Computational Micromechanics of Single Crystals and Polycrystals

part III: Micromechanics of polycrystals

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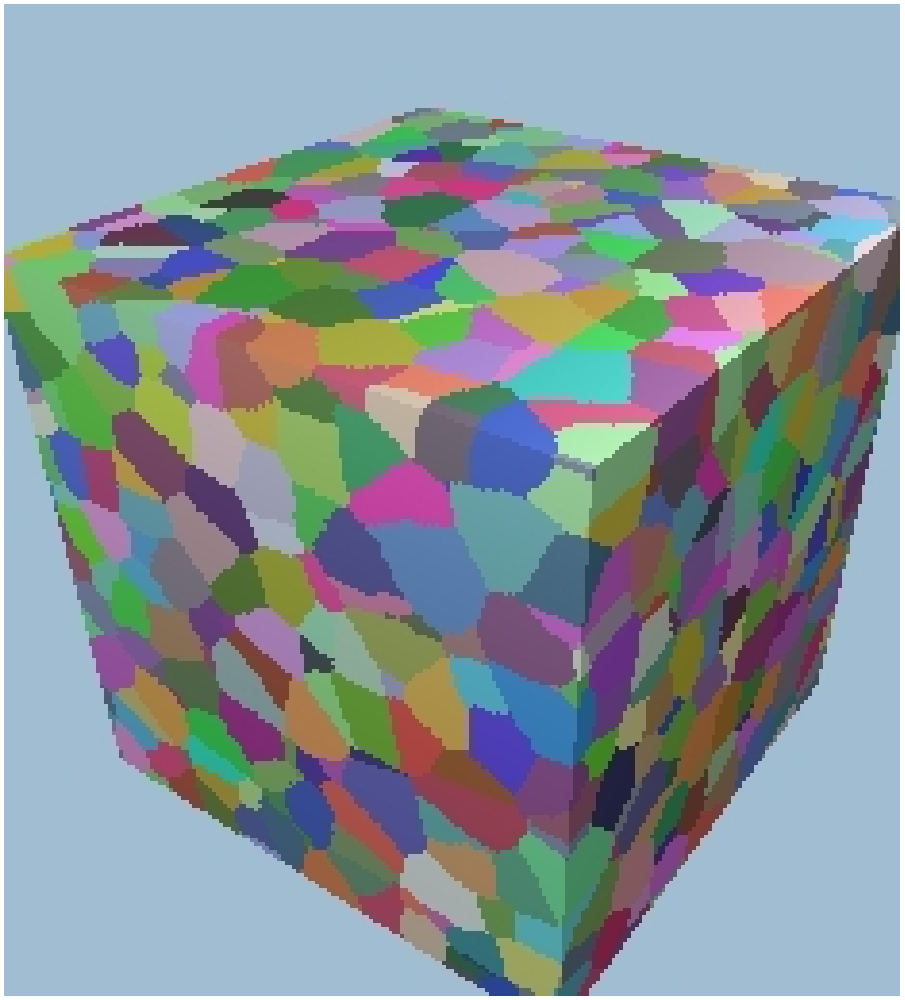
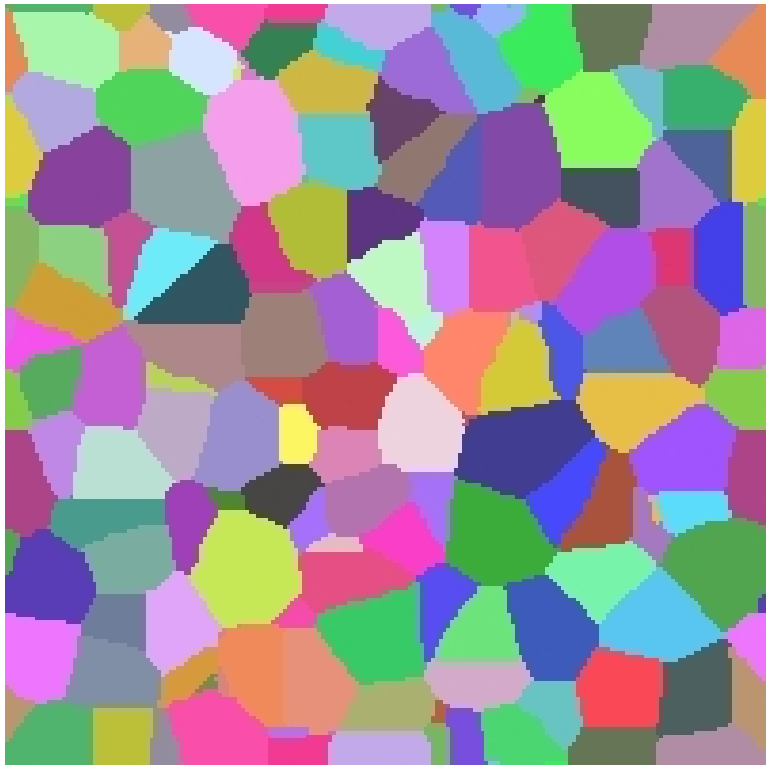
Plan

1. Computational mechanics of microstructures
   - Morphology and meshing of polycrystals
   - Exercise: boundary conditions for computing volume elements
2. Computing strain heterogeneities in polycrystals
   - Representative volume element for polycrystals
   - Parallel computing of polycrystalline aggregates
3. Homogenization models for polycrystals
4. Texture evolution during the deformation of polycrystals
5. Grain size effects in polycrystals
   - Cosserat single crystal plasticity
   - Hall–Petch behaviour

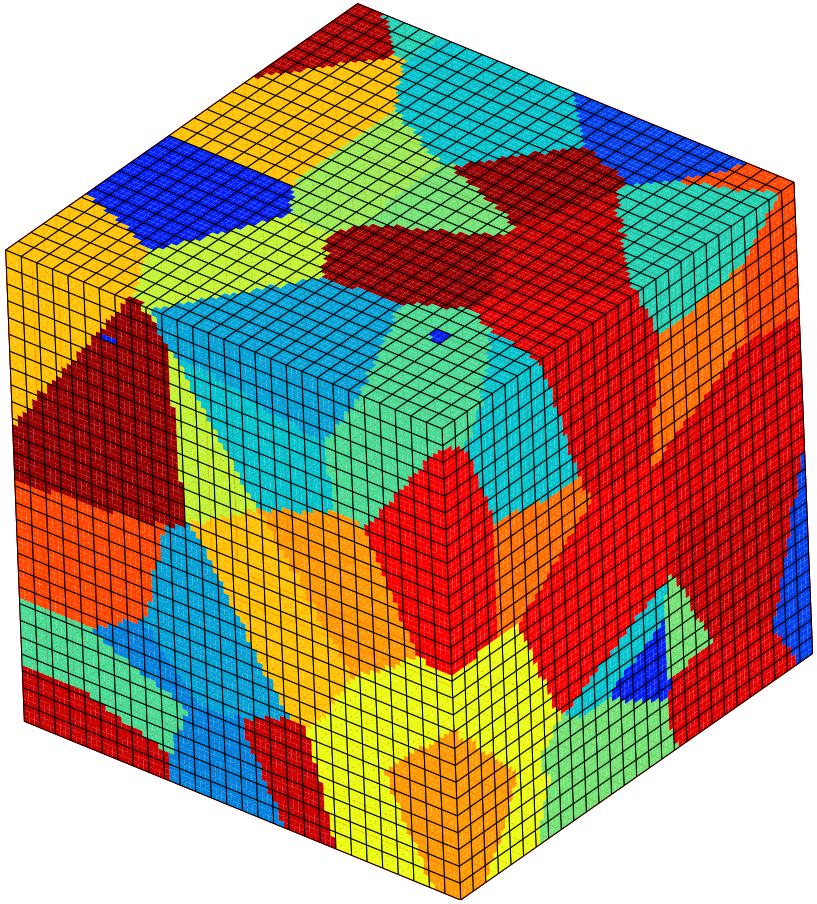
Plan

Models for polycrystals : Voronoi mosaics

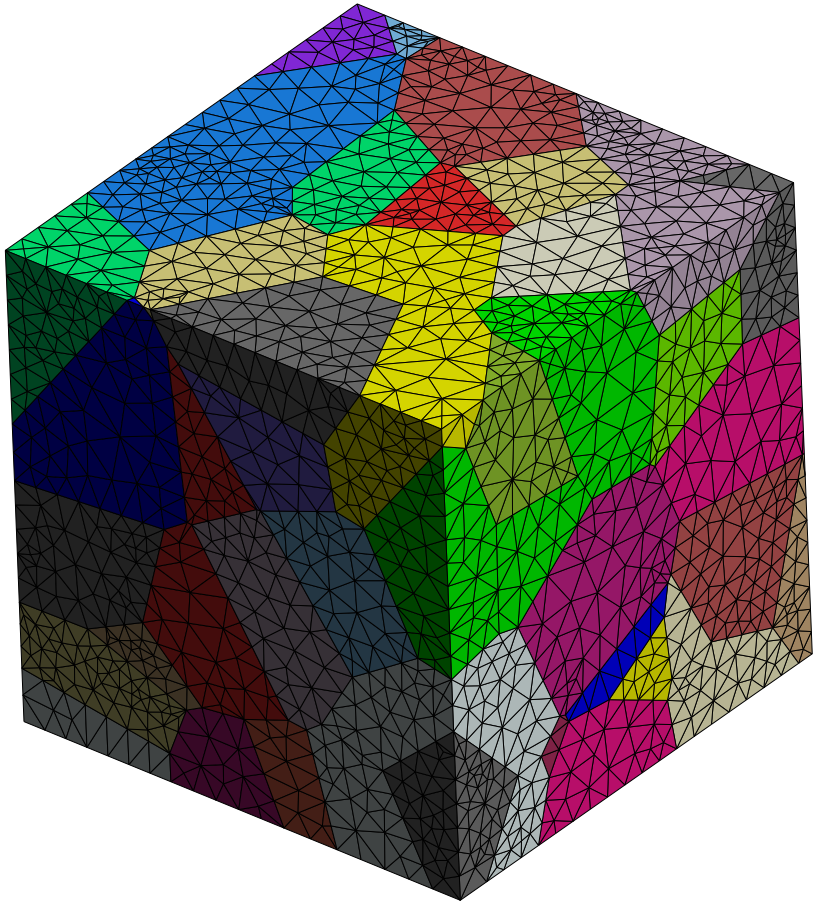




Meshing polycrystals : Voronoi cells

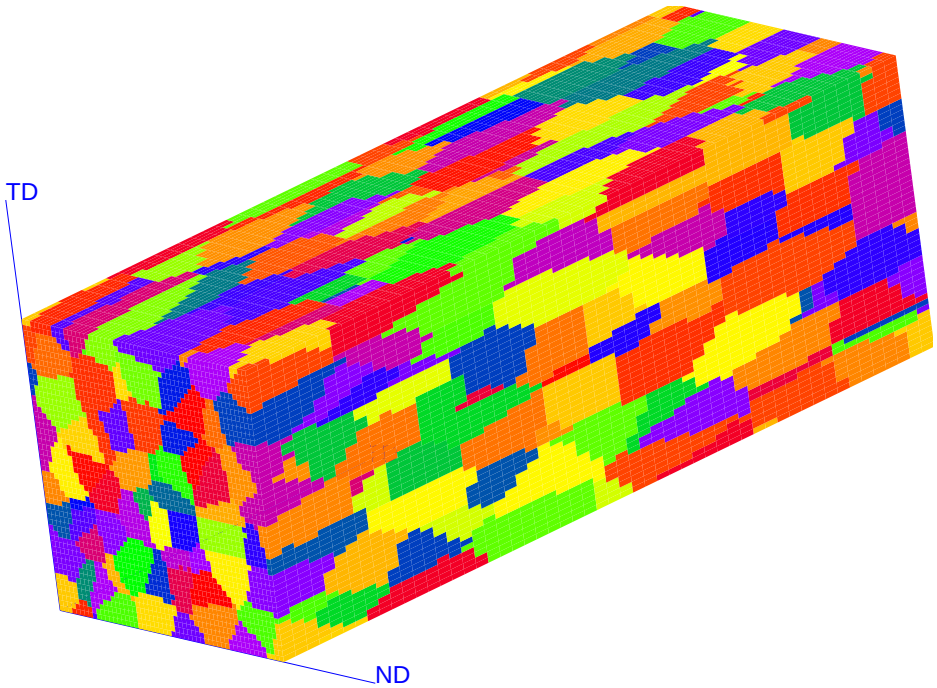


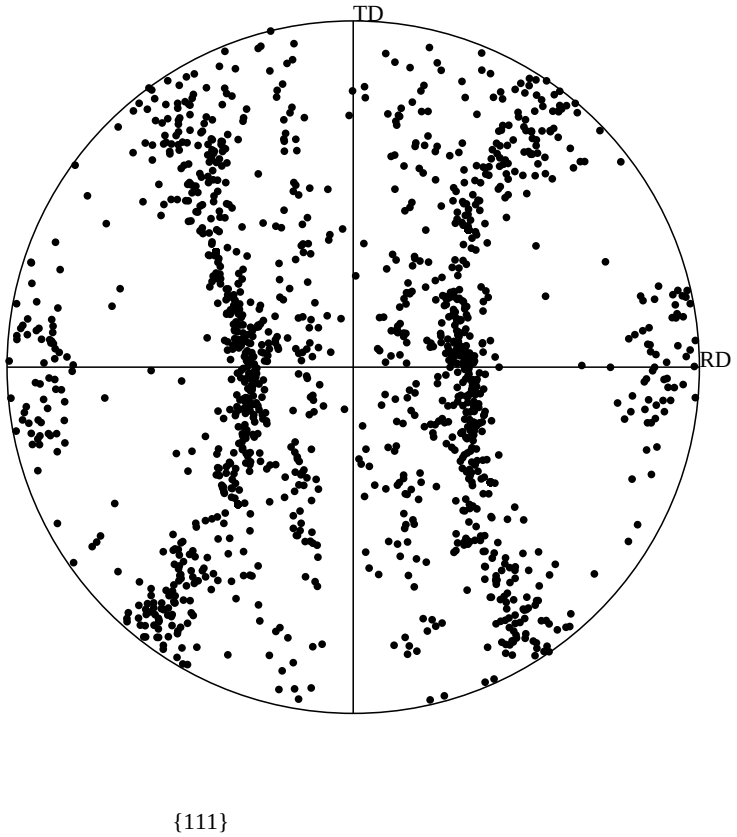
multiphase elements



free meshing

Morphological and crystallographic texture



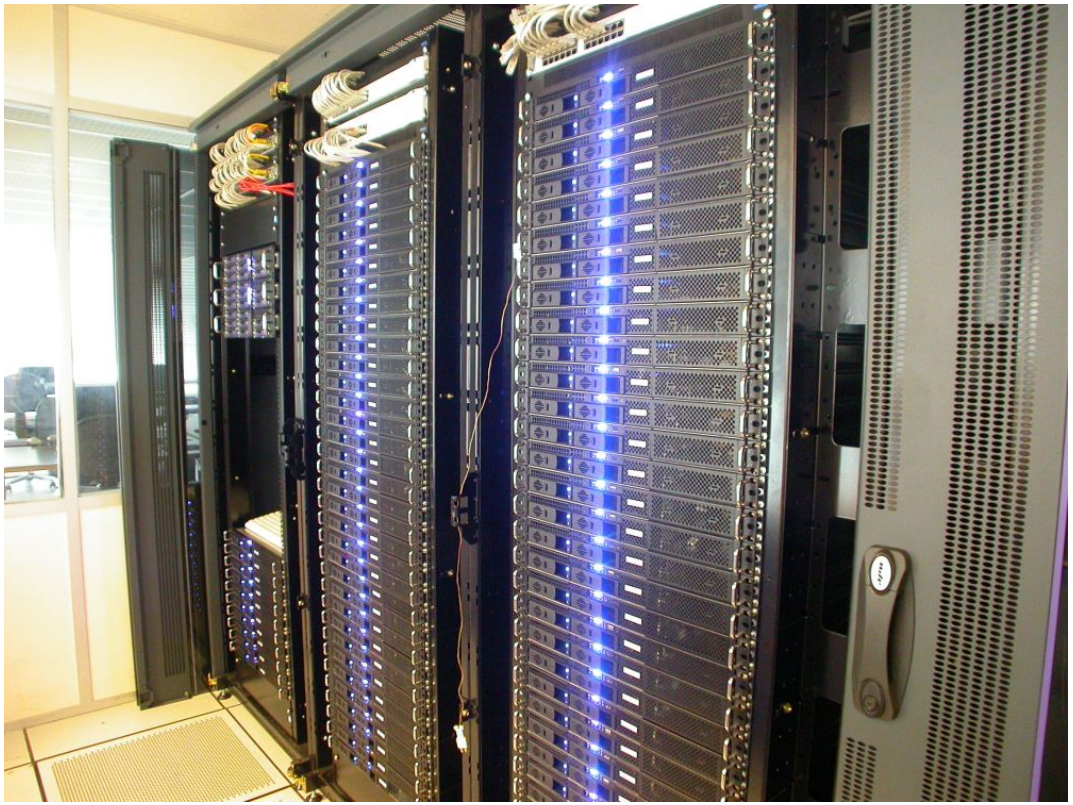


cupro–beryllium alloy

Parallel computing

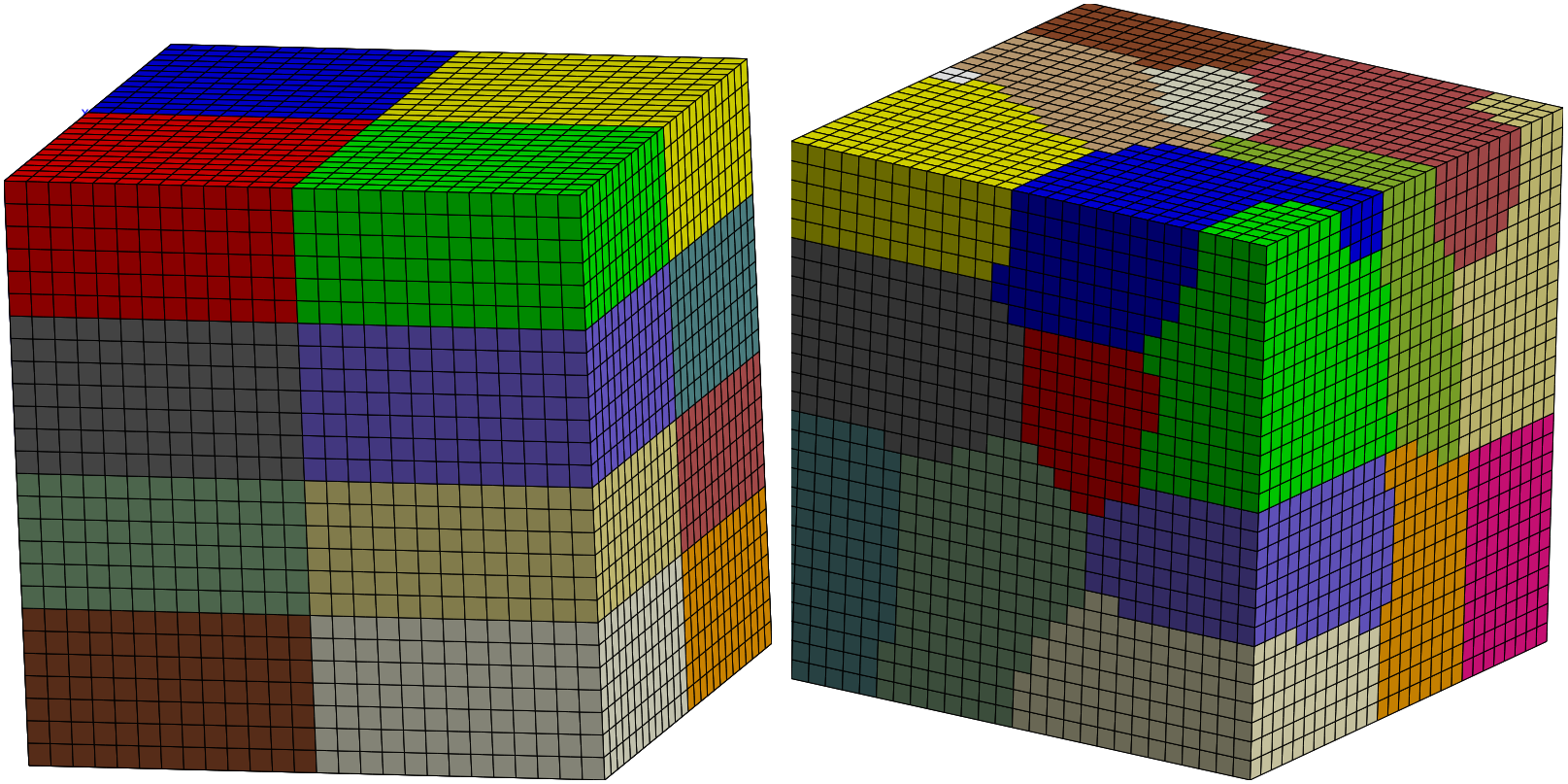
old chicken farm...
60 PC bipro
Pentium IV
768 Mo
30 Go

