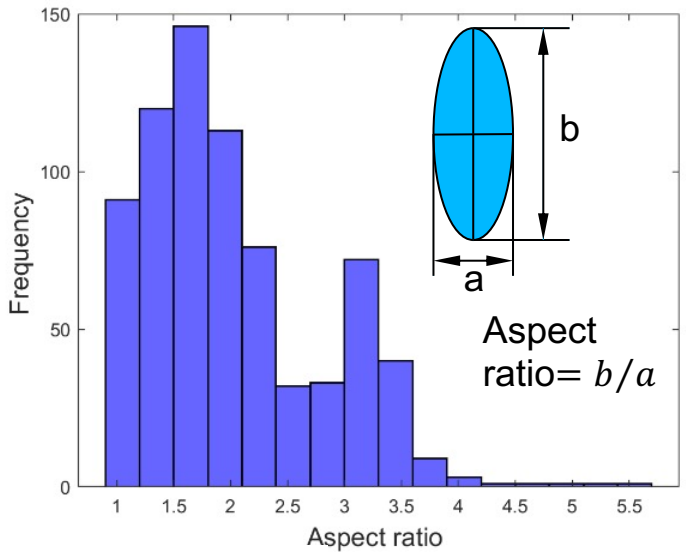


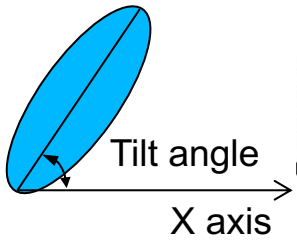
BD: Building direction
TD: Transverse direction
ND: Normal direction

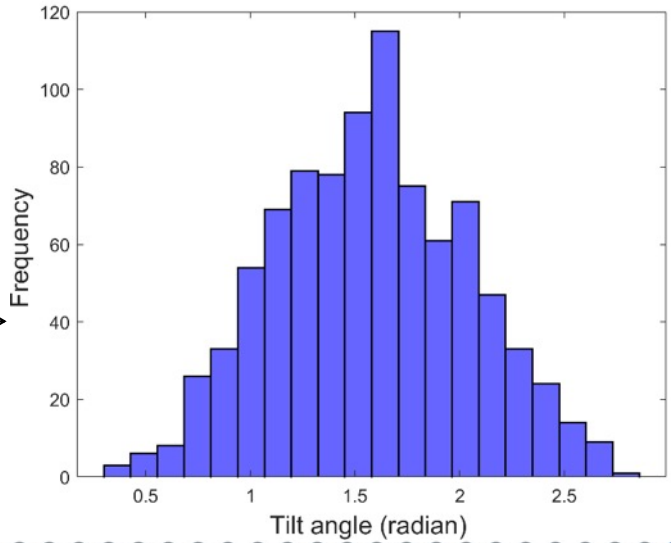
MTEX documentation
https://mtex-toolbox.github.io/Documentation.html

Elements of microstructure : Grain statistics



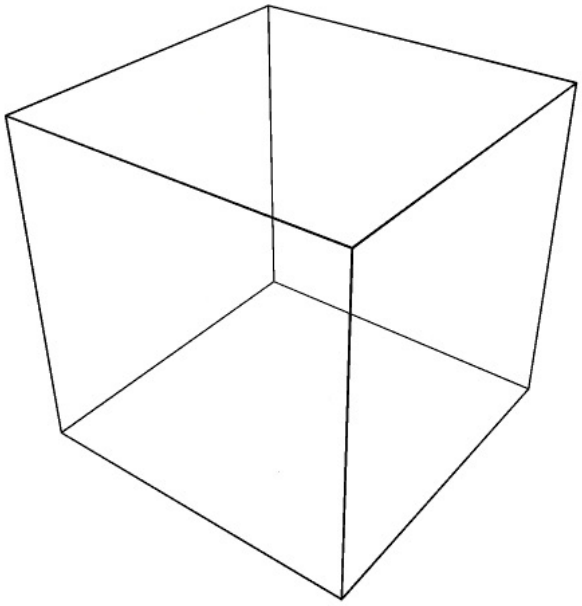




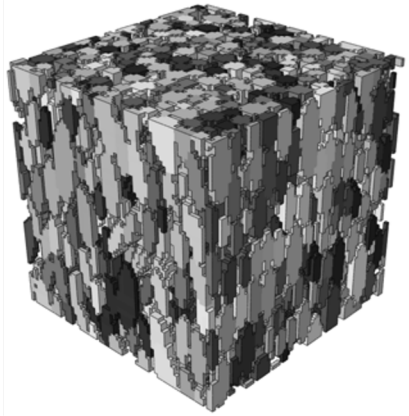


Kanapy: Synthetic microstructure generator

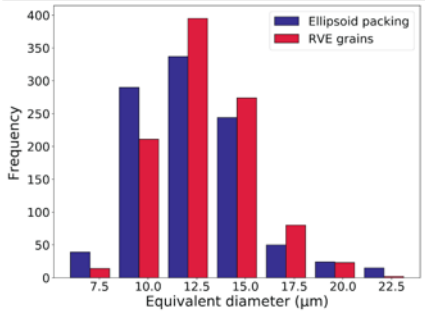
Kanapy geometry module



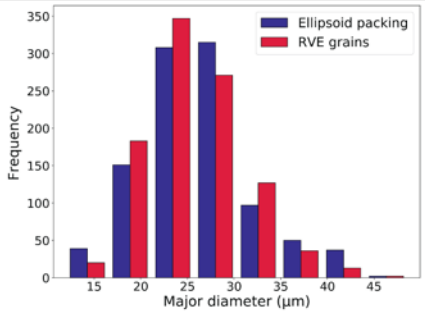
Time-driven particles packing method (advantages over RSA)



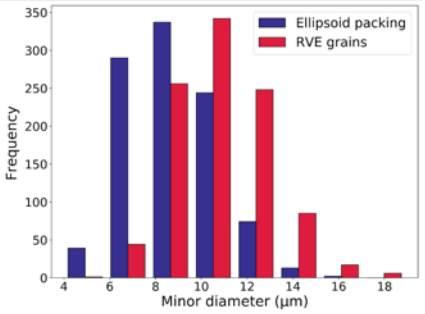
Voxelization



Equivalent diameter



Major diameter

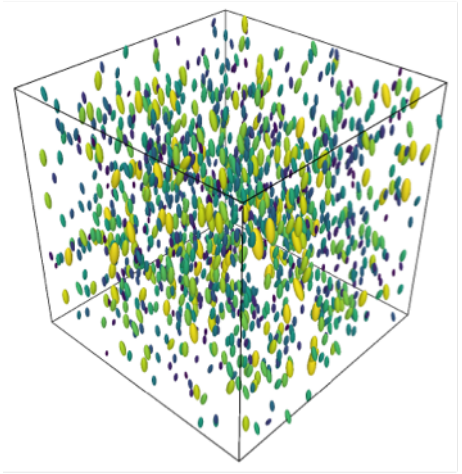


Minor diameter

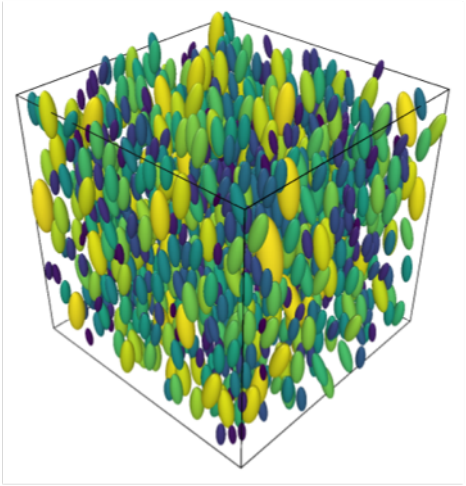
Statistical comparison of grain geometries

