

Continuum theory of crystalline defects and mechanical fields

Lecture: Phenomenological Mesoscale Field Dislocation Mechanics and Applications

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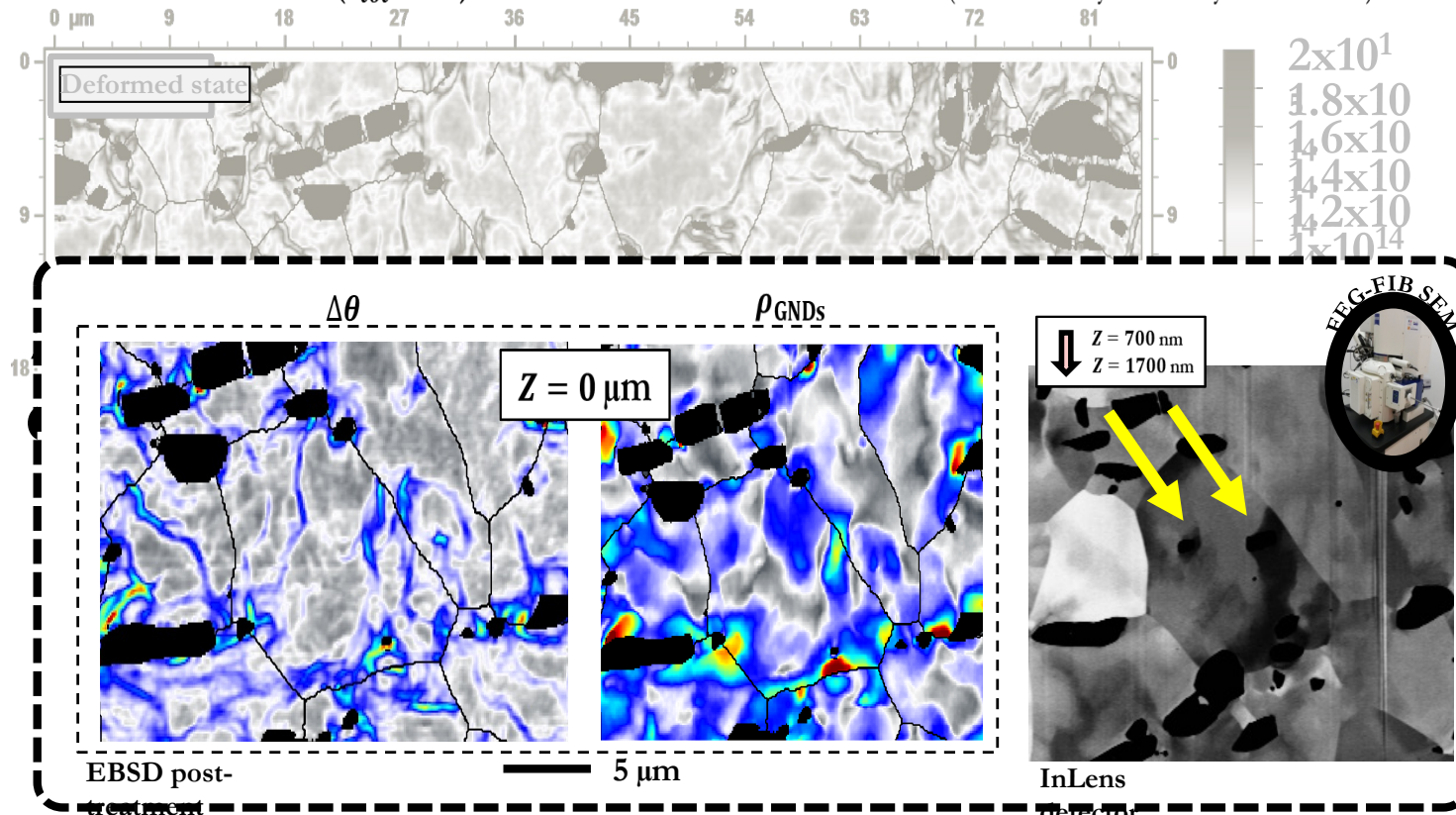
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Study of plastic deformation heterogeneities at mesoscale

Characterization of deformed state / Localization of plastic deformation /

Deformed state in tension ($\epsilon_{tot} = 4\%$) : evaluation of GND dislocations densities (Geometrically Necessary Dislocations)



Post doc J. Genée (LEM3, Labex DAMAS)