Parallel computing



new chicken farm!
80 PC bipro Opteron
8 Mo

Parallel computing



Subdomain decomposition method

Zset code (www.nwnumerics.com, www.mat.ensmp.fr): FETI method (Finite Element Tearing and Interconnecting Method)

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Boundary conditions for material volume elements

- **Kinematic uniform boundary conditions (KUBC)** :

$$\underline{\mathbf{u}} = \underset{\sim}{\mathbf{E}}.\underline{\mathbf{x}} \quad \forall \underline{\mathbf{x}} \in \partial V$$

$$< \underset{\sim}{\varepsilon} >= \frac{1}{V}\int_V \underset{\sim}{\varepsilon}\, dV = \underset{\sim}{\mathbf{E}} \quad \textit{and} \quad \underset{\sim}{\mathbf{\Sigma}} \hat{=} < \underset{\sim}{\sigma} >= \frac{1}{V}\int_V \underset{\sim}{\sigma}\, dV$$

- **Static uniform boundary conditions (SUBC)** :

$$\underset{\sim}{\sigma}.\underline{\mathbf{n}} = \underset{\sim}{\mathbf{\Sigma}}.\underline{\mathbf{n}} \quad \forall \underline{\mathbf{x}} \in \partial V$$

$$< \underset{\sim}{\sigma} >= \frac{1}{V}\int_V \underset{\sim}{\sigma}\, dV = \underset{\sim}{\mathbf{\Sigma}} \quad \textit{and} \quad \underset{\sim}{\mathbf{E}} \hat{=} < \underset{\sim}{\varepsilon} >= \frac{1}{V}\int_V \underset{\sim}{\varepsilon}\, dV$$

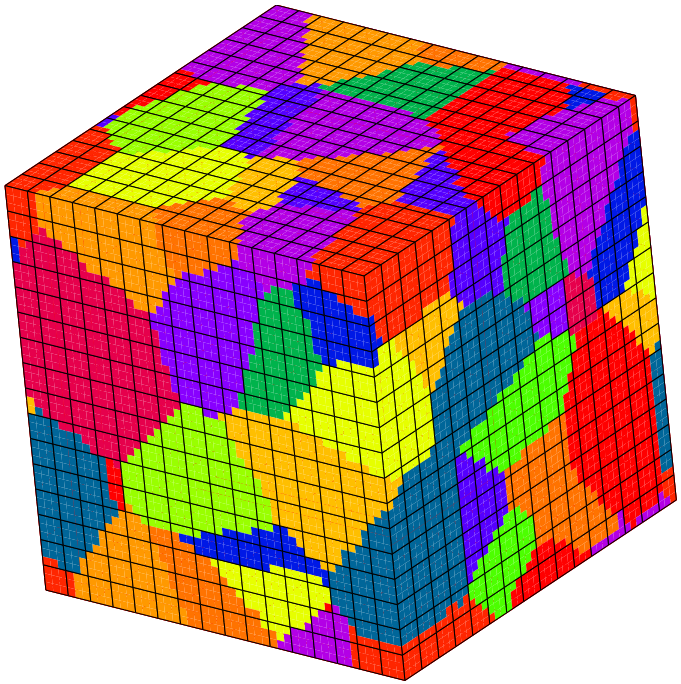
- **Periodicity conditions (PERIODIC)** :

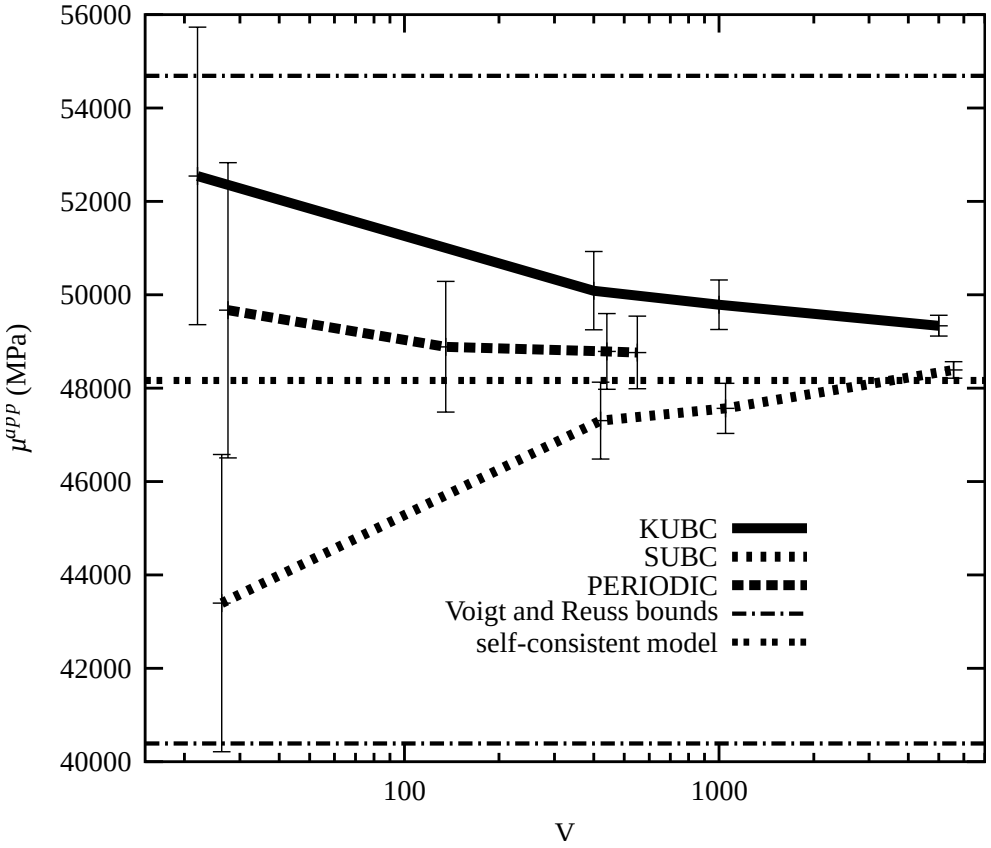
$$\underline{\mathbf{u}} = \underset{\sim}{\mathbf{E}}.\underline{\mathbf{x}} + \underline{\mathbf{v}} \quad \forall \underline{\mathbf{x}} \in V,\ \underline{\mathbf{v}}\ \textit{periodic}$$

Plan

RVE for elastic copper crystals

isotropic texture

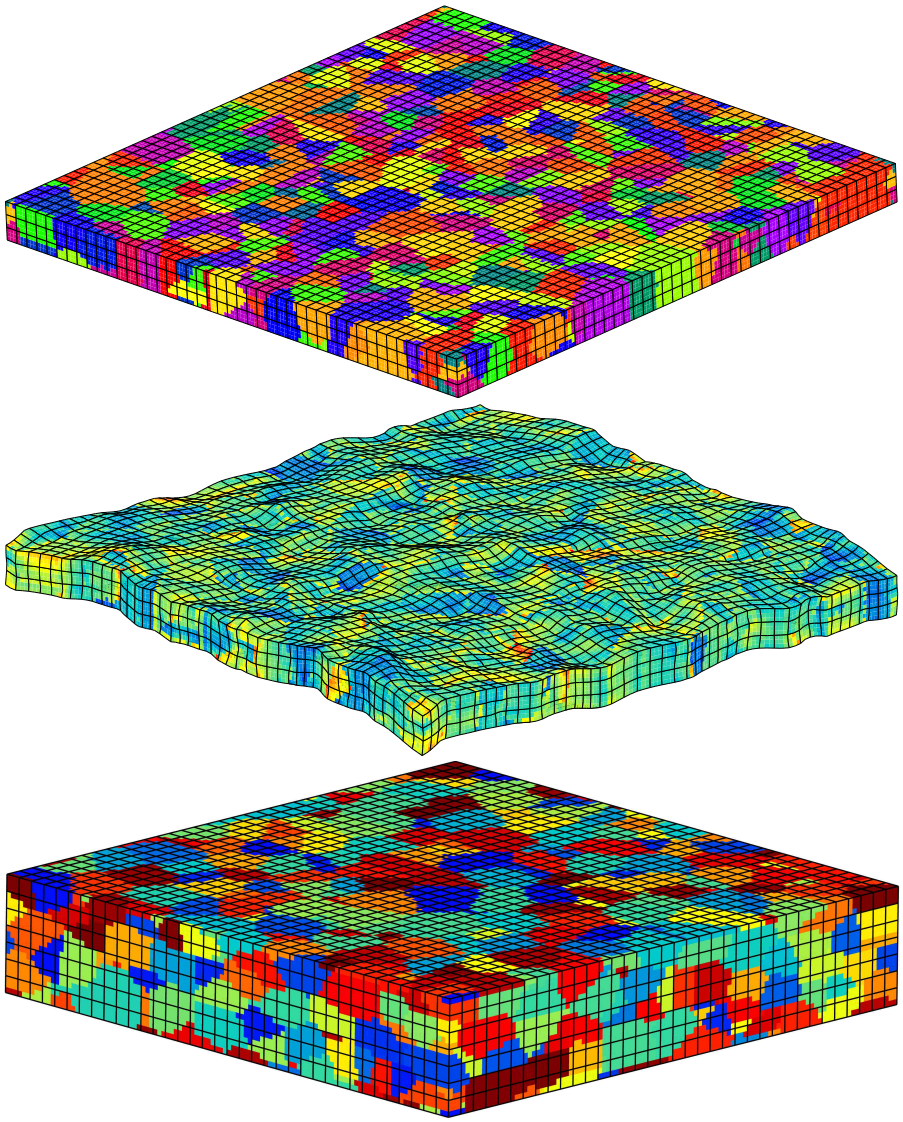




$$C_{11} = 168400 \text{ MPa}, \quad C_{12} = 121400 \text{ MPa}, \quad C_{44} = 75390 \text{ MPa}$$

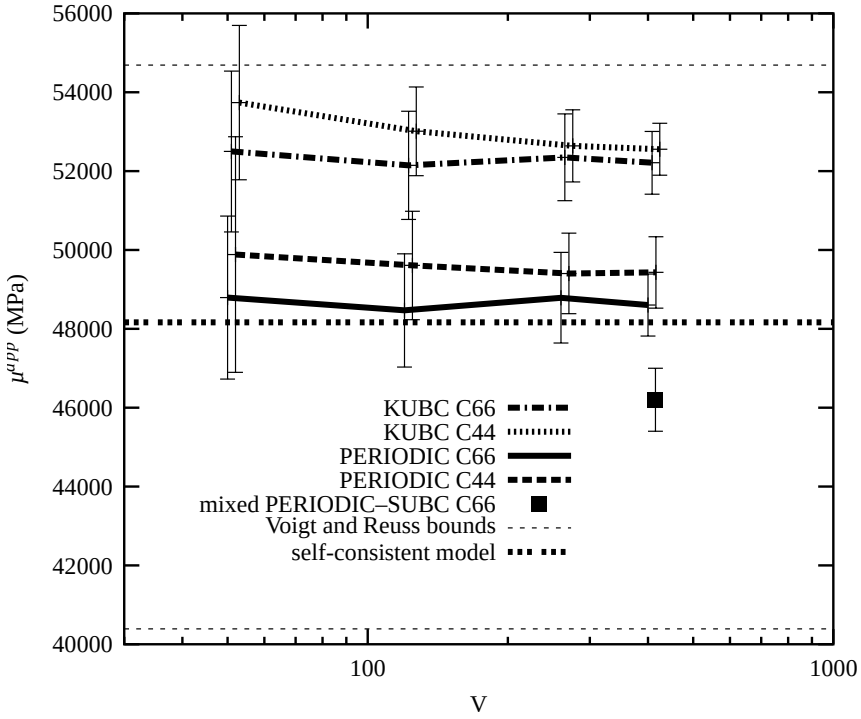
cubic elasticity $a = 2C_{44}/(C_{11} - C_{12}) = 3.2$

RVE for polycrystalline thin films?



periodic or mixed boundary conditions

The RVE does not exist for a one–grain thick polycrystalline layer

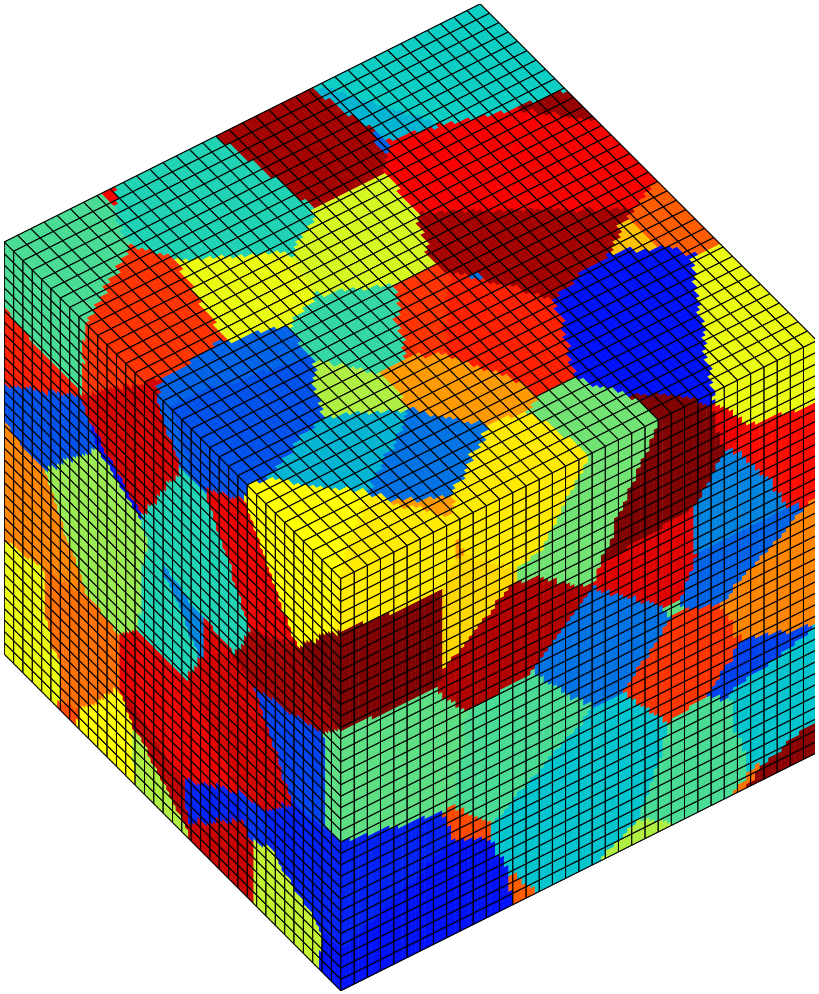


However 3 to 5 grains within the thickness are sufficient to reach bulk properties...

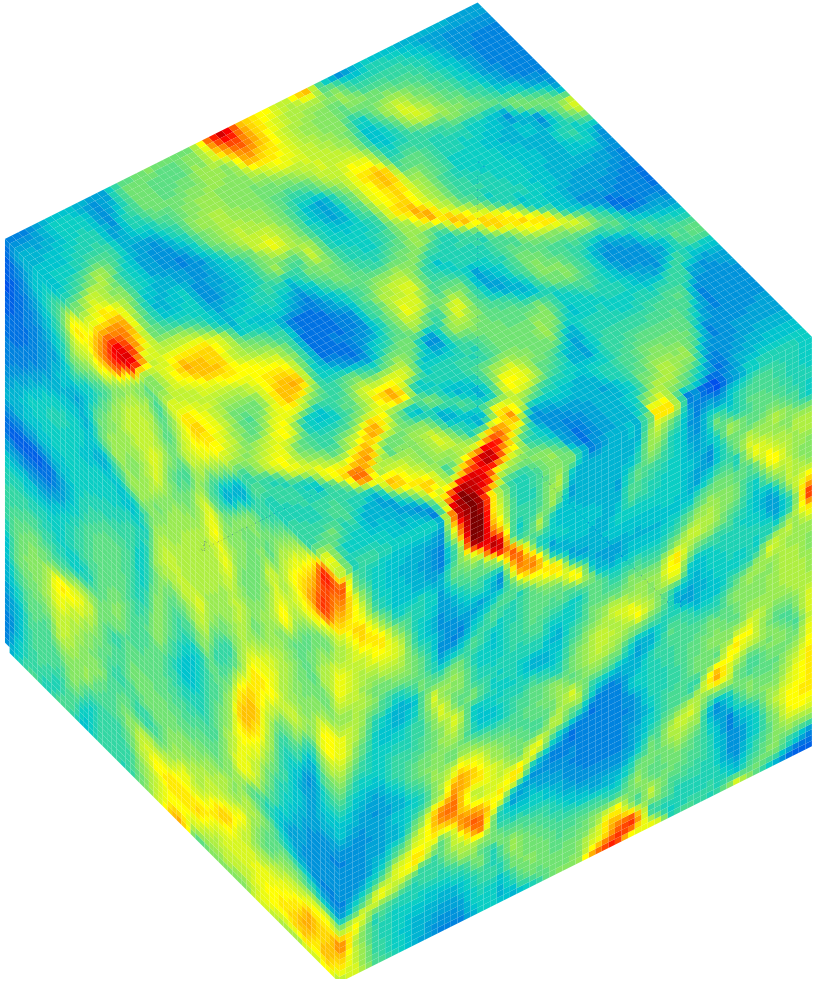
[El Houdaigui, 2004]