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

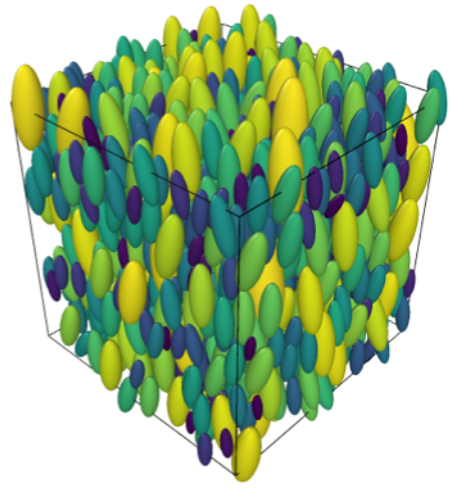
Geometry Module: Particle simulation



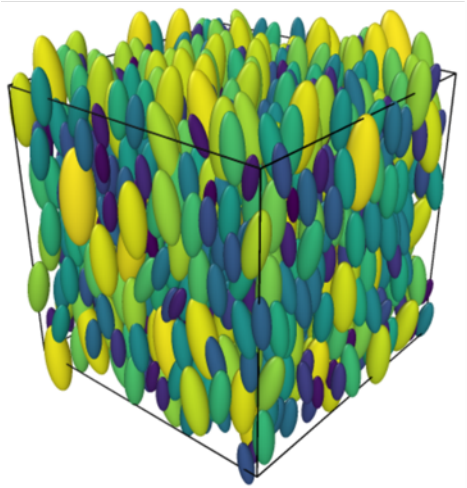
Time step : 250



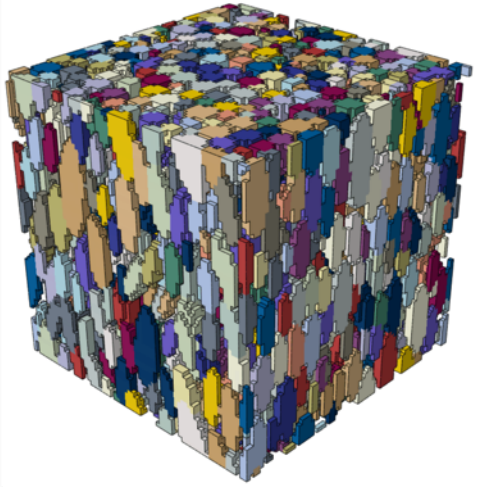
Time step : 550

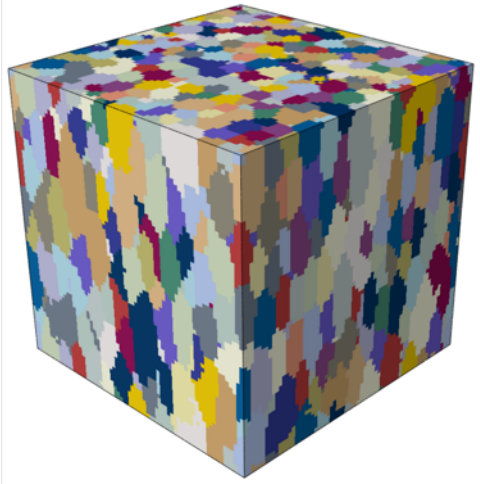


Time step : 850



Ellipsoid packing

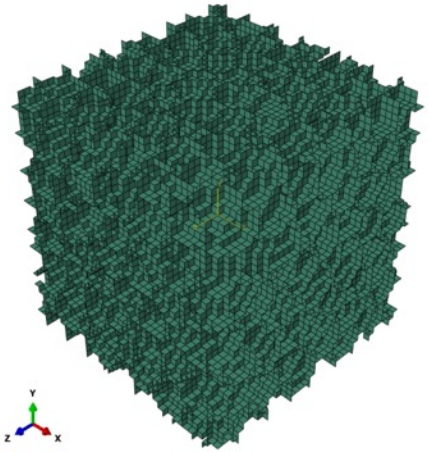




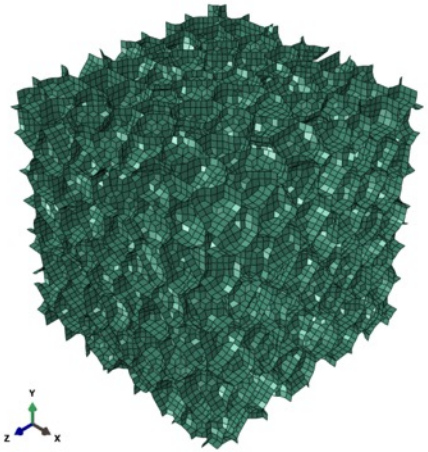
Voxelization - Hexahedral meshing

Kanapy: Synthetic microstructure generator

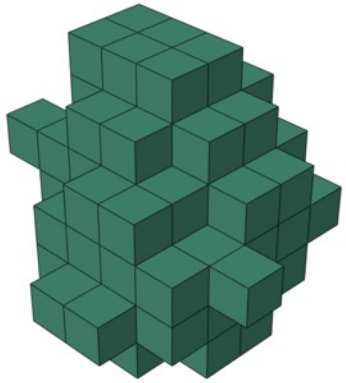
Kanapy geometry module



Voxelated grain boundaries



Smoothed grain boundaries



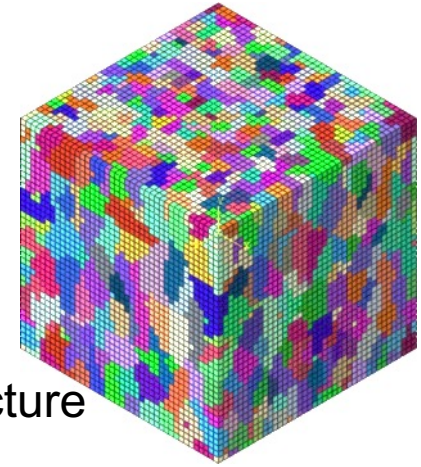
Voxelated grain

Smoothed grain

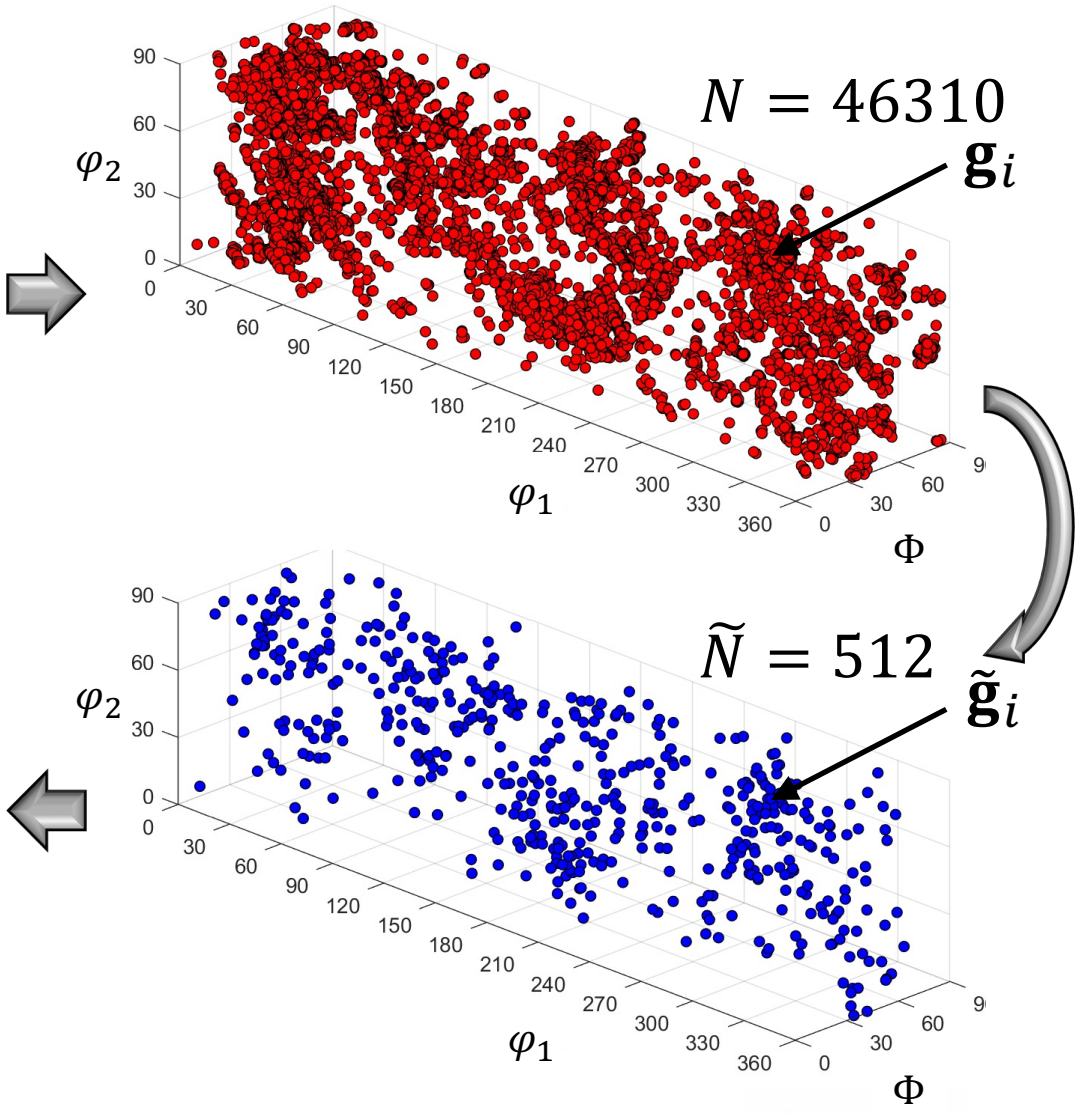
Source: https://github.com/ICAMS/Kanapy

Orientation distribution reconstruction

EBSD



Virtual microstructure



Orientation distribution reconstruction

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

Equi-spaced grid ($\Delta\theta$)

Distribute $\mathbf{g}_i$ among the grid points lying within ($\Delta\theta/2$)