Plan

Elastoplastic deformation of polycrystalline aggregates

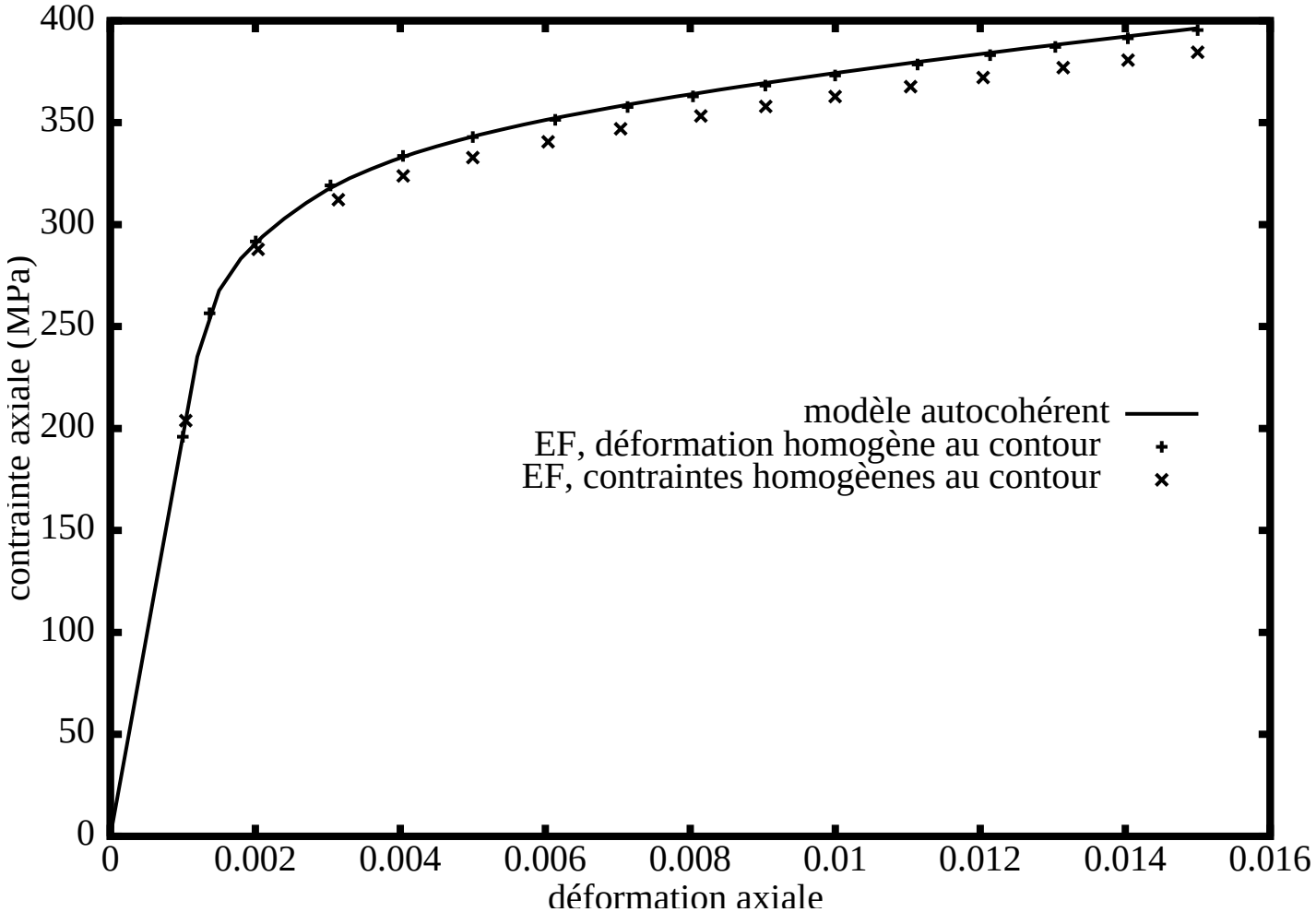


RVE for the polycrystal

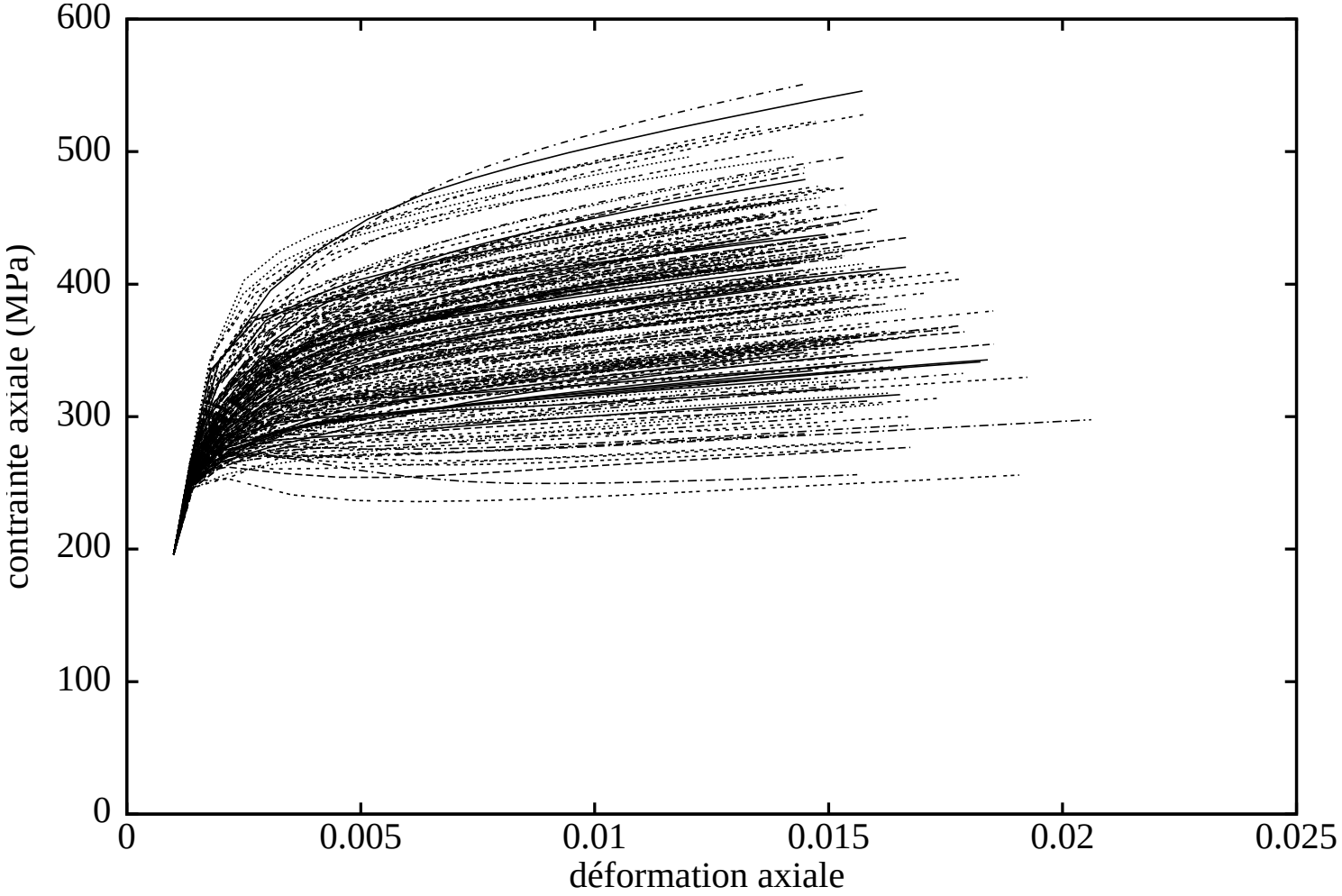


cumulative plastic strain

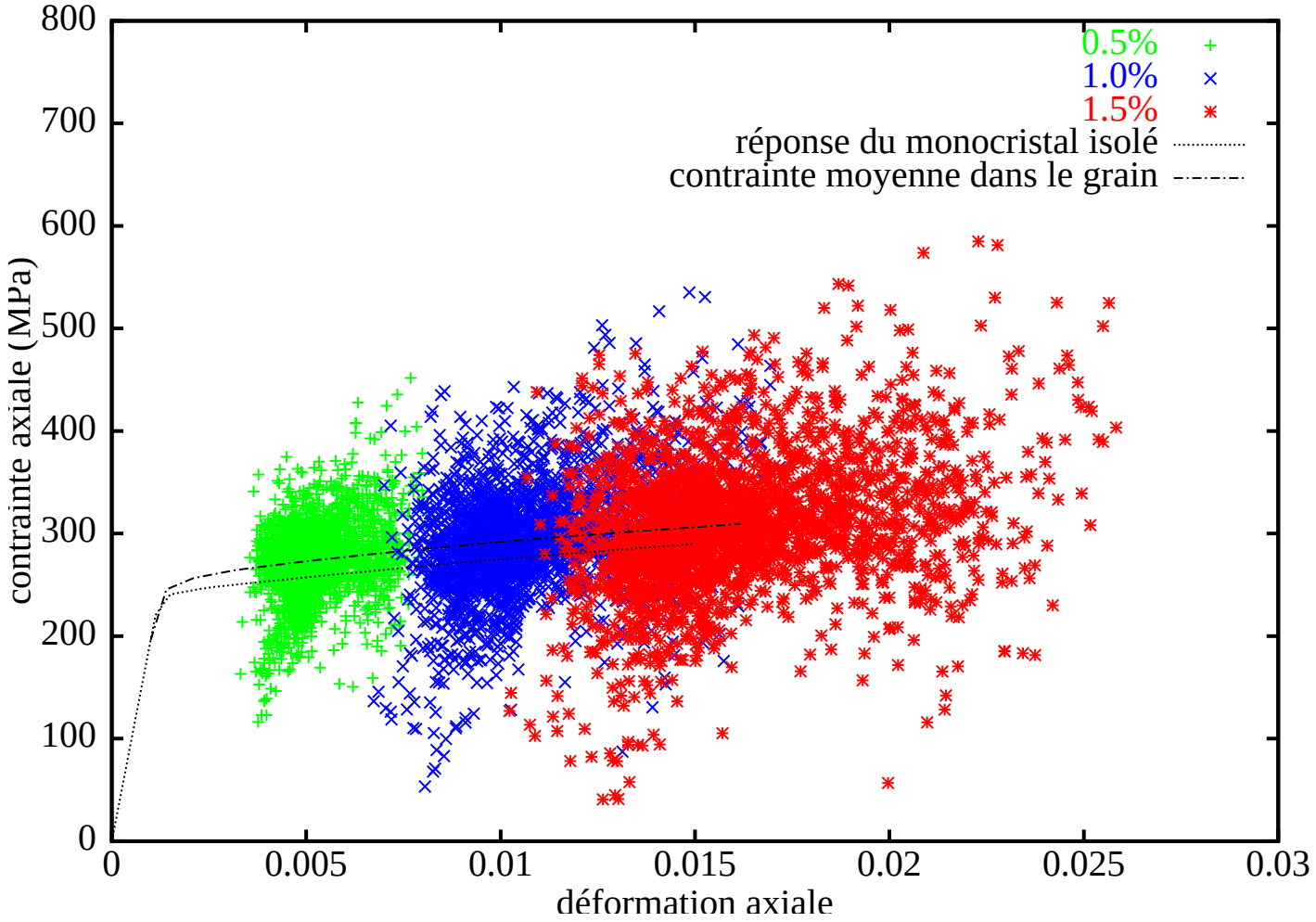
Macroscopic response



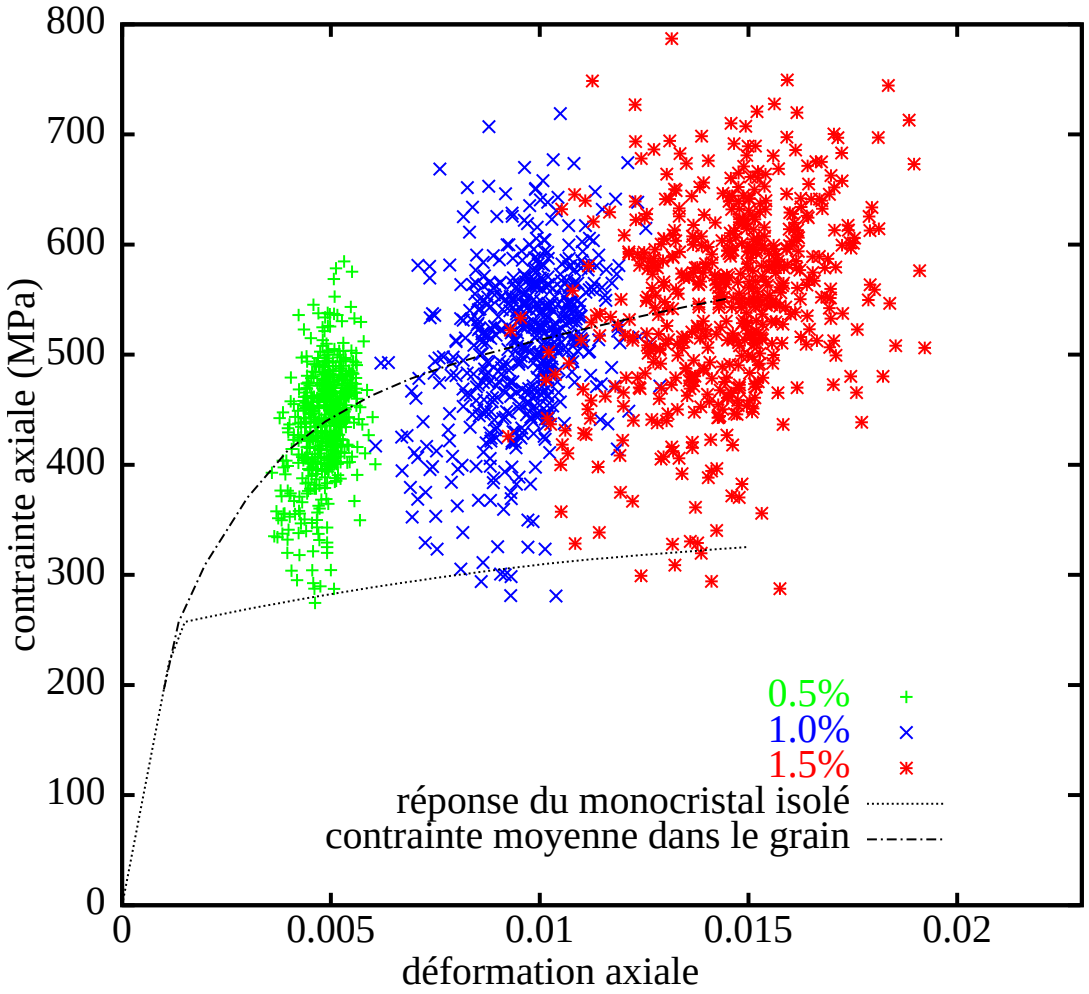
Mean response per grain



Local response in one grain



Local response in one grain



Plan

Ingredients of mean field theory

- Macroscopic quantitied

$$\underset{\sim}{\boldsymbol{\Sigma}}, \underset{\sim}{\mathbf{E}}, \underset{\sim}{\mathbf{E}}^p$$

- Mean values per phase

$$\underset{\sim}{\boldsymbol{\sigma}}^g, \underset{\sim}{\varepsilon}^{pg}, \gamma^{sg}$$

- Taylor model

$$\underset{\sim}{\varepsilon}^{pg} = \underset{\sim}{\mathbf{E}}^p \Longrightarrow \underset{\sim}{\boldsymbol{\sigma}}^g \neq \underset{\sim}{\boldsymbol{\Sigma}}$$

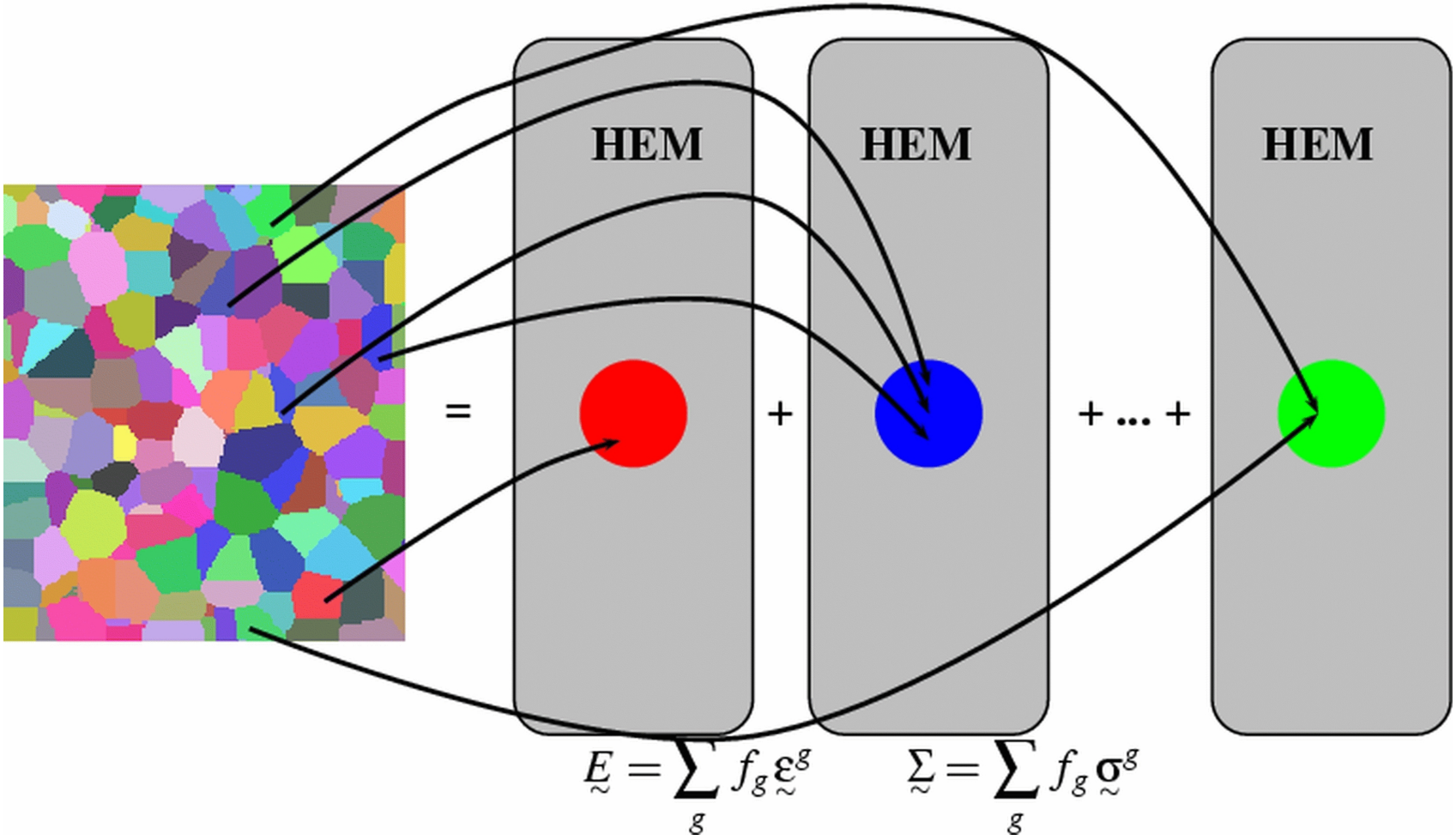
- Static model

$$\underset{\sim}{\boldsymbol{\sigma}}^g = \underset{\sim}{\boldsymbol{\Sigma}} \Longrightarrow \underset{\sim}{\varepsilon}^{pg} \neq \underset{\sim}{\mathbf{E}}^p$$

- Self–constitent estimates

$$\underset{\sim}{\boldsymbol{\sigma}}^g \neq \underset{\sim}{\boldsymbol{\Sigma}}, \quad \underset{\sim}{\varepsilon}^{pg} \neq \underset{\sim}{\mathbf{E}}^p$$

Self–consistent scheme



[Kröner, 1961]

Scale transition rules

- Secant and tangent approximations

$$\dot{\underset{\sim}{\mathbf{\Sigma}}} = \underset{\approx}{\mathbf{L}}^{eff} : \dot{\underset{\sim}{\mathbf{E}}}$$

- Lin and Kröner estimates ($\simeq$ Taylor)

$$\dot{\underset{\sim}{\boldsymbol{\sigma}}} = \dot{\underset{\sim}{\mathbf{\Sigma}}} + \mu(\dot{\underset{\sim}{\mathbf{E}}}^p - \dot{\underset{\sim}{\varepsilon}}^p)$$

- Berveiller and Zaoui's estimate (1979)

$$\underset{\sim}{\boldsymbol{\sigma}} = \underset{\sim}{\mathbf{\Sigma}} + \mu\alpha(\underset{\sim}{\mathbf{E}}^p - \underset{\sim}{\varepsilon}^p)$$

  elastoplastic accommodation coefficient α varying from 1 to 0.01 during deformation

- limitations : elastoviscoplasticity, radial and monotonic loading, no real grain morphology, limited interaction between grains, estimation that may be out of the theoretical bounds, difficult to estimate strain heterogeneities inside the grains...