$\{ \; + \; + \; \ldots \}$

$n_1 \quad n_2$

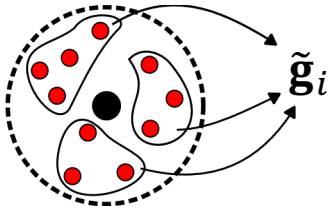
$\sum n_i = N$

Calculate scaling factor (α) using Integer approximation*

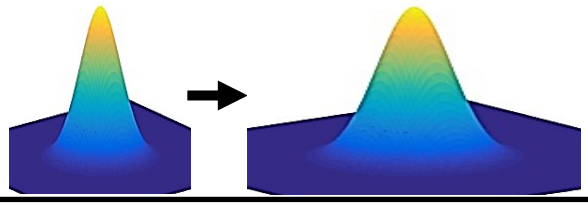
$\tilde{n}_i = round(\alpha \cdot n_i)$

$\sum \tilde{n}_i \approx \tilde{N}$

Further sub-divide for $\tilde{n}_i > 1$ and calculate mean orientations



Estimate ODF ($f(\tilde{\mathbf{g}})$) and optimize kernel ($\psi_{\tilde{\kappa}}$)



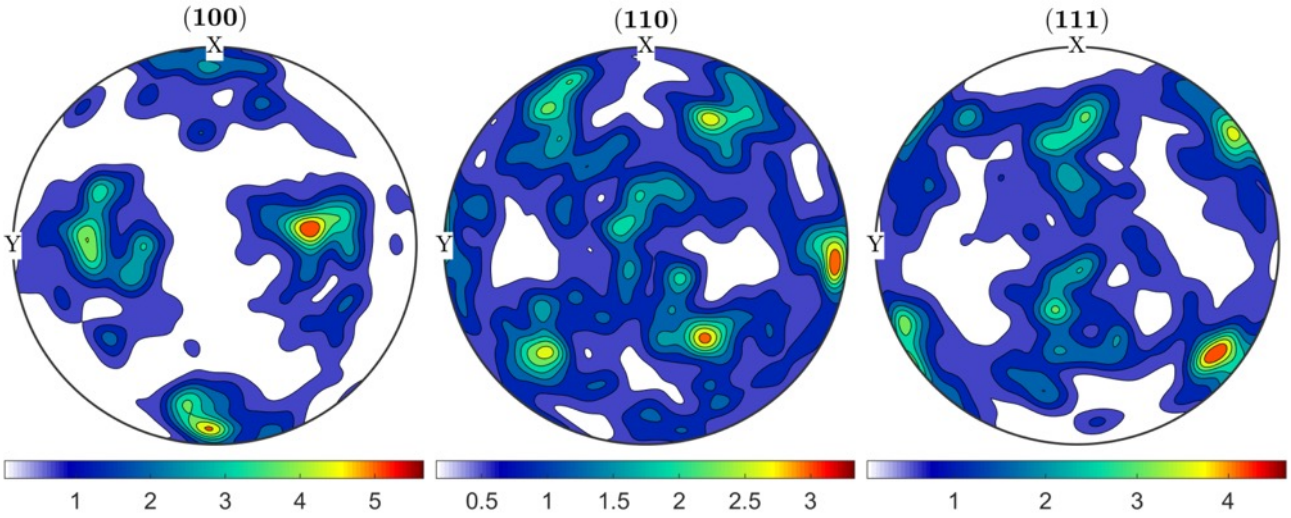
Estimate $\|f(\mathbf{g}) - f(\tilde{\mathbf{g}})\|_1$ Update $\Delta\theta$

Biswas et al., J of applied crystallography, 2020

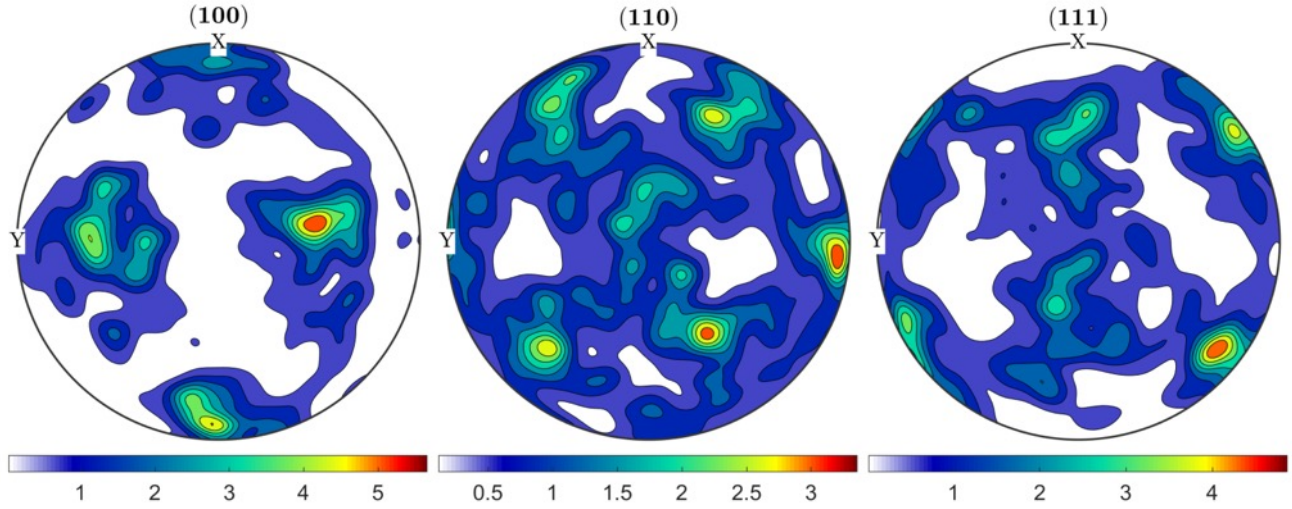
*Eisenlohr & Roters 2008 / Lefers & Jensen 1986

Orientation distribution reconstruction

$f(\mathbf{g})$



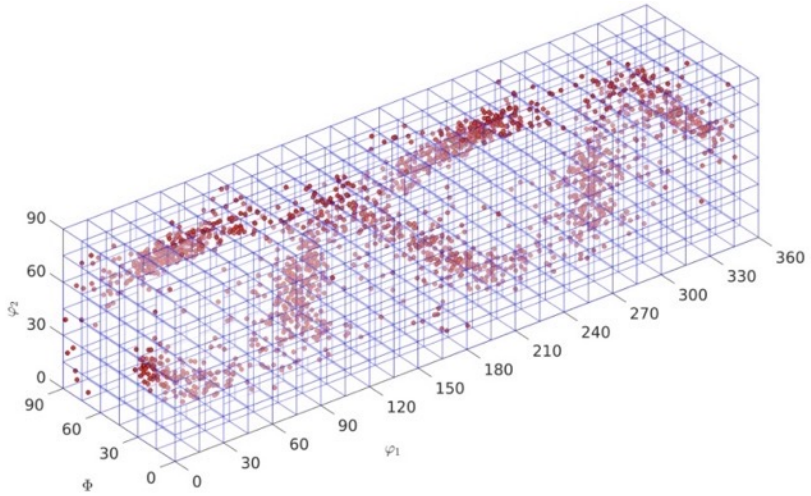
$f(\tilde{\mathbf{g}})$



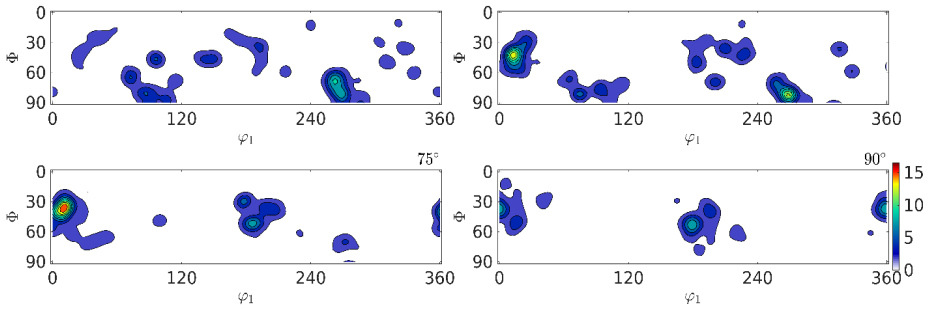
Biswas et al. J. Appl. Cryst. 12020
https://doi.org/10.1107/S1600576719017138

Kanapy: Synthetic microstructure generator

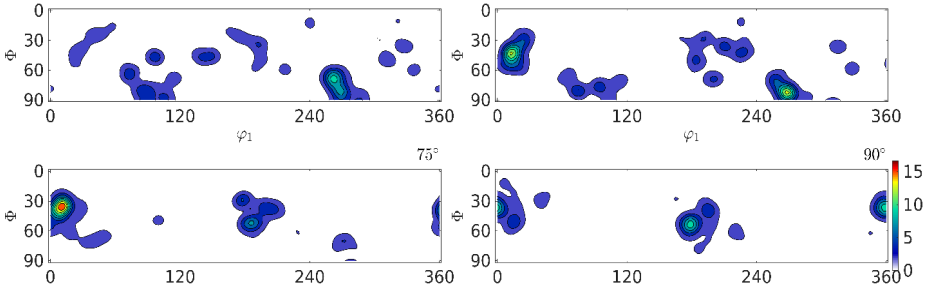
Kanapy ODF reconstruction module



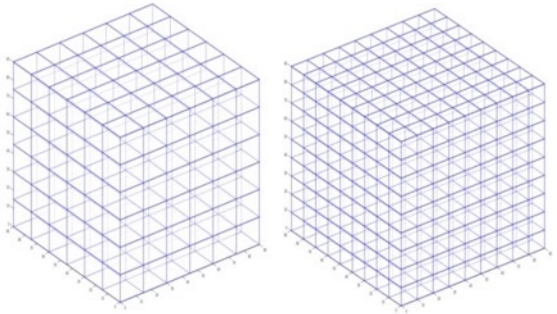
Integer Approximation (IA)



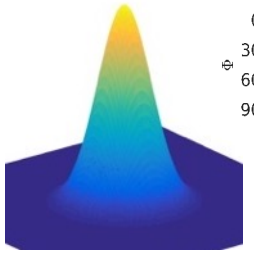
Experimental ODF



Discretized ODF



Grid spacing $\Delta\theta$ optimization

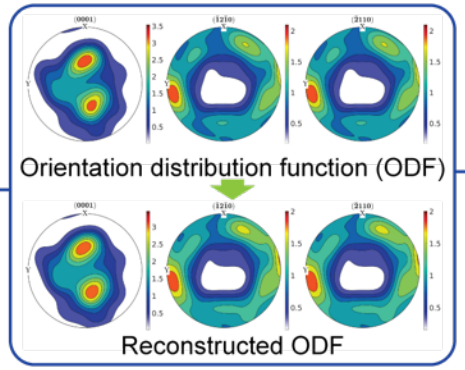


Kernel optimization

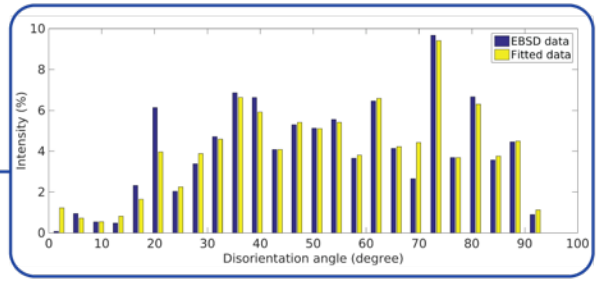
Source: Biswas et al. J. Appl. Crystallogr. 2020

Kanapy: Synthetic microstructure generator

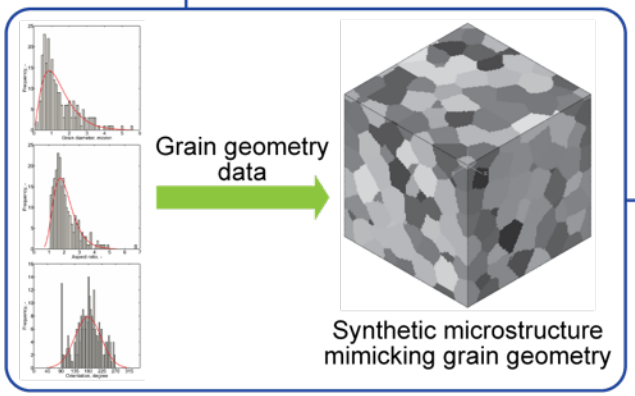
EBSD



Kanapy ODF reconstruction module

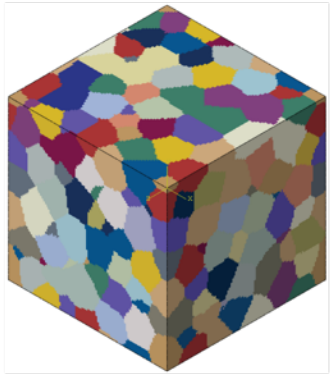


Kanapy orientation assignment module



Kanapy geometry module

Grain boundary surface area



Equiaxed grains

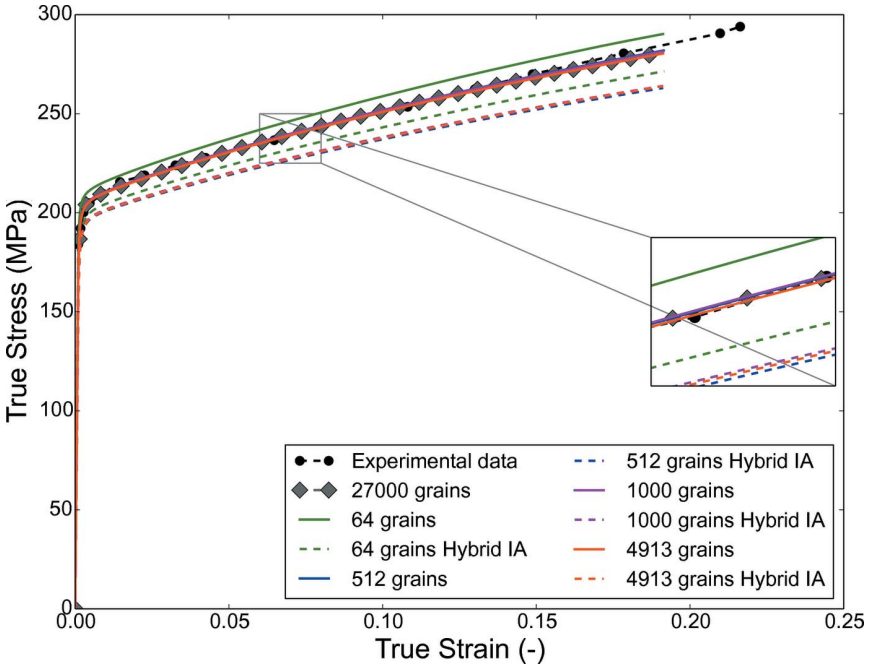
Elongated grains

Synthetic microstructure

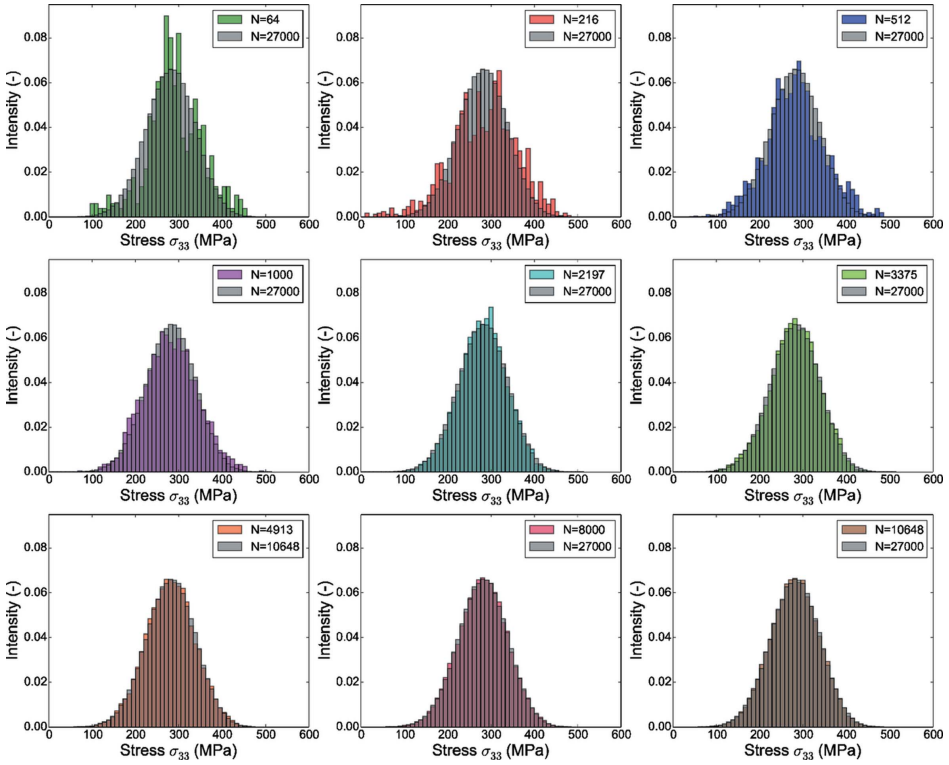
Source: https://github.com/ICAMS/Kanapy

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

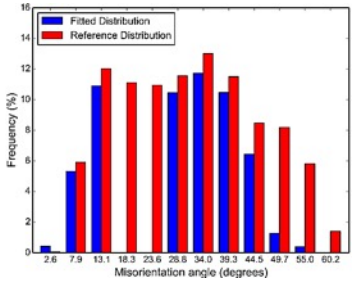
Kanapy orientations assignment module

Inputs

- Orientation set
- Grain boundary area
- Grain neighbors
- Misorientation statistical distribution

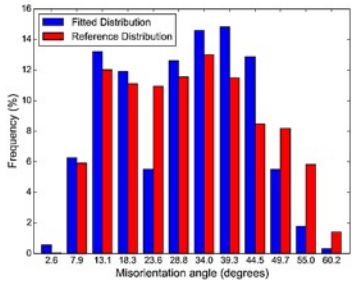
First stage

- Misorientation calculation
- Prioritization of misorientation data
- Strict orientation assignment to neighbors