Identification of scale transition rules

$$\underset{\sim}{\mathbf{E}} = \underset{\sim}{\mathbf{E}}^e + \underset{\sim}{\mathbf{E}}^p, \quad \underset{\sim}{\boldsymbol{\Sigma}} = \underset{\sim}{\underset{\sim}{\mathbf{C}}} : \underset{\sim}{\mathbf{E}}^e, \quad \underset{\sim}{\boldsymbol{\Sigma}} = \sum_{g=1}^{N_g} f_g \, \underset{\sim}{\boldsymbol{\sigma}}^g, \quad \dot{\underset{\sim}{\mathbf{E}}}^p = \sum_{g=1}^{N_g} f_g \, \dot{\underset{\sim}{\varepsilon}}^{pg}$$

$\underset{\sim}{\boldsymbol{\sigma}}^g \longrightarrow \dot{\underset{\sim}{\varepsilon}}^{pg}$ according to the constitutive equations of single crystal plasticity

Example of efficient parametrized scale transition rule:

$$\underset{\sim}{\boldsymbol{\sigma}}^g = \underset{\sim}{\boldsymbol{\Sigma}} + C\left(\underset{\sim}{\mathbf{B}} - \underset{\sim}{\boldsymbol{\beta}}^g\right), \quad \underset{\sim}{\mathbf{B}} = \sum_{g=1}^{N_g} f_g \, \underset{\sim}{\boldsymbol{\beta}}^g, \quad \dot{\underset{\sim}{\boldsymbol{\beta}}}^g = \dot{\underset{\sim}{\varepsilon}}^{pg} - D\dot{\varepsilon}_{eq}^{pg} \underset{\sim}{\boldsymbol{\beta}}^g$$

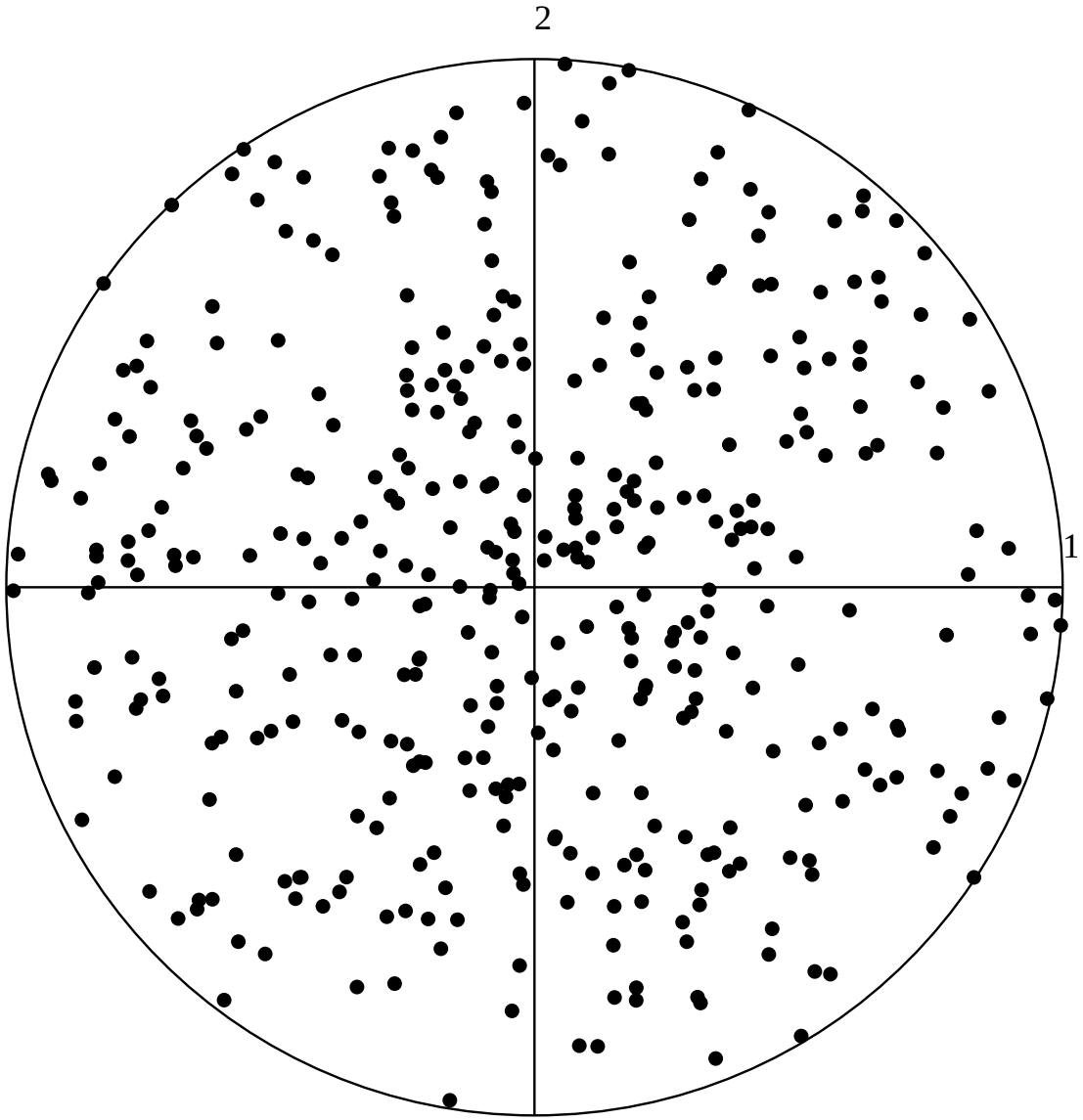
intergranular plastic accommodation variables $\underset{\sim}{\boldsymbol{\beta}}$ with the nonlinear evolution law

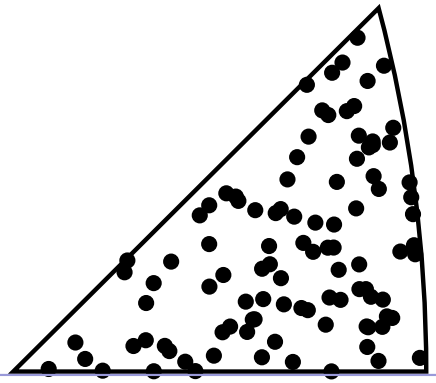
scale transition parameters : $C, D \neq$ material parameters

identification procedure, inverse approach

Plan

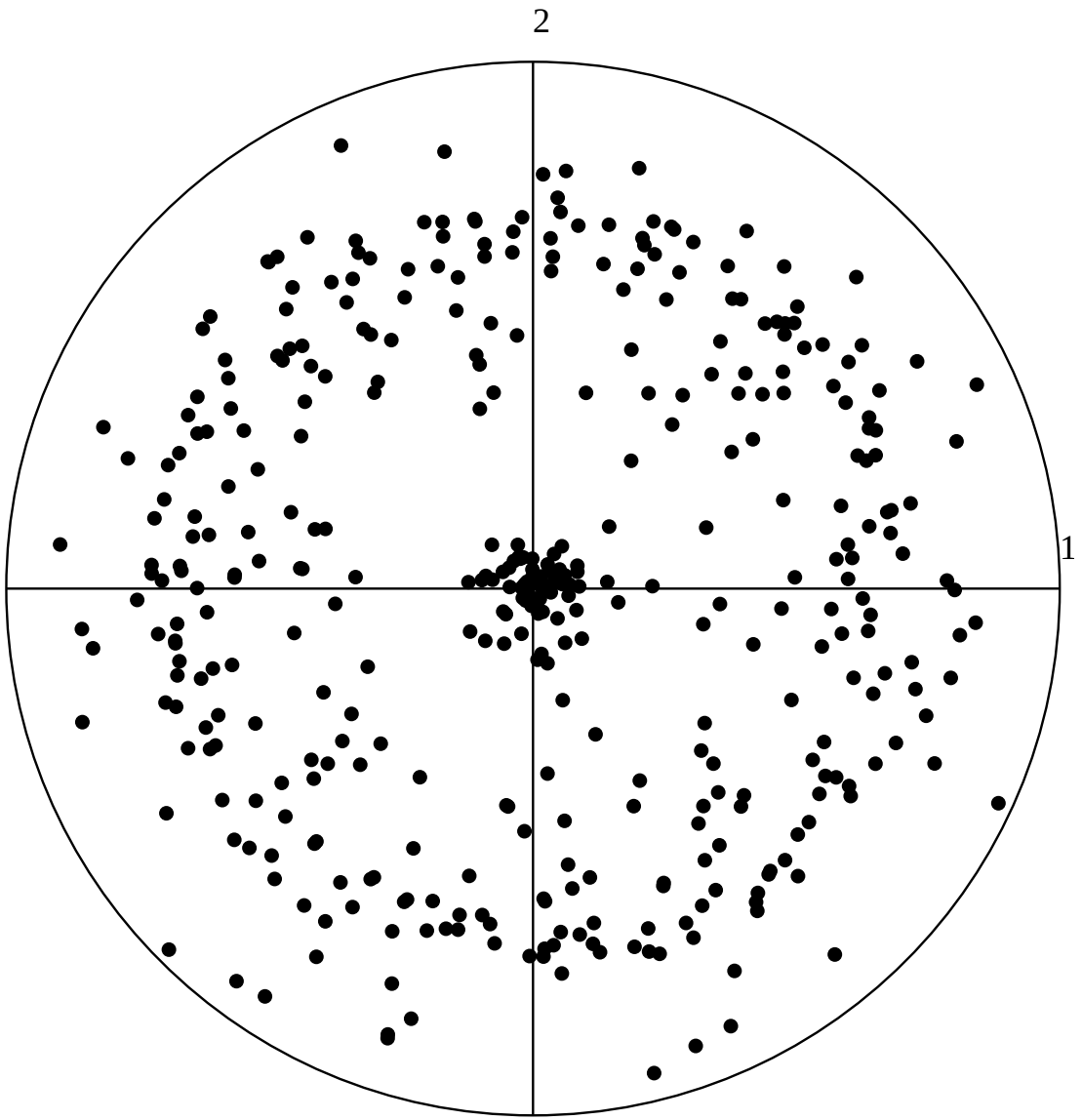
Texture evolution (FCC)

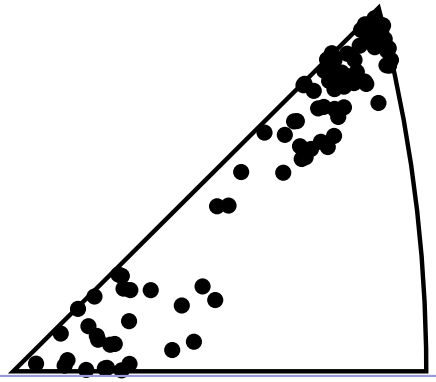




planes : {111}

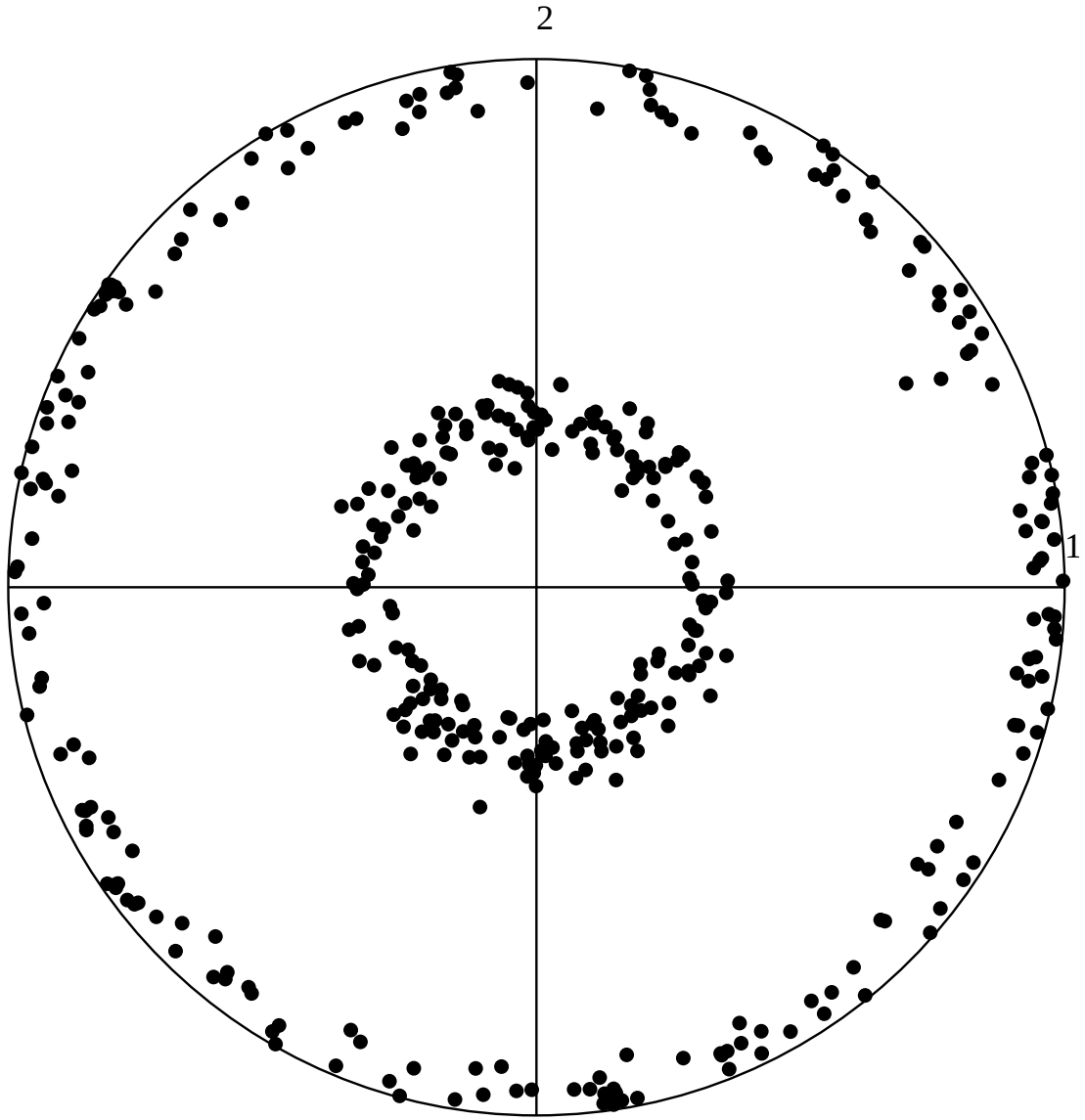
Texture evolution (FCC) (tension $F_{33} = 1.7$)

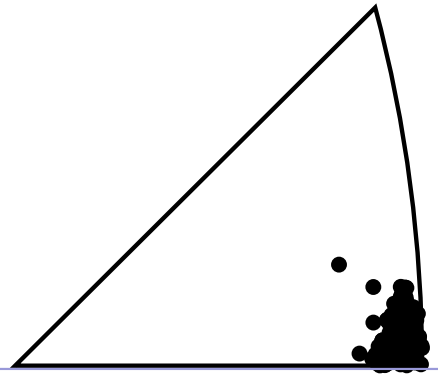




planes : {111}

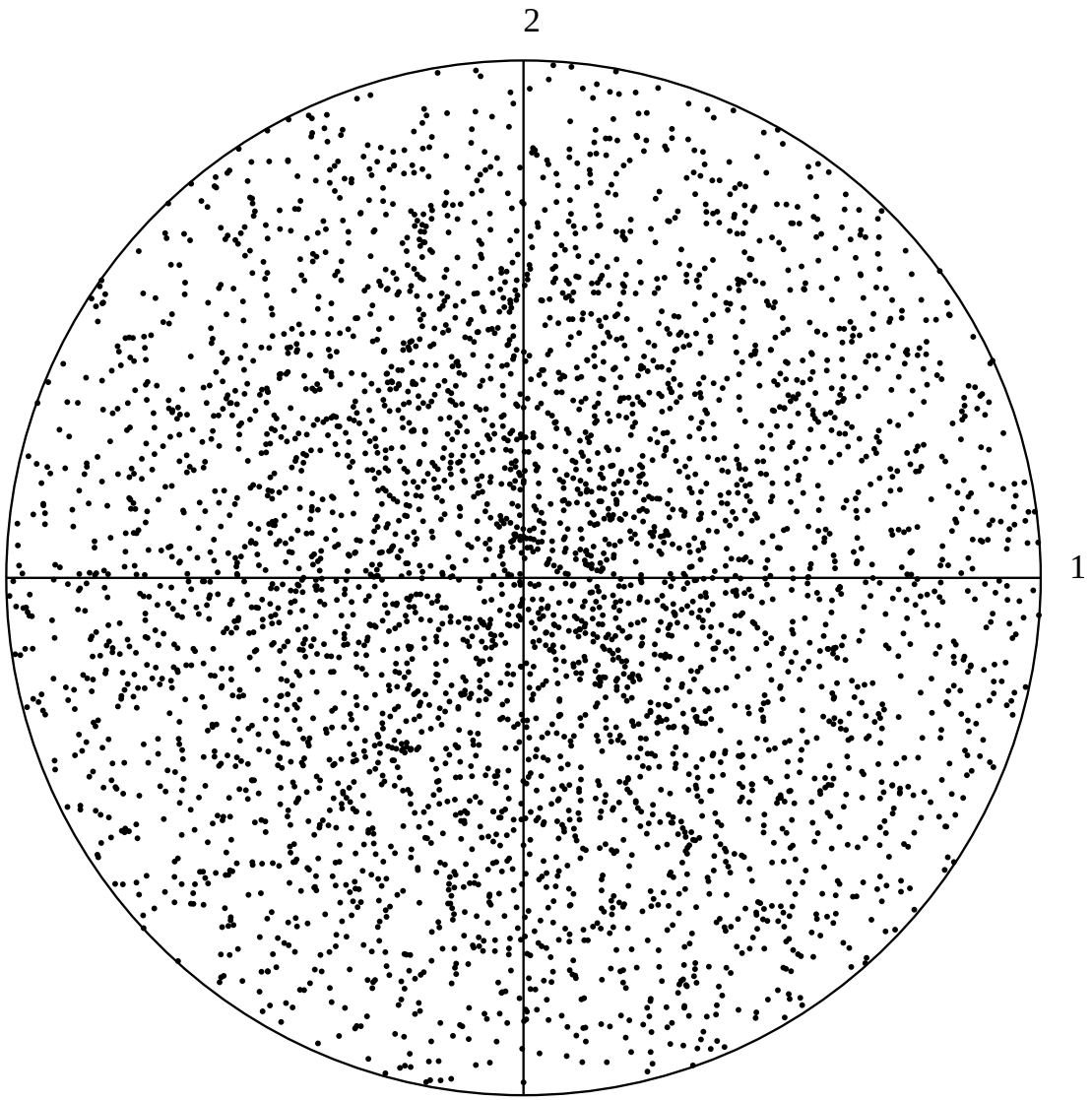
Texture evolution (FCC) (compression $F_{33} = 0.3$)

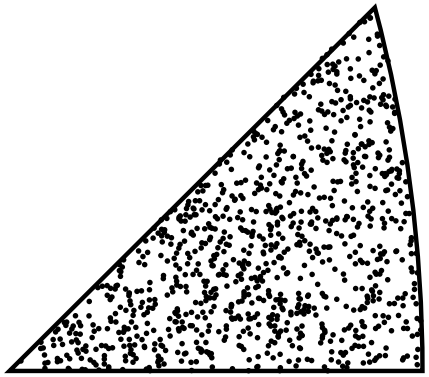




planes : {111}

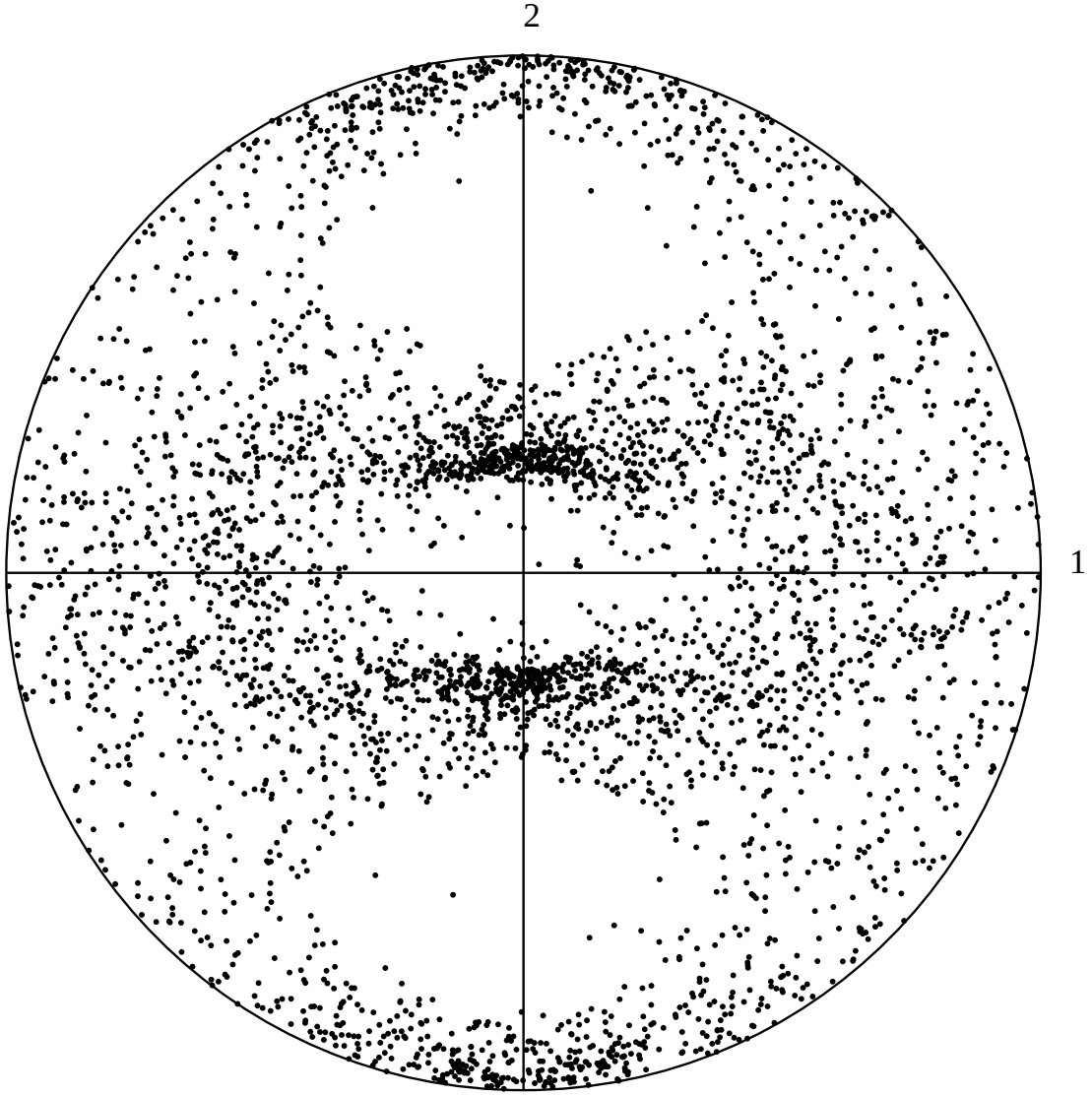
Texture evolution (FCC)