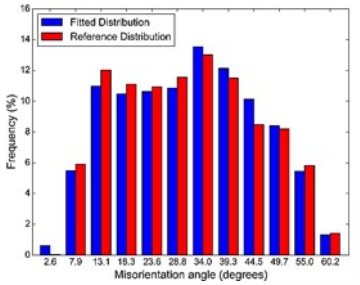
Second stage

- Rearrangement of priority array
- Identify empty neighbors for each grain
- Relaxed orientation assignment to neighbors



Third stage

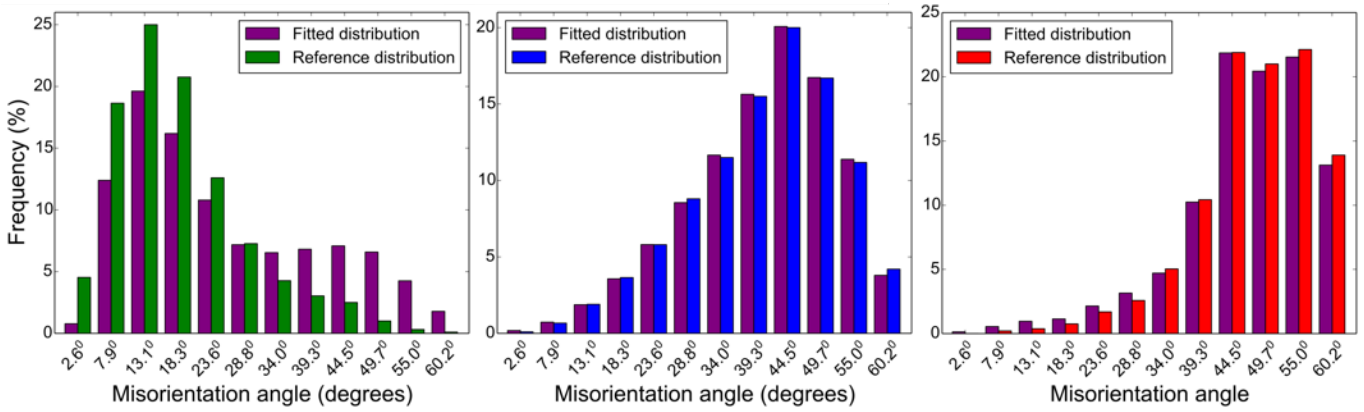
- Error estimation
- Weight calculation
- Score estimation and update



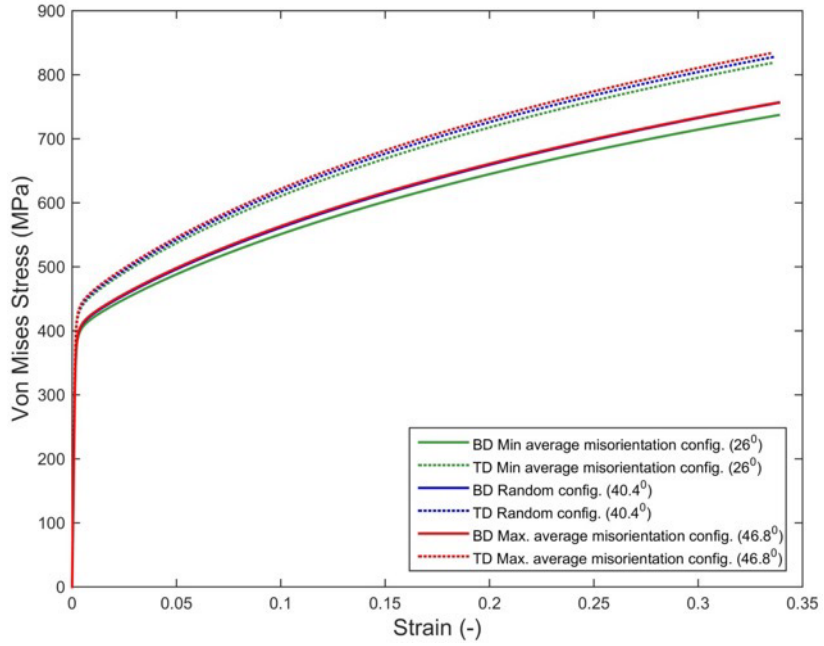
Order of orientation assignment

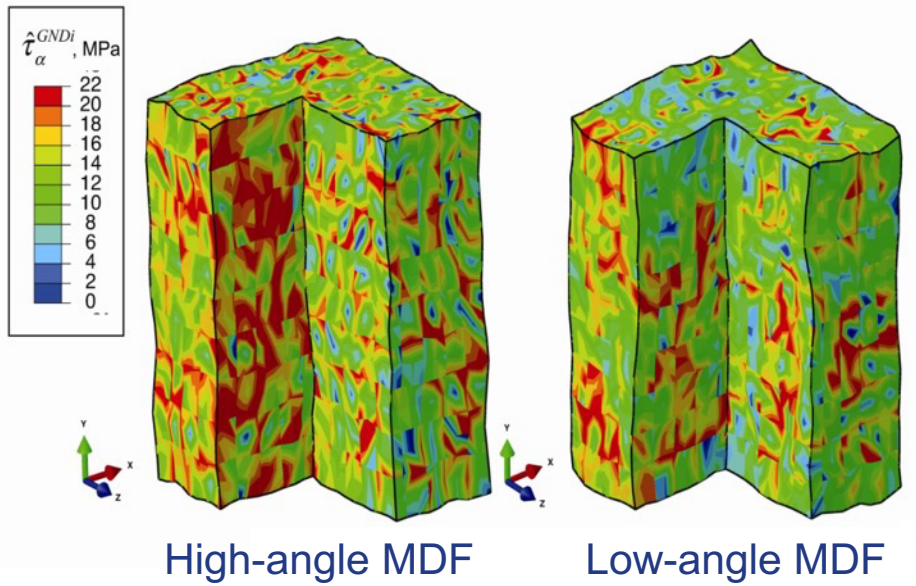
A. Biswas et al. Adv. Eng. Mater. 2019

Influence of misorientation distribution (MDF)



Low-angle MDF | Random MDF | High-angle MDF





High-angle MDF | Low-angle MDF

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

Outline

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- Porous microstructures

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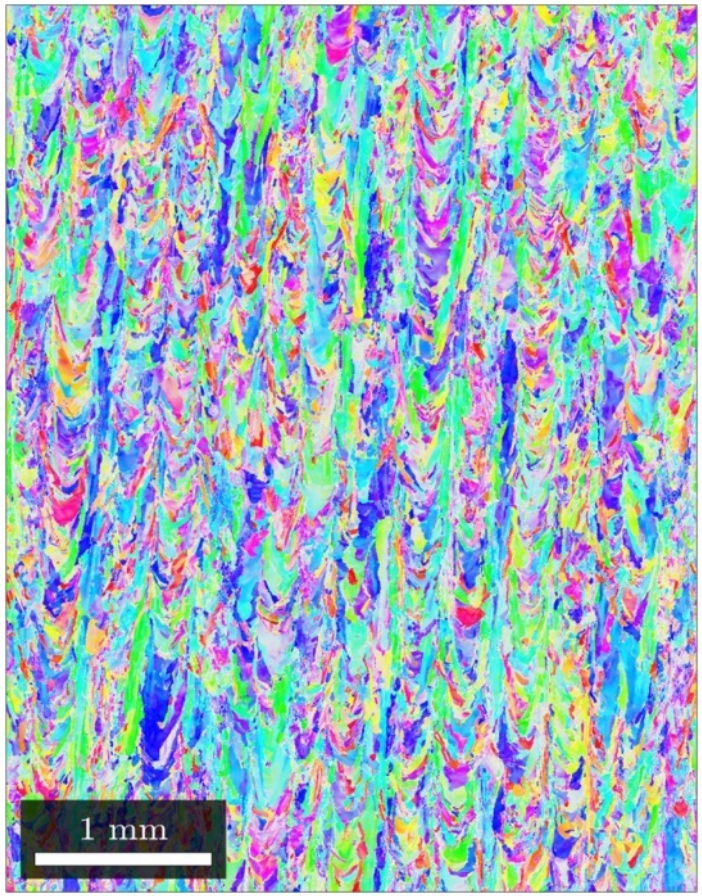
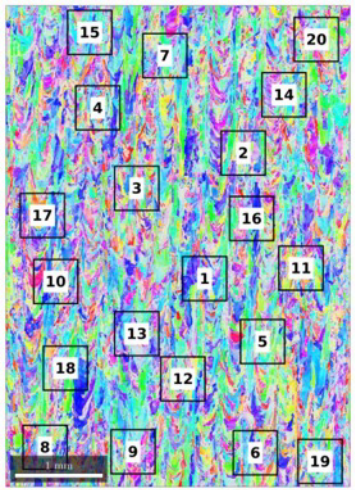
- Demonstration 2: Polycrystals and crystallographic texture