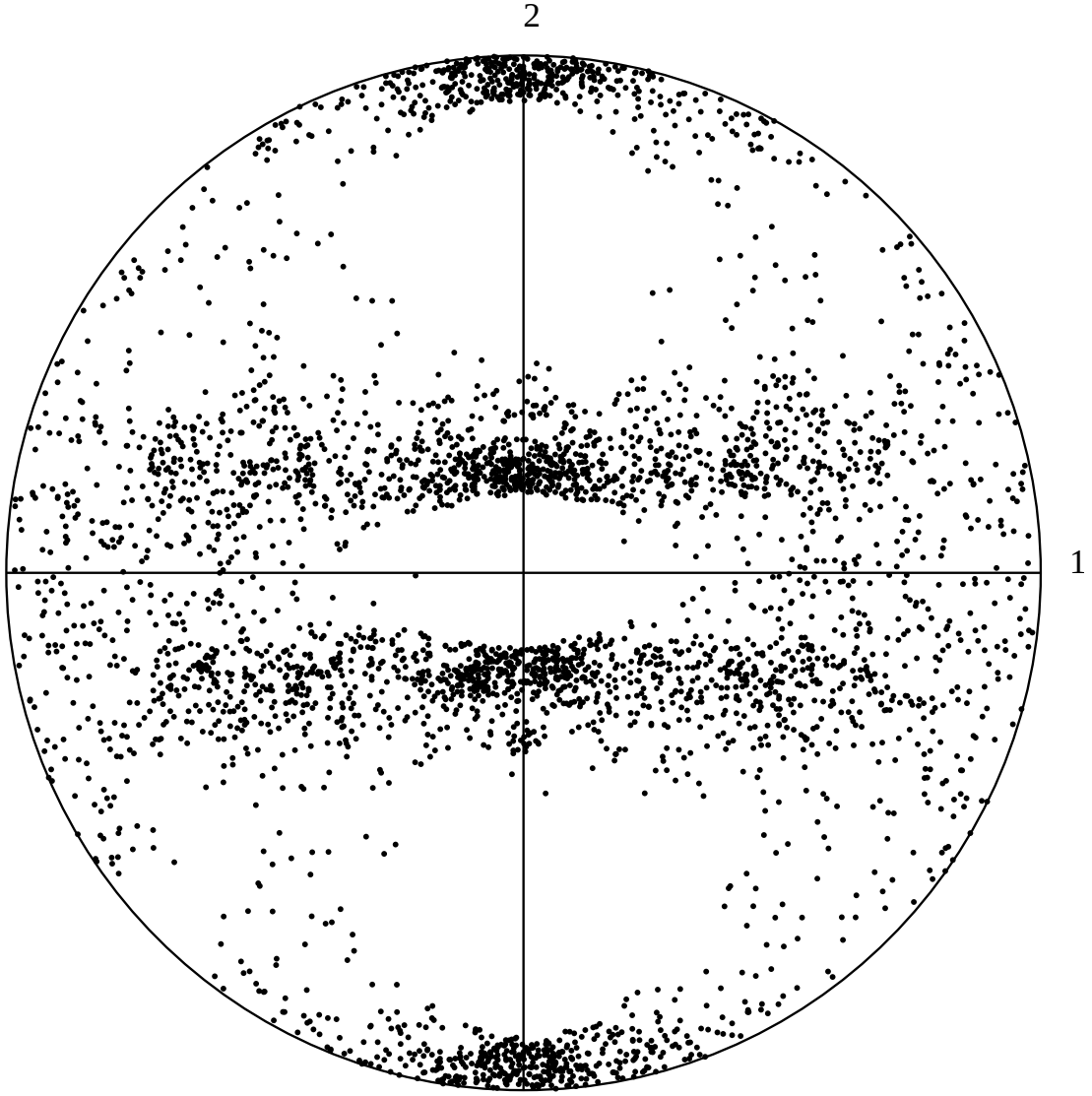
planes : {111}

Texture evolution (FCC) (rolling $F_{33} = 0.66$)



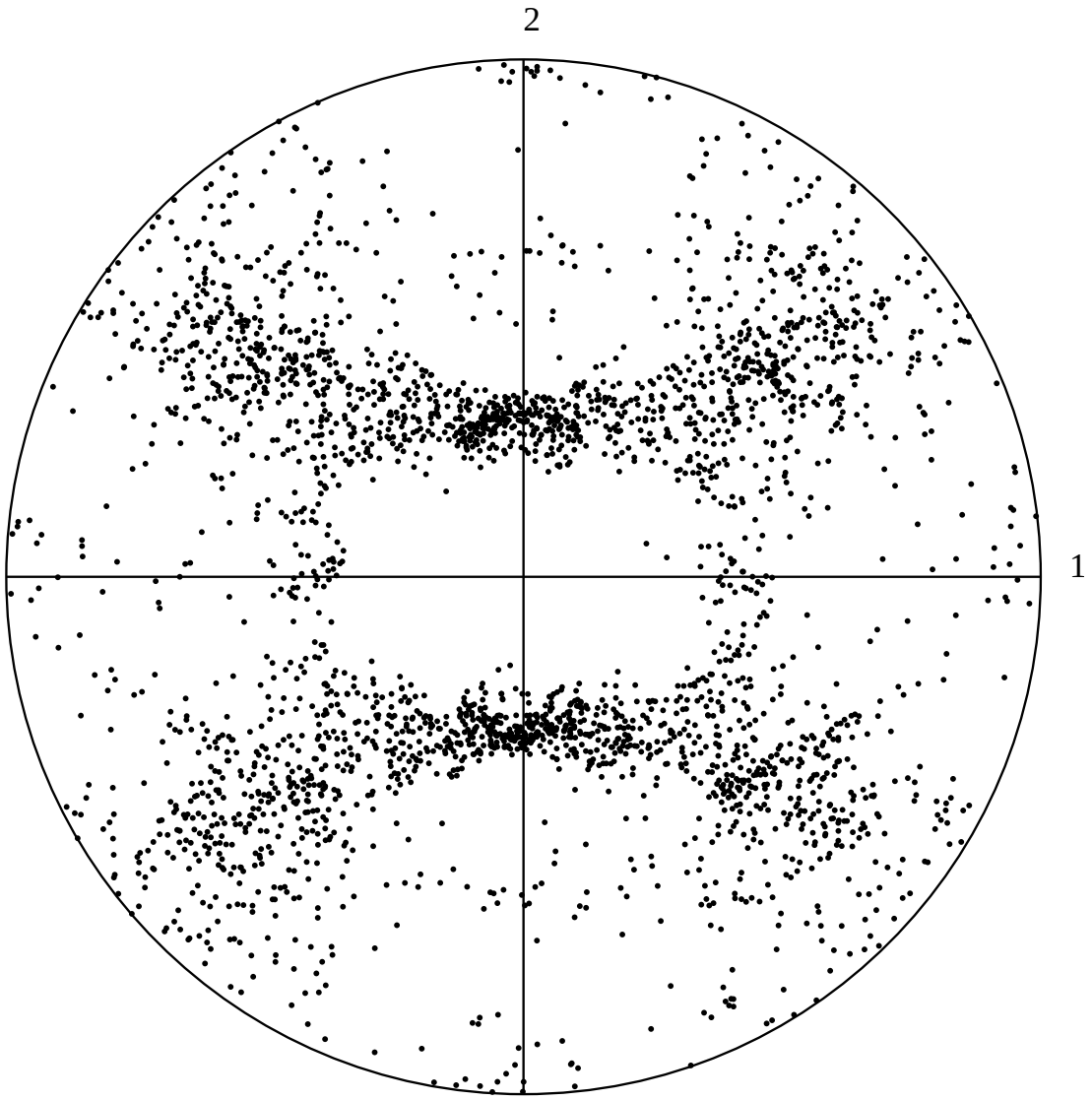
planes : {111}

Texture evolution (FCC) (rolling $F_{33} = 0.43$)



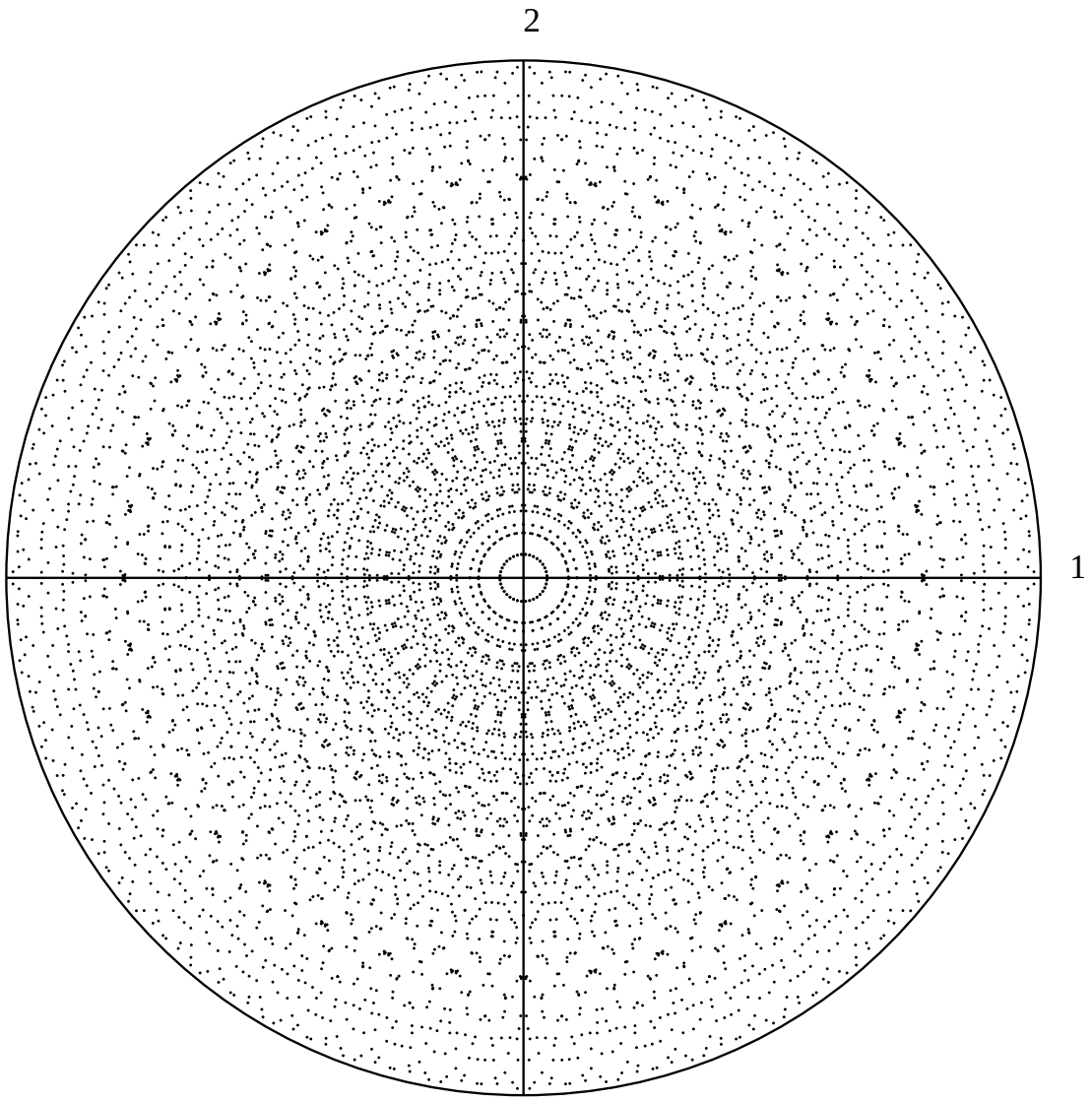
planes : {111}

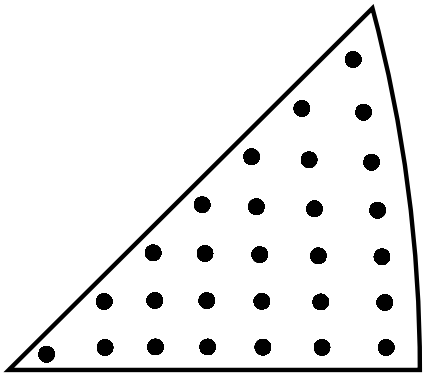
Texture evolution (FCC) (rolling $F_{33} = 0.43$)



planes : {200}

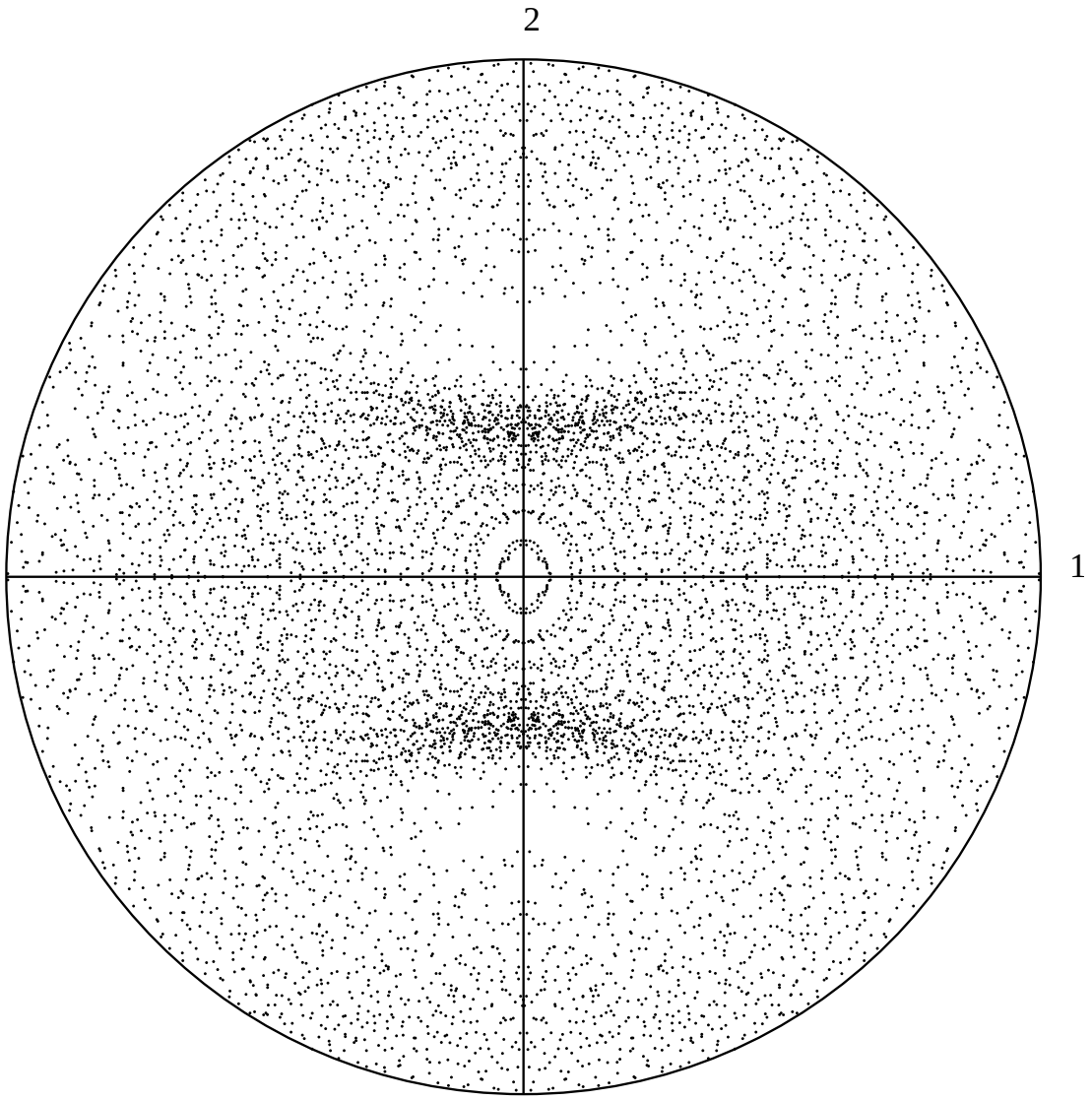
Texture evolution (FCC)





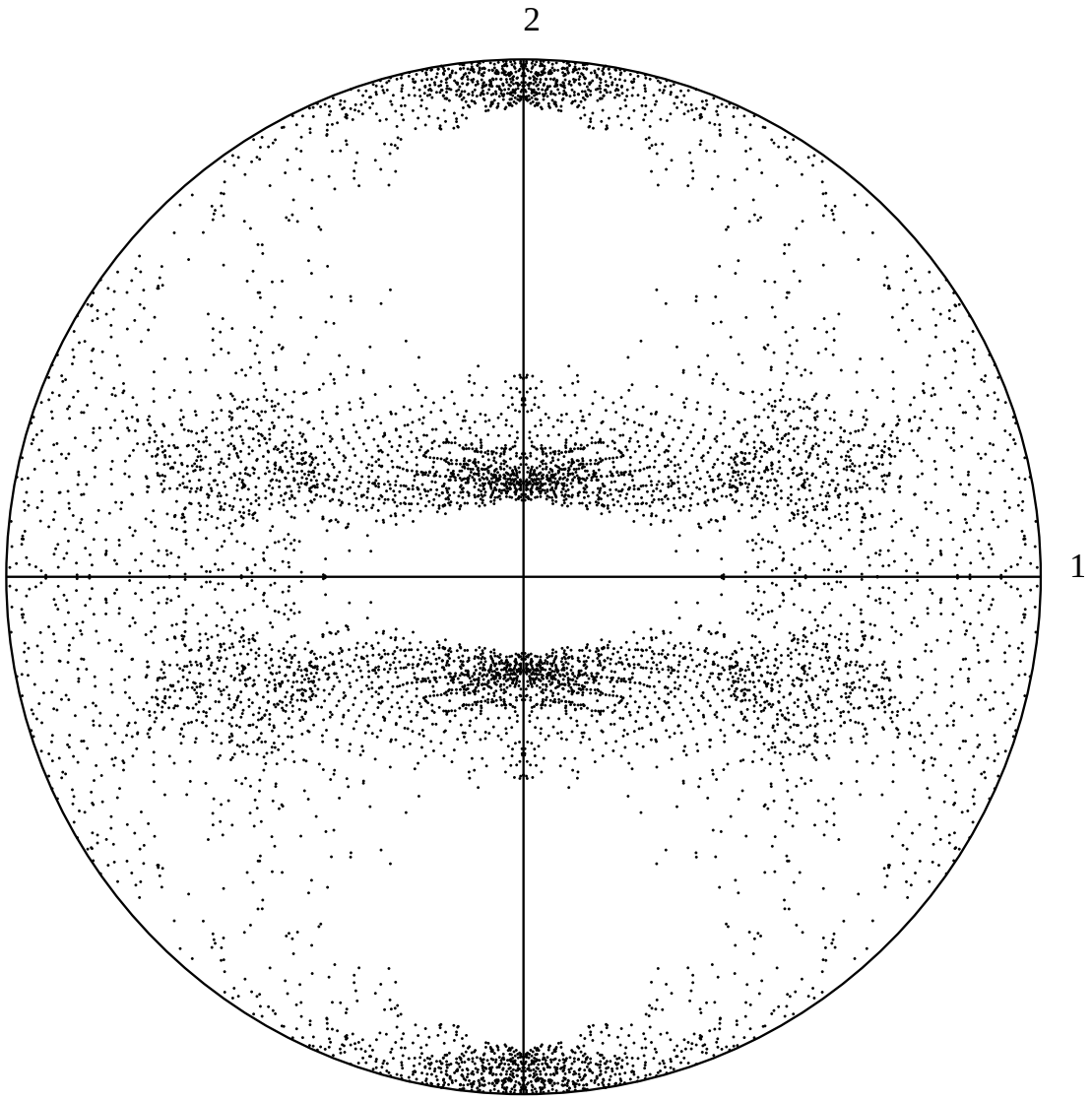
planes : {111}

Texture evolution (FCC) (rolling $F_{33} = 0.88$)