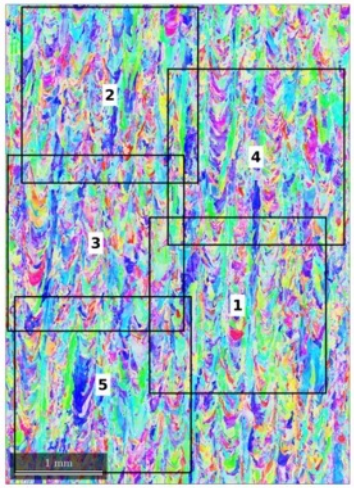
Effect of grain statistics on micromechanical modeling



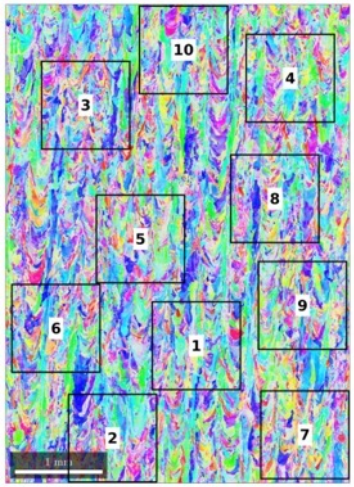
4x5 mm² EBSD



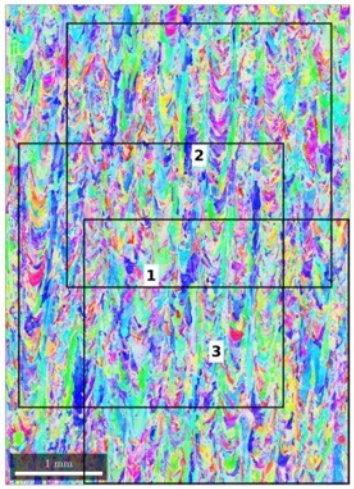
0.5x0.5 mm²



2x2 mm²



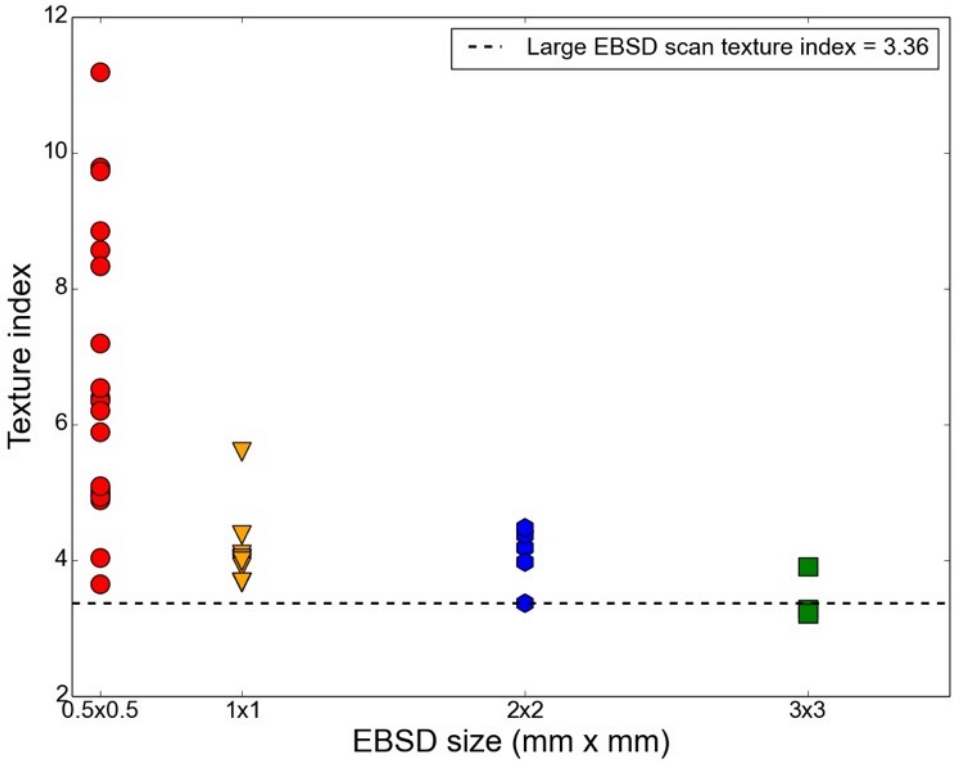
1x1 mm²

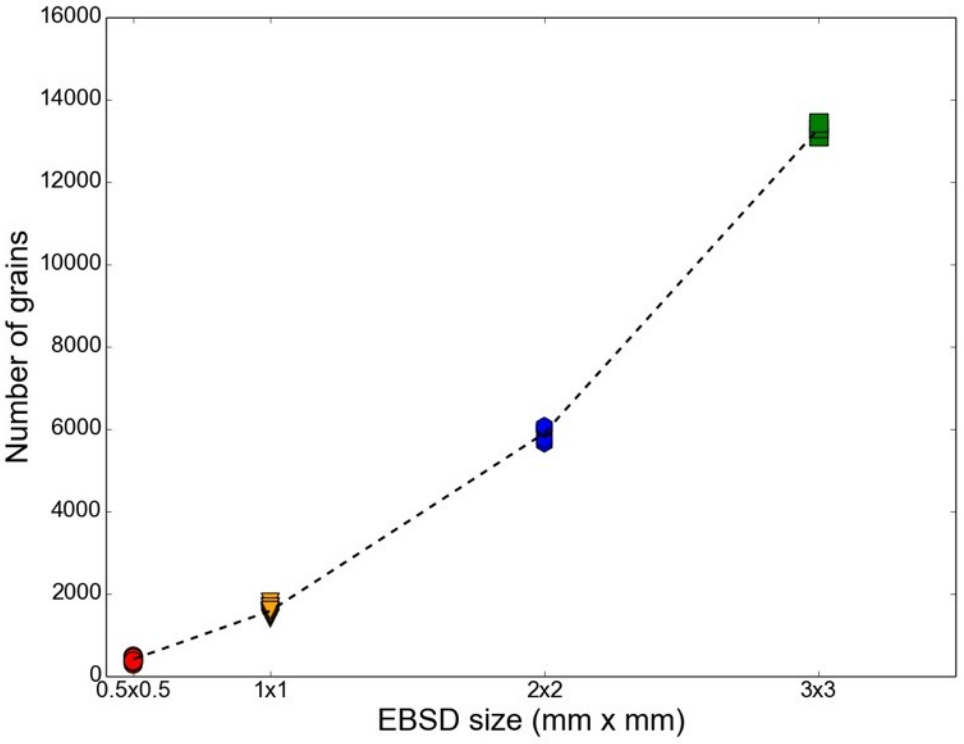


3x3 mm²

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

Effect of grain statistics on micromechanical modeling



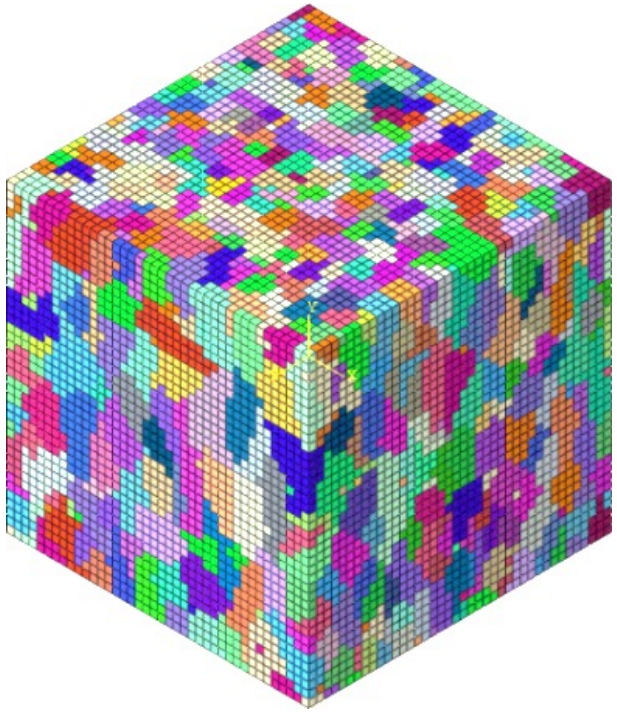


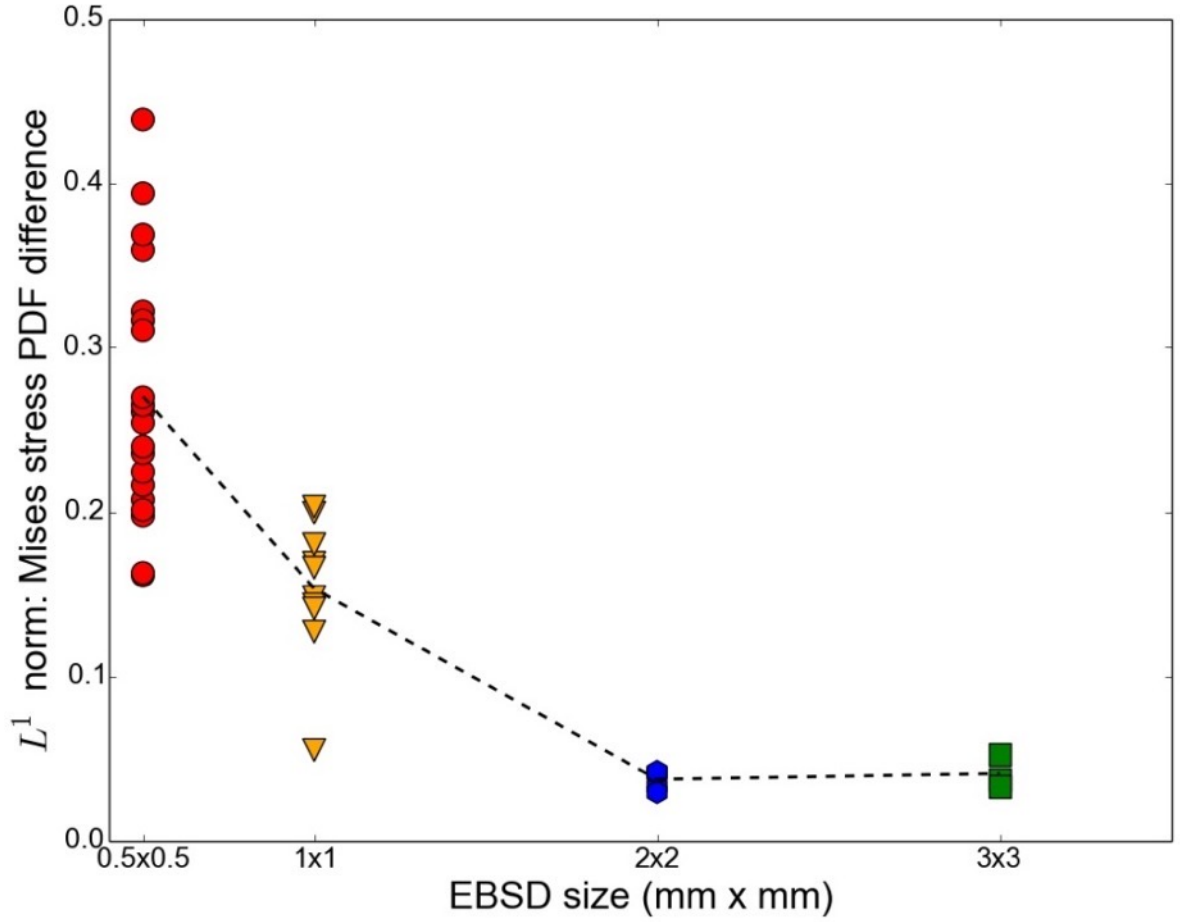
$\bar{f}$: ODF estimated from cropped EBSD

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

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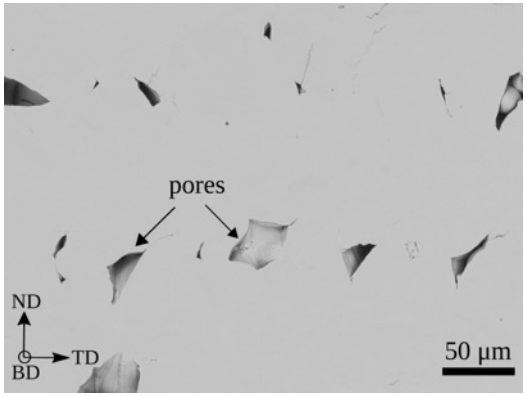
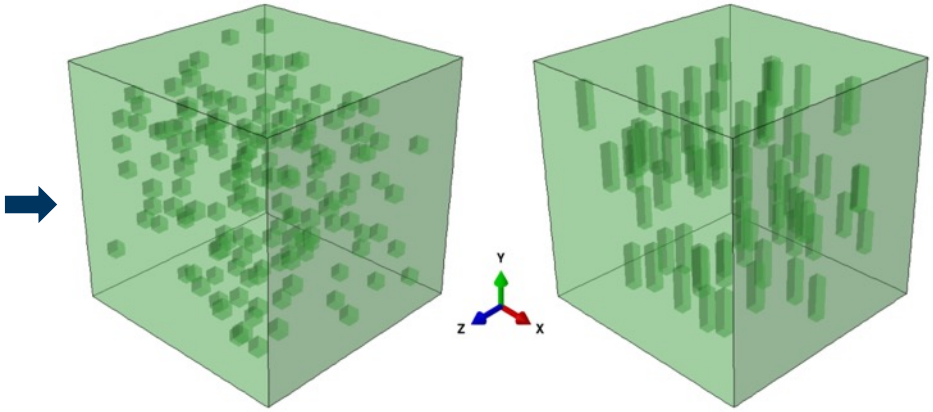
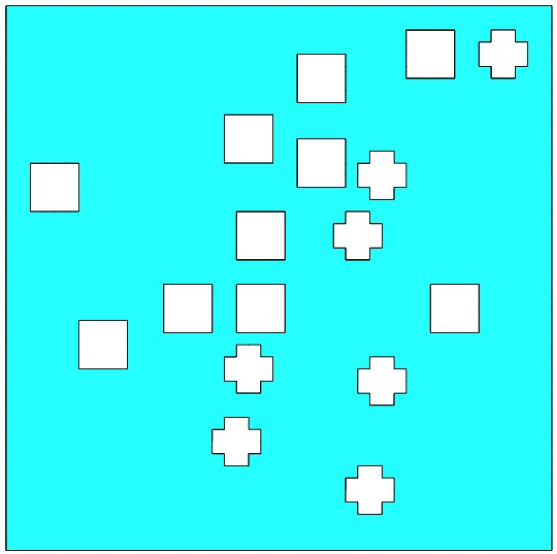
Micromechanical modeling – Modeling pores and Damage



Pores

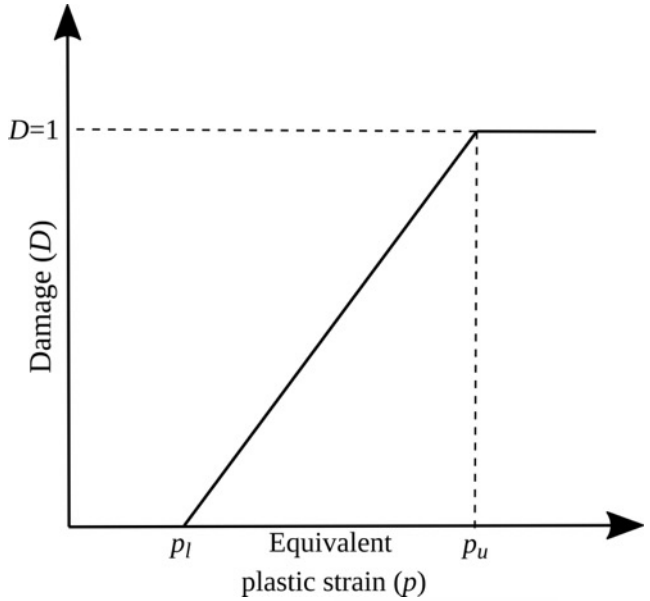


RVEs containing equiaxed and elongated pores



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

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



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

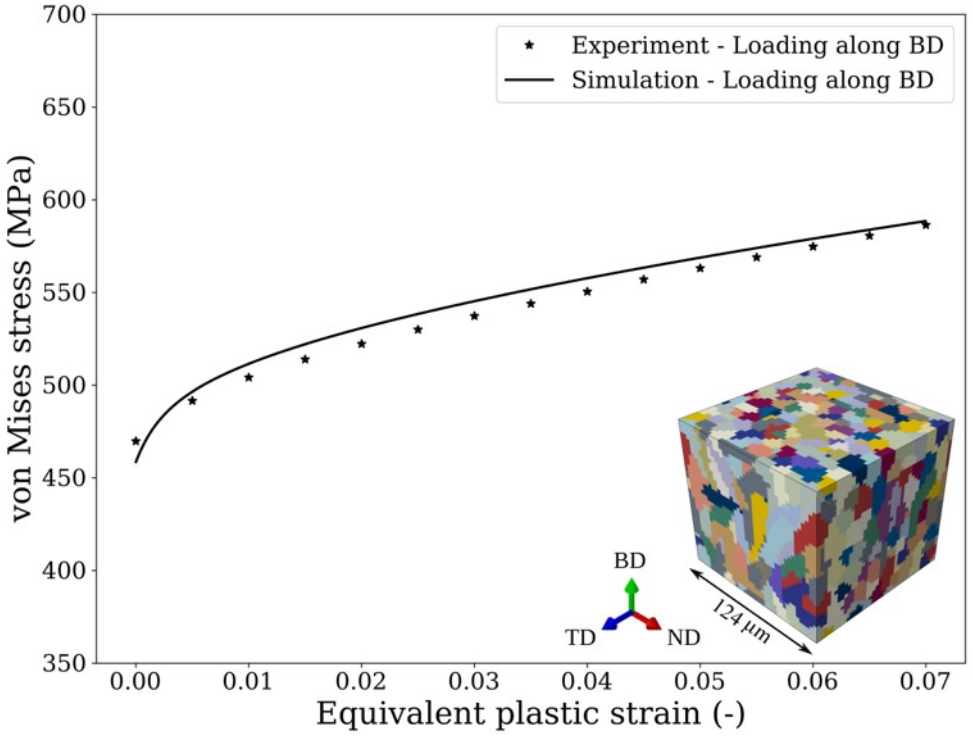
$$\dot{\hat{\tau}}_\alpha = \sum_{\beta=1}^{N} h_0 \chi_{\alpha\beta} \left(1 - \frac{\hat{\tau}_\alpha}{\hat{\tau}_{sat}}\right)^{p_2} |\dot{\gamma}_\beta|$$