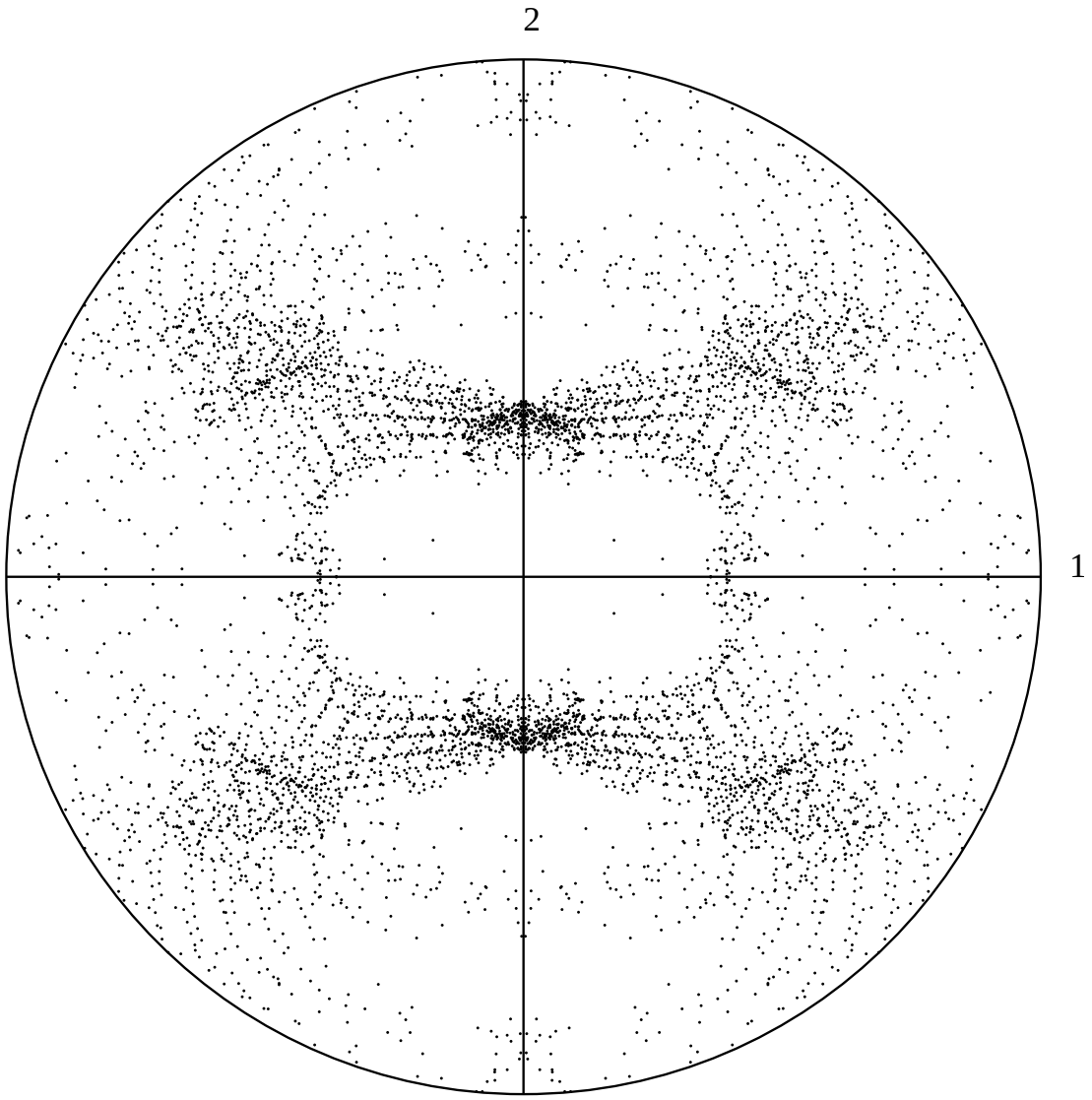
planes : {111}

Texture evolution (FCC) (rolling $F_{33} = 0.43$)



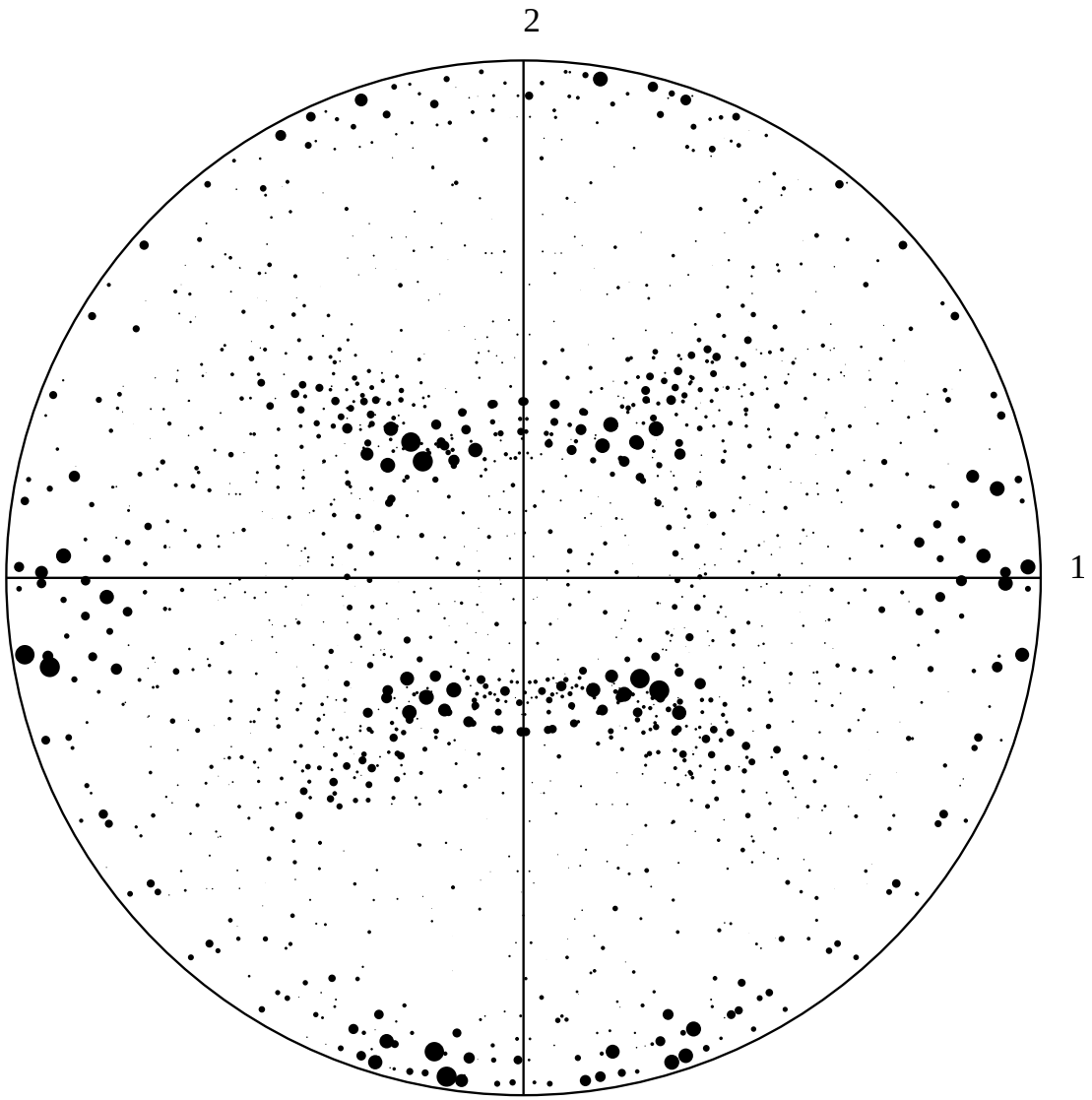
planes : {111}

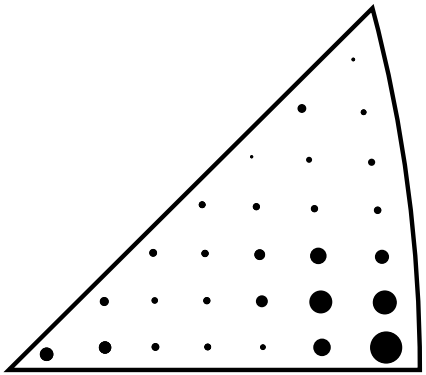
Texture evolution (FCC) (rolling $F_{33} = 0.43$)



planes : {200}

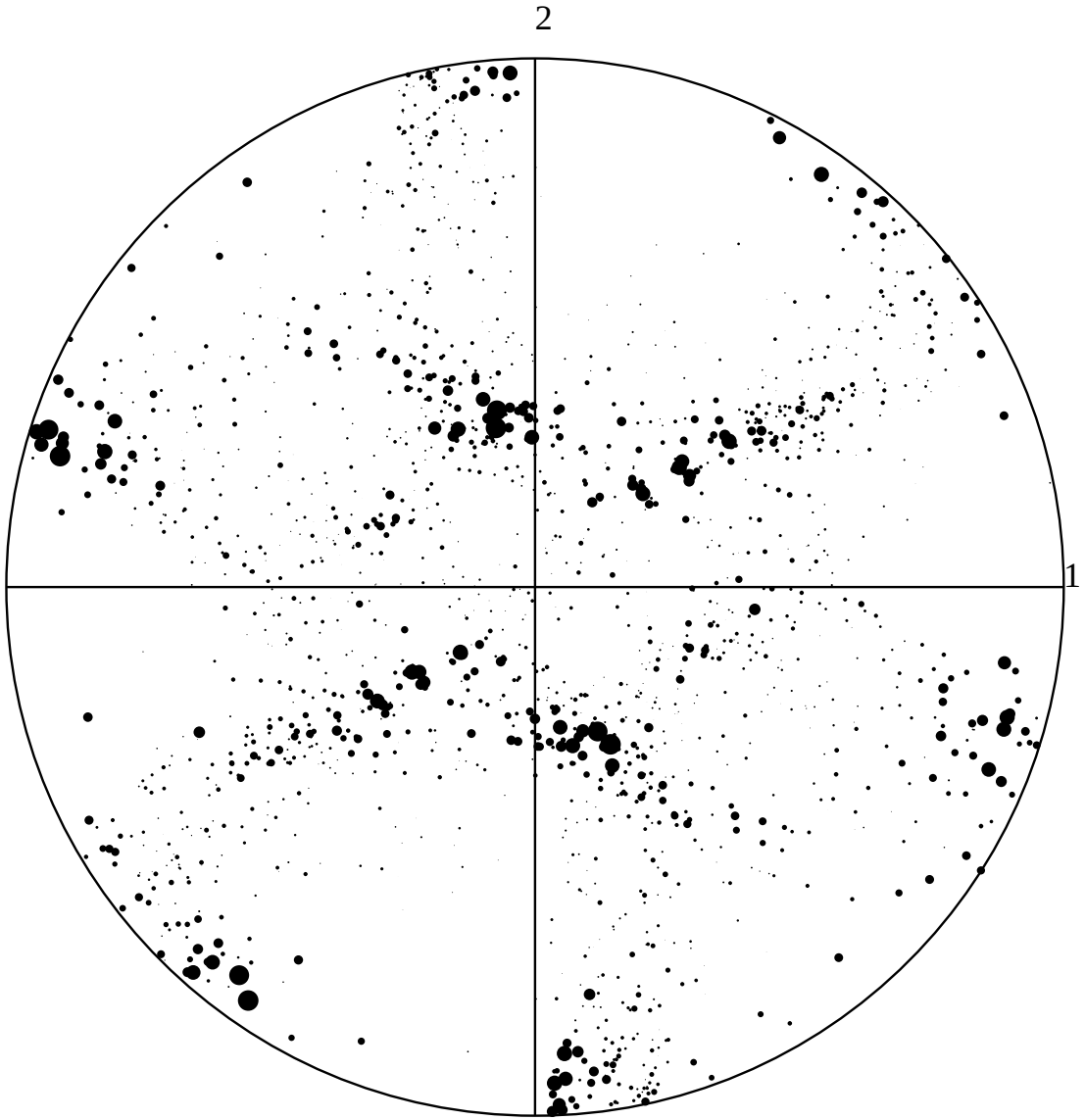
Texture evolution (FCC) (anisotropic initial texture)





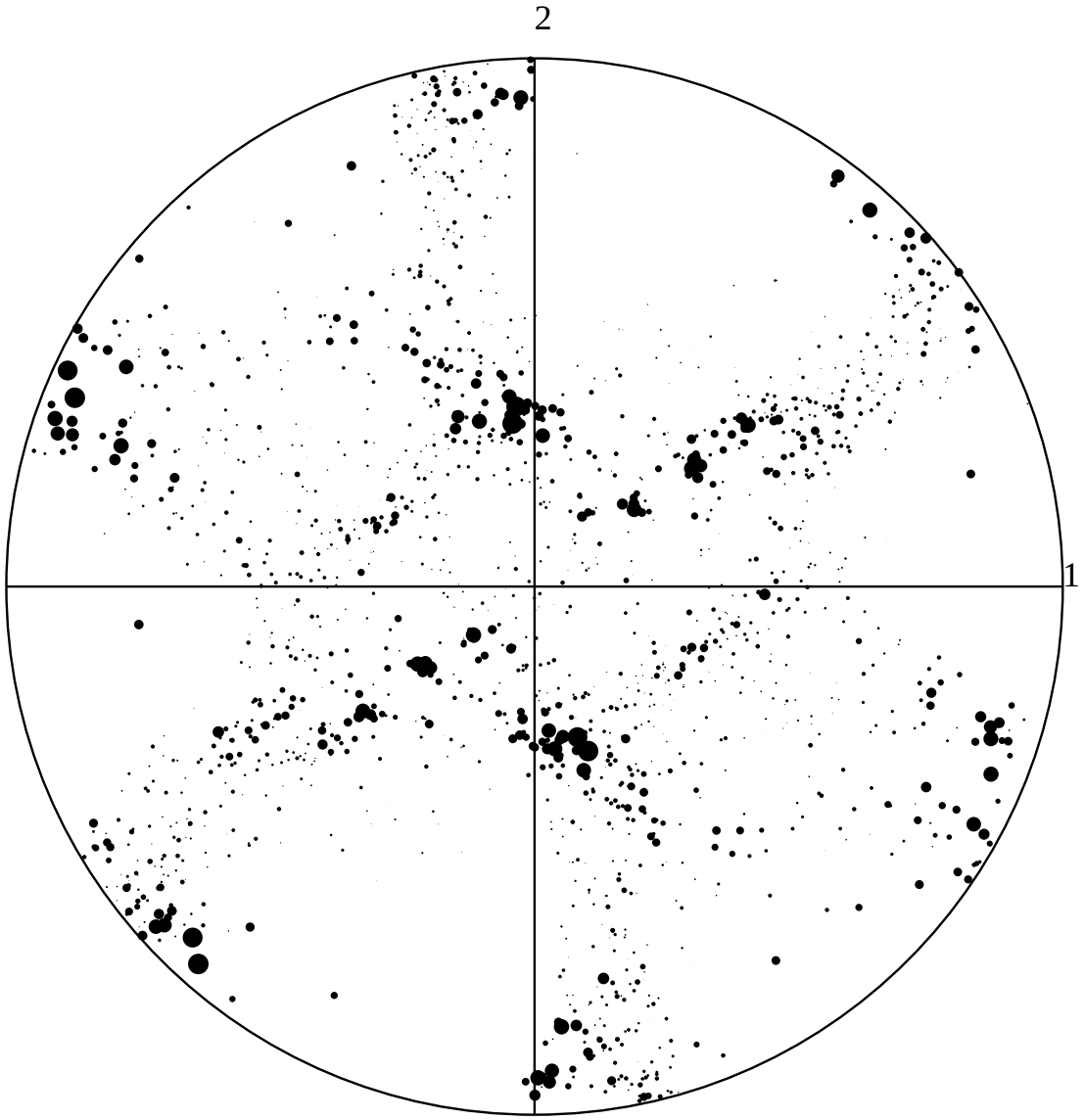
planes : {111}

Texture evolution (FCC) (torsion $F_{12} = 0.55$)



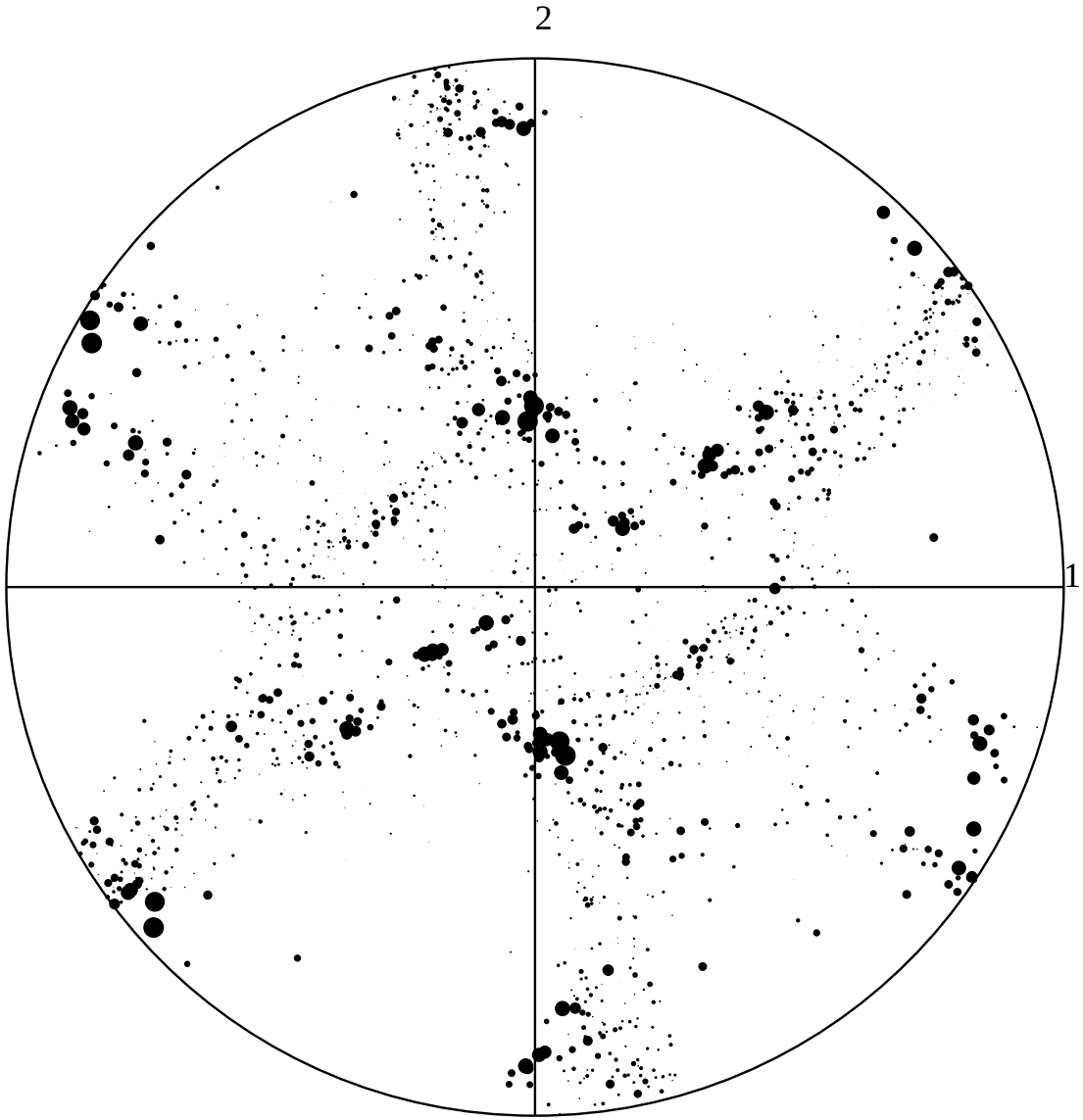
planes : {111}

Texture evolution (FCC) (torsion $F_{12} = 0.77$)



planes : {111}

Texture evolution (FCC) (torsion $F_{12} = 1.00$)