Kinematic hardening

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

Isotropic hardening

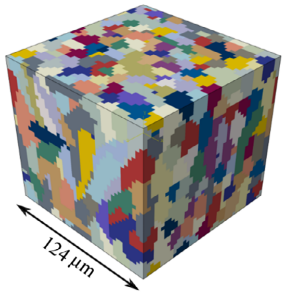
$$\hat{\tau}_\alpha^{\mathrm{GNDi}} = c_1 \mu b \sqrt{\sum_{\beta=1}^{9} \chi_{\alpha\beta}^{\mathrm{GND}} |\bar{\rho}_\beta|}$$



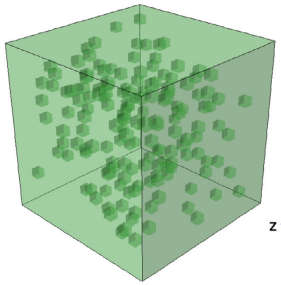
Ma & Hartmaier. Phil Mag (2014)

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

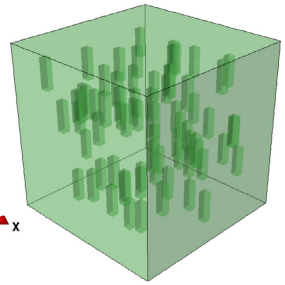
Influence of pore shape on anisotropy



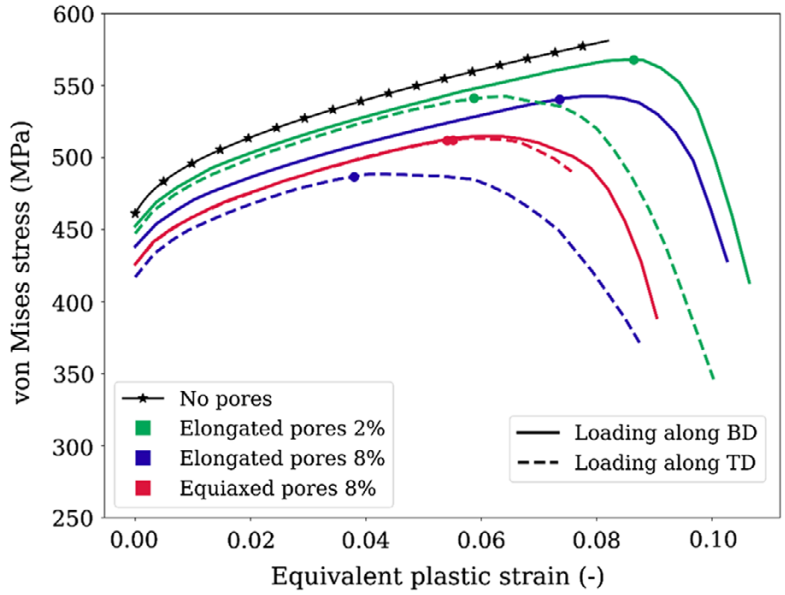
Synthetic microstructure



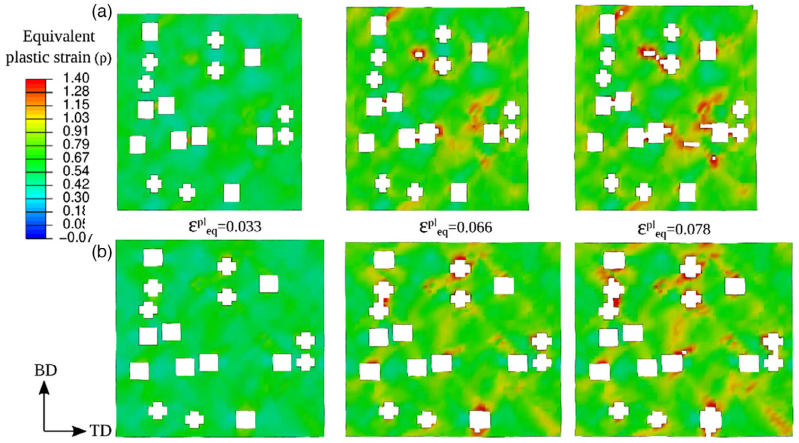
Equiaxed pores



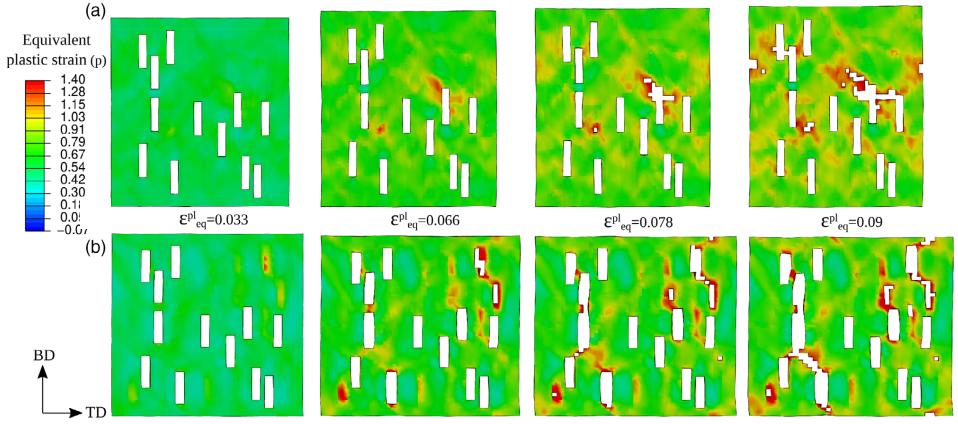
Elongated pores



Flow curves



Equiaxed pores

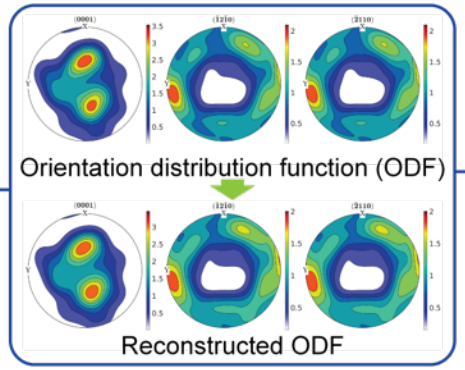


Elongated pores

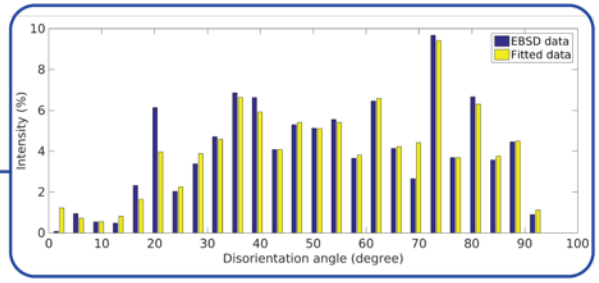
Source: Prasad et al., Adv. Eng. Mater. 2020

Summary

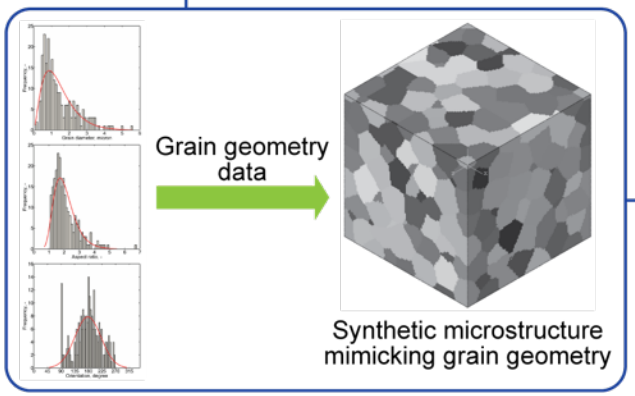
EBSD



Kanapy ODF reconstruction module

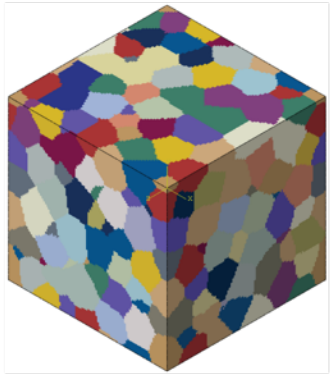


Kanapy orientation assignment module



Kanapy geometry module

Grain boundary surface area



Equiaxed grains

Elongated grains

Synthetic microstructure

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

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