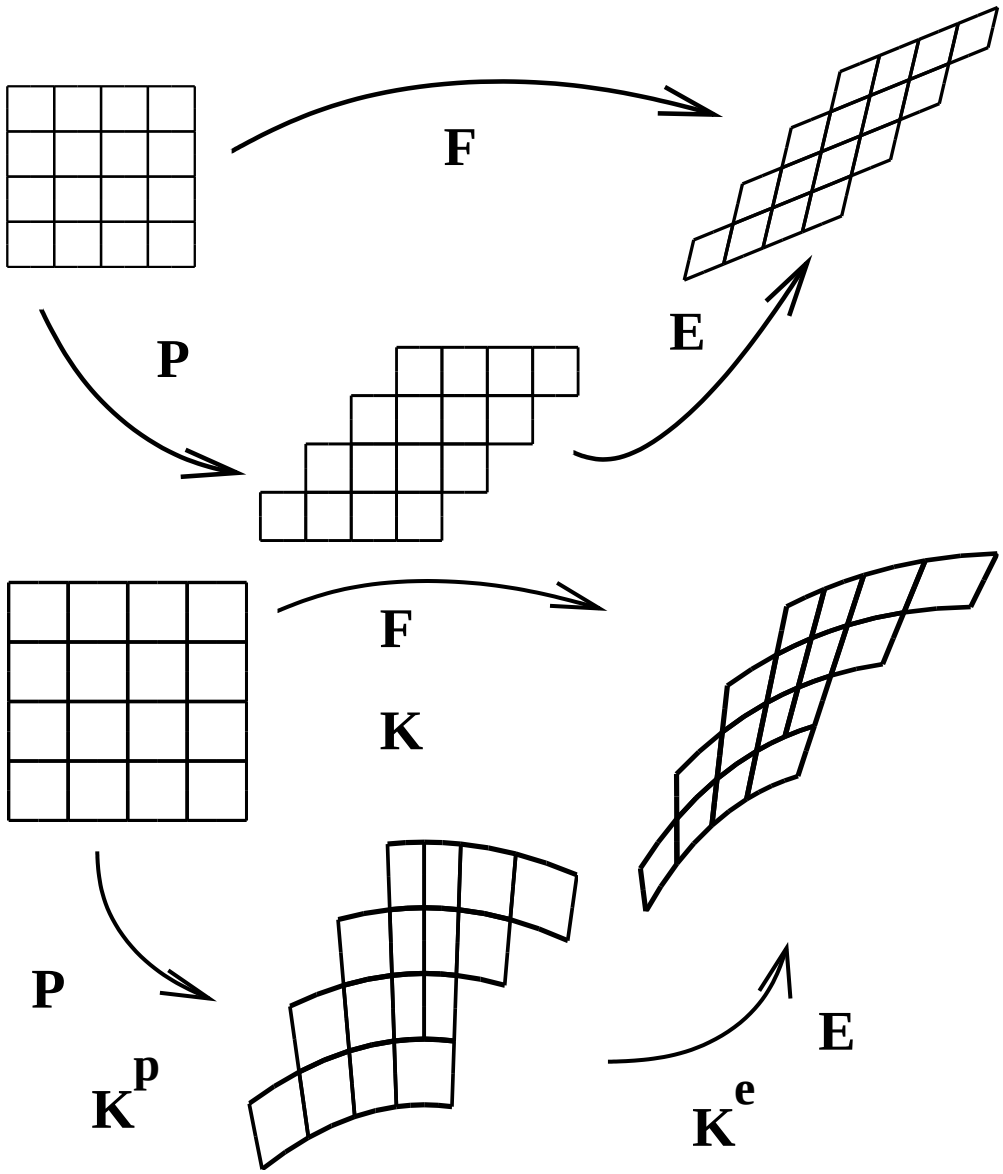


planes : {111}

Plan

Plan

Dislocation density tensor



resulting Burgers vector

$$\underline{\mathbf{b}} = \oint_c \underset{\sim}{\mathbf{E}}^{-1}.\, d\underline{\mathbf{x}}$$

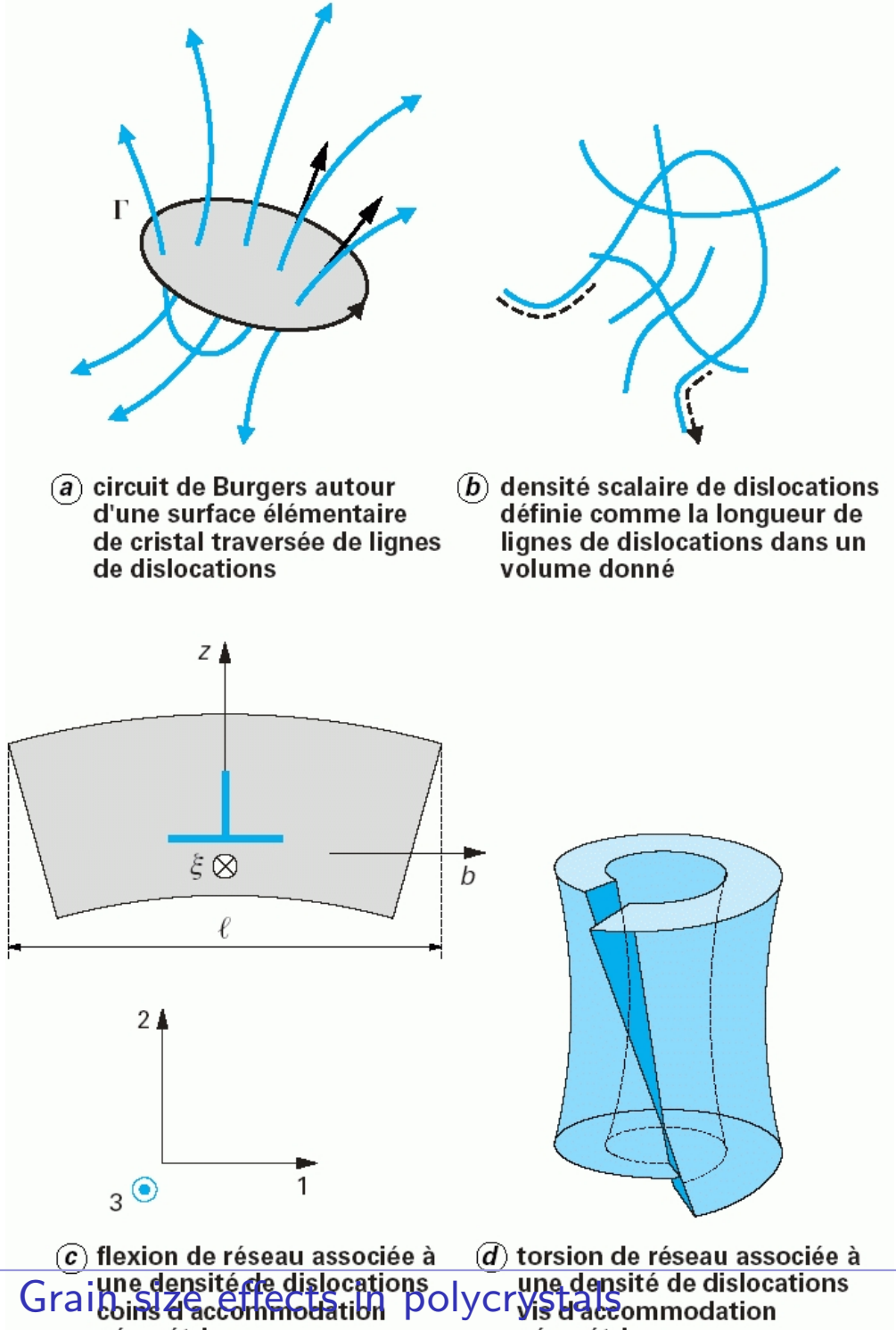
$$\underline{\mathbf{b}} = \int_S \underset{\sim}{\boldsymbol{\alpha}}\, .\underline{\mathbf{n}}\; dS$$

with

$$\underset{\sim}{\boldsymbol{\alpha}} = -\mathbf{curl}\, \underset{\sim}{\mathbf{E}}^{-1}$$

in other words,

$$\underset{\sim}{\boldsymbol{\alpha}} = < \underline{\mathbf{b}} \otimes \underline{\boldsymbol{\xi}} >$$



(a) circuit de Burgers autour d'une surface élémentaire de cristal traversée de lignes de dislocations

(b) densité scalaire de dislocations définie comme la longueur de lignes de dislocations dans un volume donné

(c) flexion de réseau associée à une densité de dislocations coins d'accommodation

(d) torsion de réseau associée à une densité de dislocations vis d'accommodation

Nye's relation (1953)

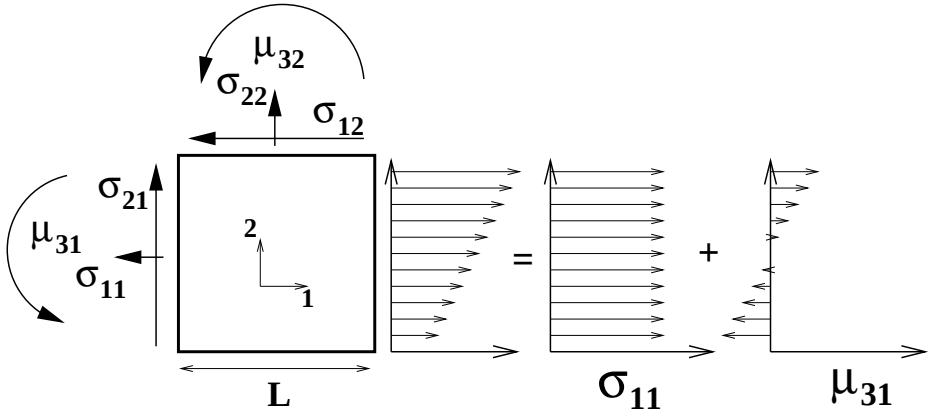
$$\underset{\sim}{\alpha} = \underset{\sim}{\mathbf{K}}^T - (\mathrm{trace}\,\underset{\sim}{\mathbf{K}})\underset{\sim}{\mathbf{1}}$$

lattice curvature tensor

$$\underset{\sim}{\mathbf{K}} = \underline{\phi} \otimes \boldsymbol{\nabla}$$

lattice curvature due to edge dislocations
lattice torsion due to screw dislocations

Cosserat continuum mechanics



isotropic elasticity :

$$\underset{\sim}{\boldsymbol{\sigma}} = \lambda \underset{\sim}{\mathbf{1}} \operatorname{Tr} \underset{\sim}{\mathbf{e}}^e + 2\mu \, {}^{\{}\underset{\sim}{\mathbf{e}}^{e\}} + 2\mu_c \, {}^{\}}\underset{\sim}{\mathbf{e}}^{e\{}$$

$$\underset{\sim}{\boldsymbol{\mu}} = \alpha \underset{\sim}{\mathbf{1}} \operatorname{Tr} \underset{\sim}{\boldsymbol{\kappa}}^e + 2\beta \, {}^{\{}\underset{\sim}{\boldsymbol{\kappa}}^{e\}} + 2\gamma \, {}^{\}}\underset{\sim}{\boldsymbol{\kappa}}^{e\{}$$

kinematics

d.o.f. $\underline{\mathbf{u}}$, $\underline{\mathbf{\Phi}}$

Cosserat deformation :

$$e_{ij} = u_{i,j} + \epsilon_{ijk}\Phi_k$$

curvature tensor :

$$\kappa_{ij} = \Phi_{i,j}$$

statics

balance of momentum :

$$\sigma_{ij,j} + f_i = 0$$

balance of moment of momentum :

$$\mu_{ij,j} - \epsilon_{ijk}\sigma_{jk} + c_i = 0$$

Cosserat crystal plasticity model

$$ {}^{\sharp}\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{R}}^T.\underset{\sim}{\mathbf{F}}, \quad {}^{\sharp}\underset{\sim}{\mathbf{K}} = \underset{\sim}{\mathbf{R}}^T.\underset{\sim}{\mathbf{K}} $$

multiplicative/additive decomposition

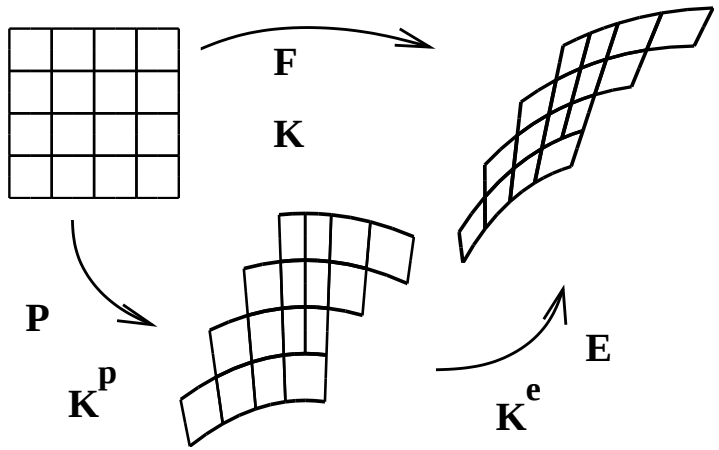
$$ {}^{\sharp}\underset{\sim}{\mathbf{F}} = {}^{\sharp}\underset{\sim}{\mathbf{F}}^e.{}^{\sharp}\underset{\sim}{\mathbf{F}}^p, \qquad {}^{\sharp}\underset{\sim}{\mathbf{K}} = {}^{\sharp}\underset{\sim}{\mathbf{K}}^e.{}^{\sharp}\underset{\sim}{\mathbf{F}}^p + {}^{\sharp}\underset{\sim}{\mathbf{K}}^p $$

$$ {}^{\sharp}\dot{\underset{\sim}{\mathbf{F}}}^p.{}^{\sharp}\underset{\sim}{\mathbf{F}}^{p-1} = \sum_{s=1}^{n} \dot{\gamma}^s {}^{\sharp}\underset{\sim}{\mathbf{P}}^s $$

$$ {}^{\sharp}\dot{\underset{\sim}{\mathbf{K}}}^p.{}^{\sharp}\underset{\sim}{\mathbf{F}}^{p-1} = \sum_{s=1}^{n} \left(\frac{\dot{\theta}^s_{\perp}}{l_{\perp}} {}^{\sharp}\underset{\sim}{\mathbf{Q}}^s{}_{\perp} + \frac{\dot{\theta}^s_{\odot}}{l_{\odot}} {}^{\sharp}\underset{\sim}{\mathbf{Q}}^s{}_{\odot} \right) $$

$$ {}^{\sharp}\underset{\sim}{\mathbf{P}}^s = {}^{\sharp}\underline{\mathbf{m}}^s \otimes {}^{\sharp}\underline{\mathbf{n}}^s $$

$$ {}^{\sharp}\underset{\sim}{\mathbf{Q}}_{\perp} = {}^{\sharp}\underline{\boldsymbol{\xi}} \otimes {}^{\sharp}\underline{\mathbf{m}}, \; {}^{\sharp}\underset{\sim}{\mathbf{Q}}_{\odot} = \frac{1}{2}\underset{\sim}{\mathbf{1}} - {}^{\sharp}\underline{\mathbf{m}} \otimes {}^{\sharp}\underline{\mathbf{m}} $$



generalized Schmid law

$$ \tau^s = \underset{\sim}{\mathbf{P}}^s : \underset{\sim}{\boldsymbol{\sigma}}^s $$

$$ \nu^s = \underset{\sim}{\mathbf{Q}}^s : \underset{\sim}{\boldsymbol{\mu}}^s $$

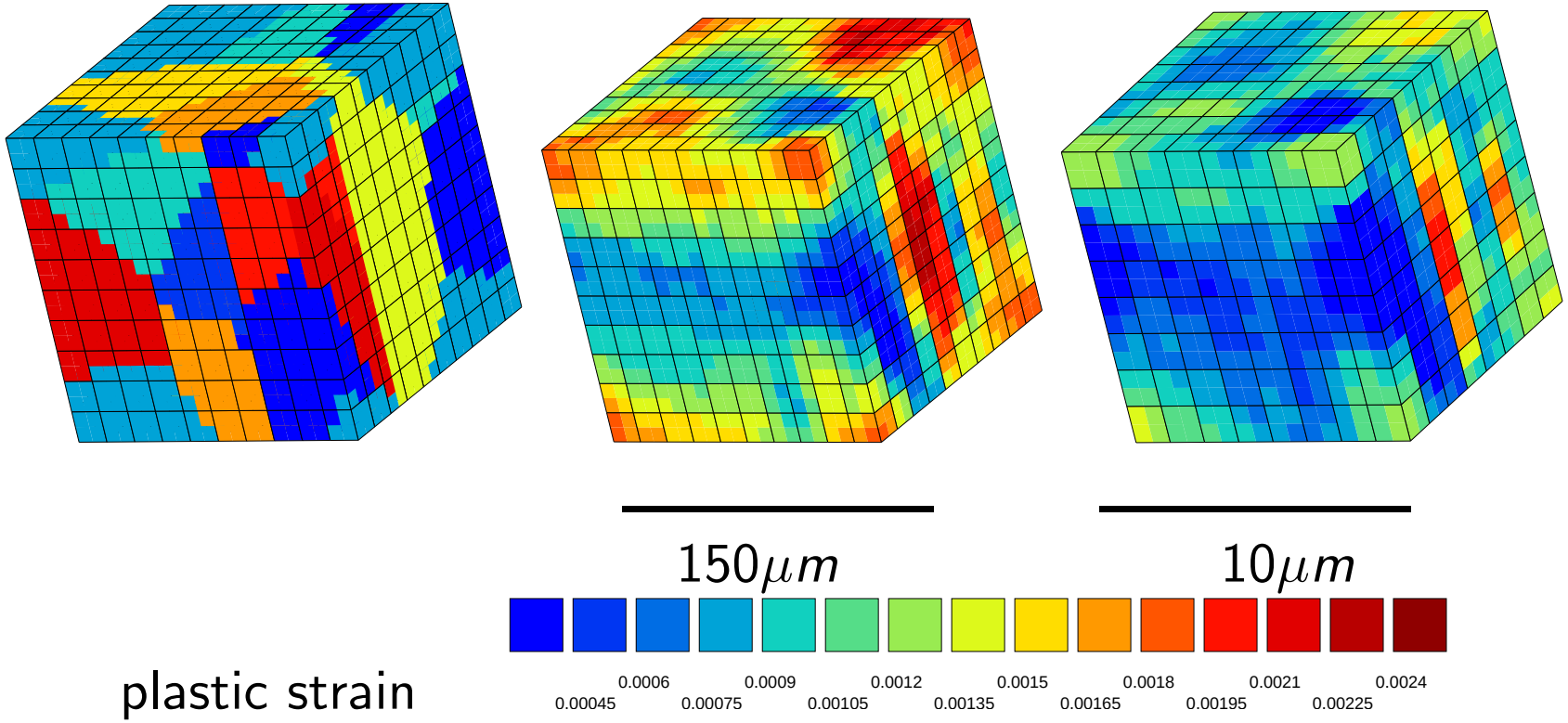
$$ \dot{\gamma}^s = < \frac{\mid \tau^s \mid - r^s}{k} >^n \operatorname{sign}\tau^s $$

$$ \dot{\theta}^s = < \frac{\mid \nu^s \mid - l_{\perp} r^s_c}{l_{\perp} k_c} >^{n_c} \operatorname{sign}(\nu^s) $$

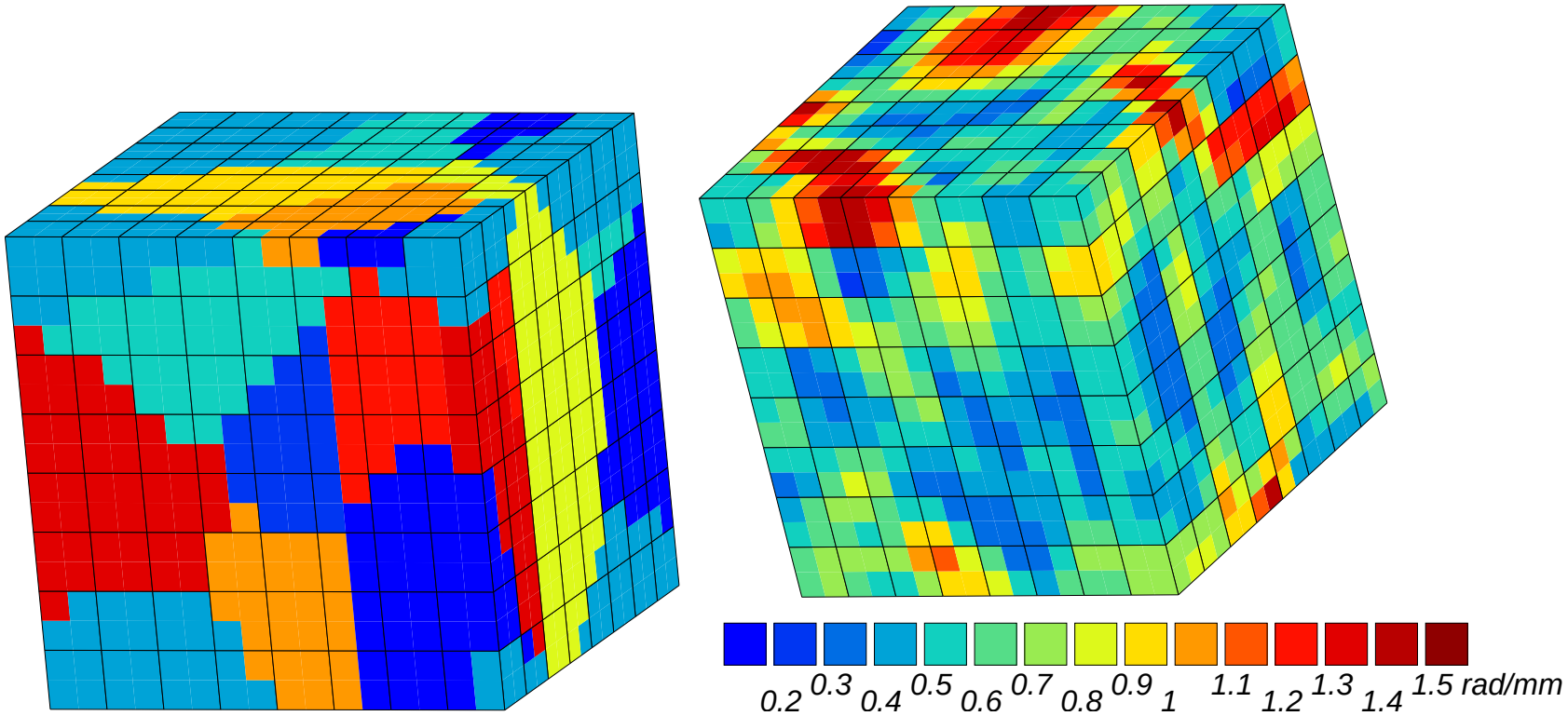
hardening law $\quad r^s = r_0 + q \sum_{r=1}^{n} h^{sr}(1 - \exp(-bv^r)) + R(\mid \theta^s \mid), \quad r^s_c = r_{c0}$

Plan

Grain size effects in polycrystals



Lattice curvature in a ferritic steel



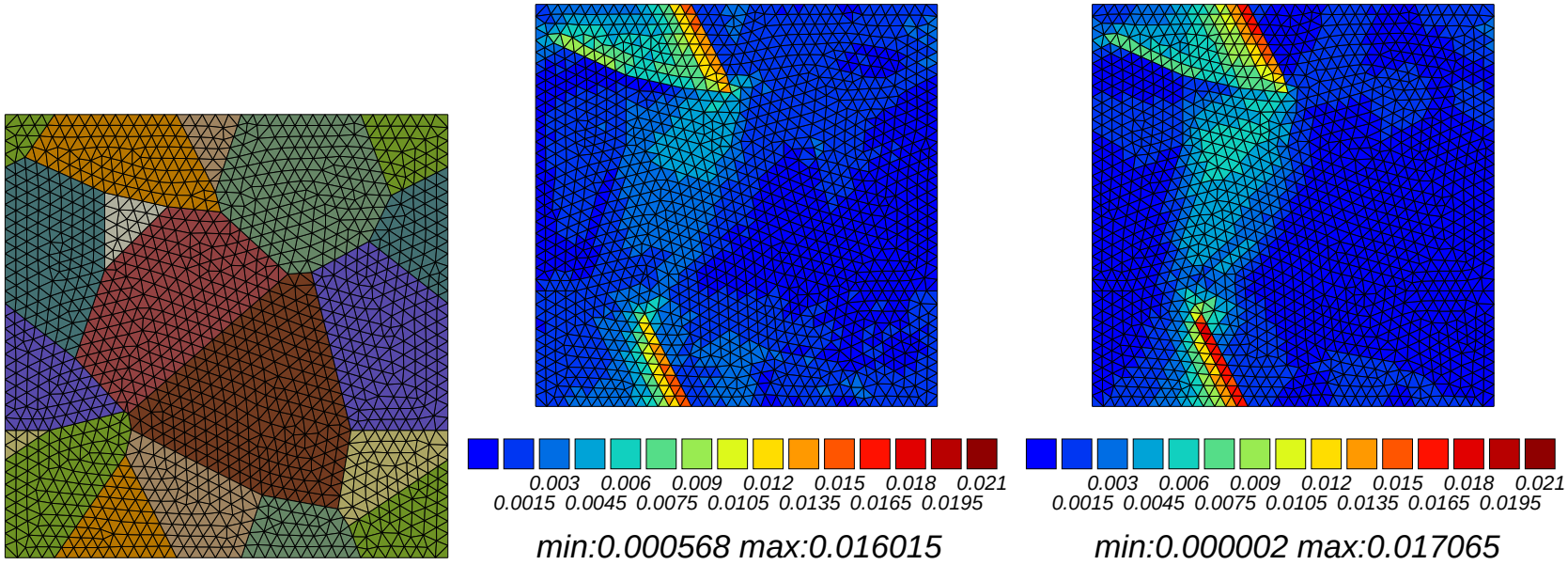
$\simeq 1 - 10^\circ/\mu m$

additional hardening $R^s(\theta^s) = Q_c \sqrt{\sum_r |\theta^r|}$

[Zeghadi, 2004]

Grain size effect in a ferritic steel

Microplasticity: plastic strain

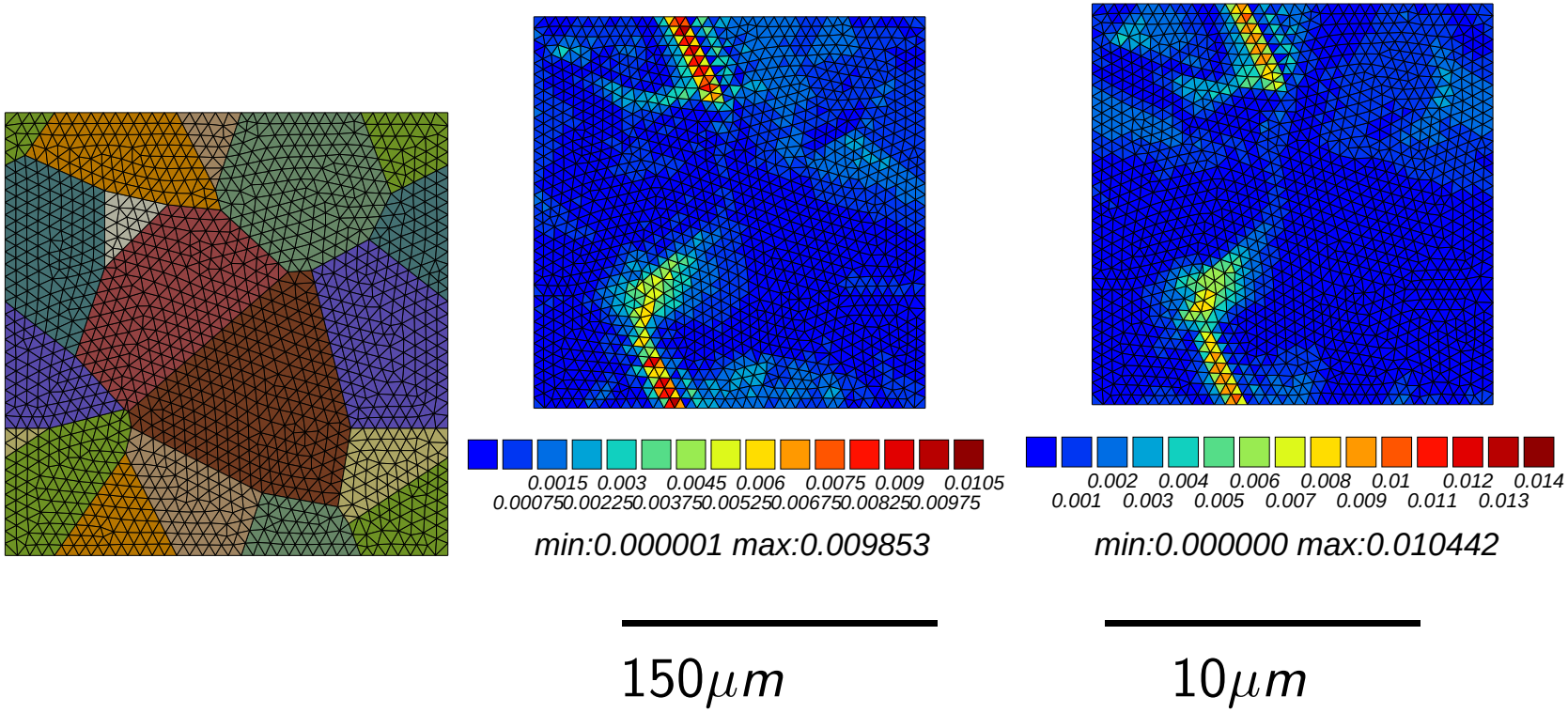


$150\mu m$ $10\mu m$

[Zeghadi, 2004]

Grain size effect in a ferritic steel

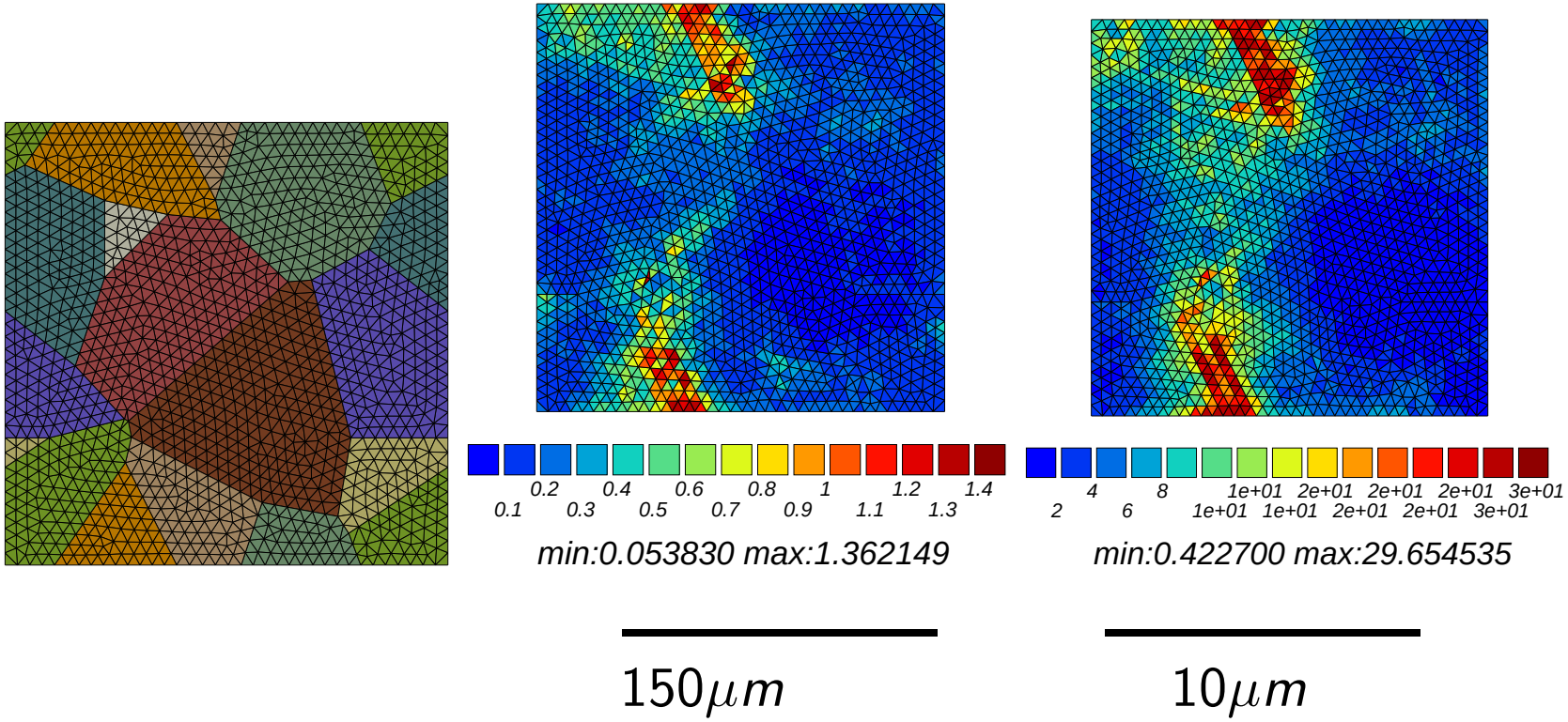
Microplasticity: lattice rotation



[Zeghadi, 2004]

Grain size effect in a ferritic steel

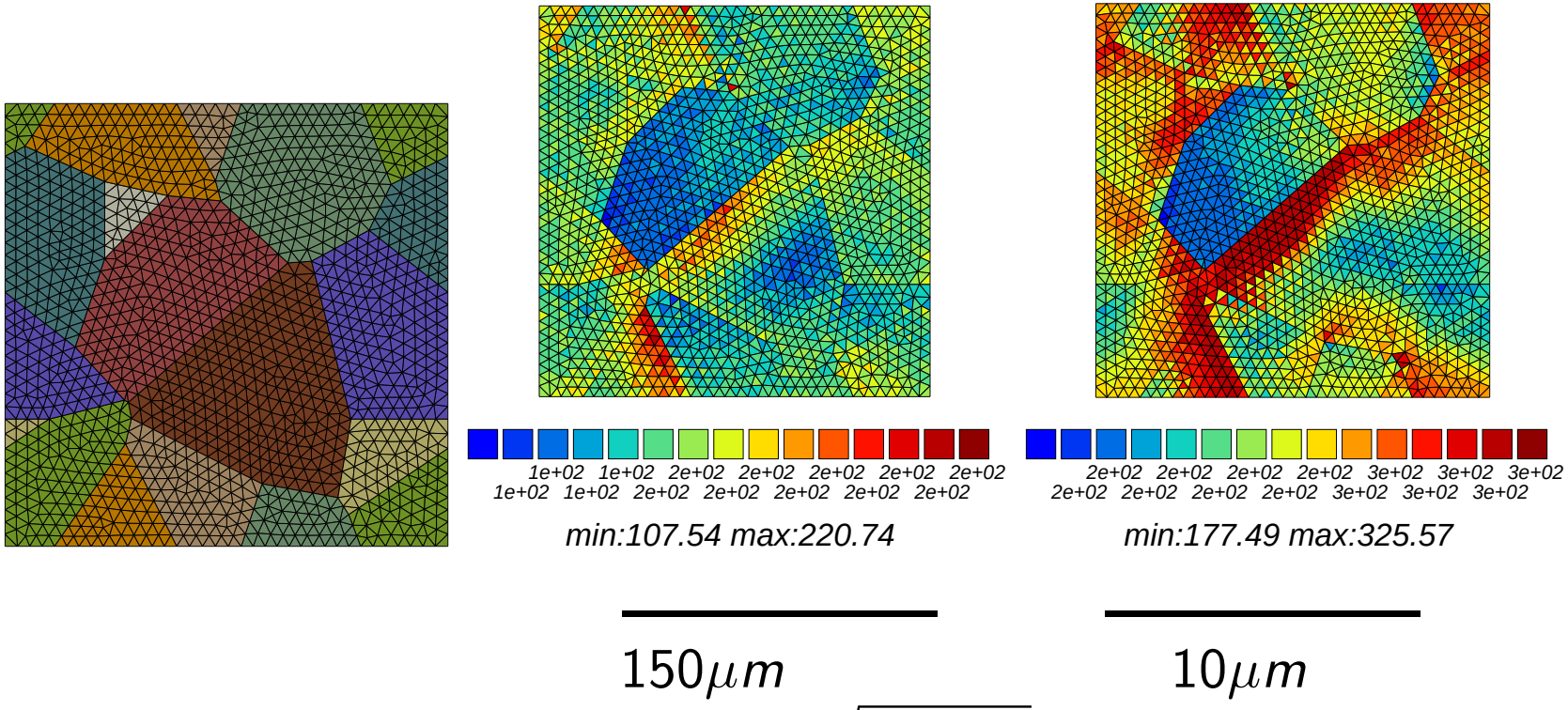
Microplasticity: lattice curvature



[Zeghadi, 2004]

Grain size effect in a ferritic steel

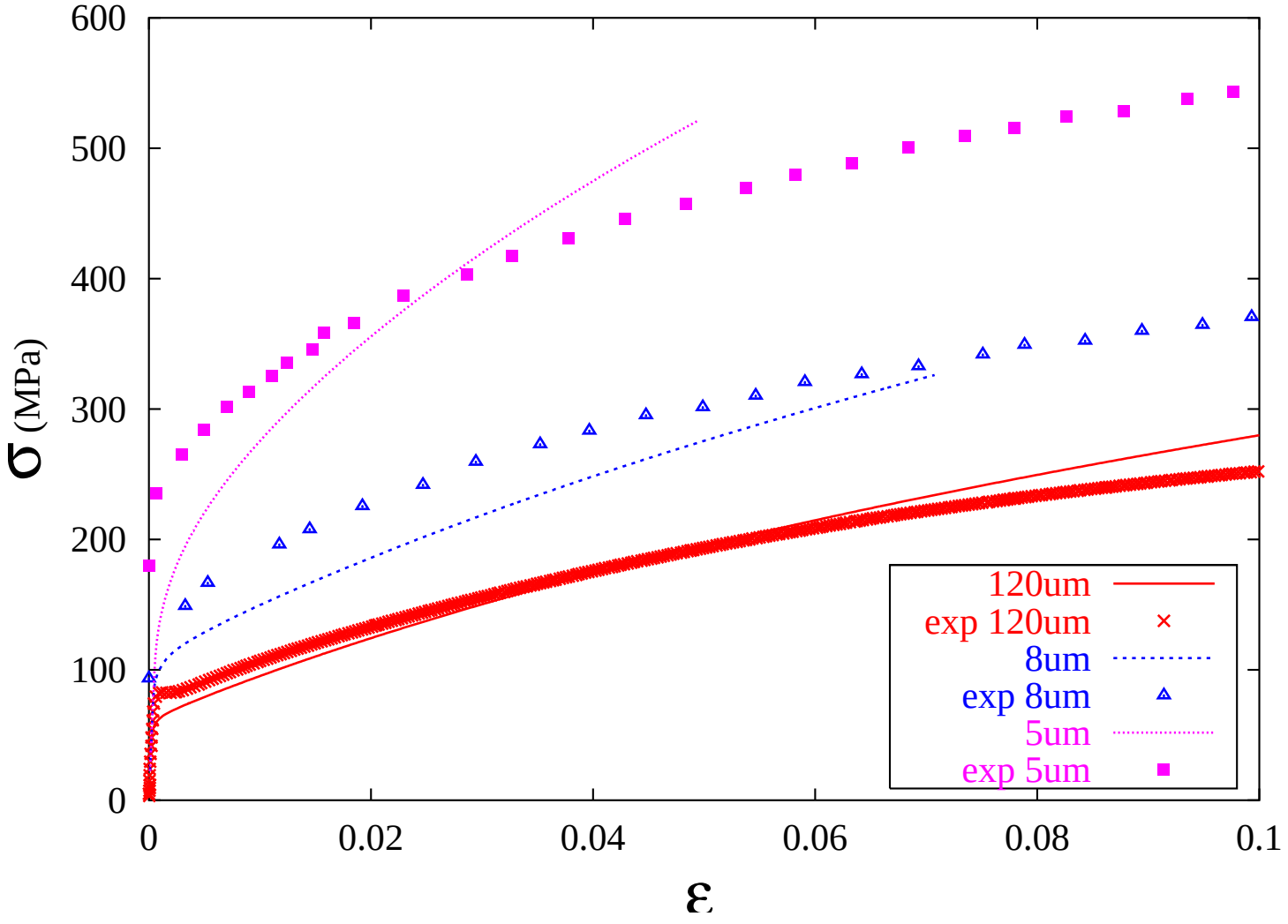
Microplasticity : local stresses



additional hardening $R^s(\theta^s) = Q_c \sqrt{\sum_r |\theta^r|}$

[Zeghadi, 2004]

Grain size effects in a ferritic steel



[Bouaziz, 2002]