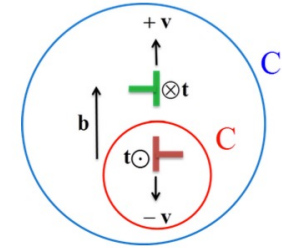
Genée et al. J. Mater. Sci. (2021)

Outline

- Mesoscopic Field Dislocation Mechanics (PMFDM)
- Numerical implementation based on an elastoviscoplastic FFT scheme (PMFDM-EVPFFT)
- Applications of PMFDM-EVPFFT
- References

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Phenomenological Mesoscopic Field Dislocation Mechanics



- **Evolution of plastic distortion:** $\dot{\mathbf{U}}^p = \boldsymbol{\alpha} \times \mathbf{v} + \mathbf{L}^p$

Acharya and Roy (2006)

- **SSD (Statistically stored dislocations) and Crystal plasticity** (*Asaro, 1983*)

$$\mathbf{L}^p = \sum_{s=1}^N \dot{\gamma}^s \mathbf{m}^s \otimes \mathbf{n}^s \quad \text{with} \quad \dot{\gamma}^s = \dot{\gamma}^0 \left(|\tau^s| / \hat{\tau}_c \right)^{1/m} \text{sign}(\tau^s)$$

- **GND (Geometrically Necessary Dislocation) density transport equation**

$$\dot{\boldsymbol{\alpha}} = -\text{Curl} \left(\boldsymbol{\alpha} \times \mathbf{v} + \mathbf{L}^p \right)$$

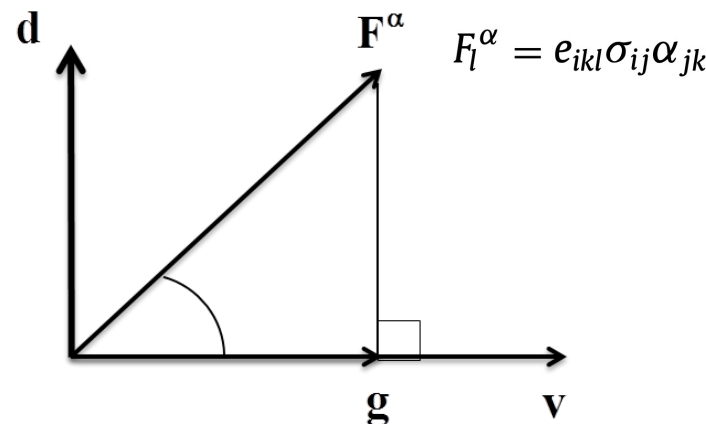
- **Intrinsic Dissipation** $\mathbf{D} = \int_V \boldsymbol{\sigma} : \mathbf{L}^p dV + \int_V \mathbf{F}^\alpha \cdot \mathbf{v} dV$ with: $\mathbf{F}^\alpha = \mathbf{X} : (\boldsymbol{\sigma} \cdot \boldsymbol{\alpha})$

Constitutive equations (GNDs)

$$\mathbf{v} = \frac{\mathbf{g}}{|\mathbf{g}|} \bar{v} \quad \bar{v} \geq 0$$

$$\mathbf{g} = \mathbf{F}^\alpha - \left(\mathbf{F}^\alpha \cdot \frac{\mathbf{d}}{|\mathbf{d}|} \right) \frac{\mathbf{d}}{|\mathbf{d}|}$$

$$\bar{v} = \frac{\eta^2 b}{N} \left(\frac{\mu}{\hat{\tau}_c} \right)^2 \sum_{s=1}^N |\dot{\gamma}^s|$$



$\mathbf{g}$: glide force $\mathbf{X}$: Levi-Civita
 $\mathbf{F}^\alpha$: Peach-Koehler driving force

$\mathbf{d}$: dilatant direction

$\bar{v}$: GND velocity magnitude

η : materials parameter

N : number of slip systems
 here $N=12$ for fcc metals
 $(111)\langle 110 \rangle$

Crystal plasticity-based strain-hardening models

PMFDM-EVP-FFT vs. Conventional Crystal Plasticity (CP-EVP-FFT)

- **Classic Crystal Plasticity (CP-EVP-FFT)** : no hardening due to GNDs (classic incremental Voce law, hardening due to SSDs)

$$\dot{\hat{\tau}}_c = \theta_0 \frac{\tau_s - \hat{\tau}_c}{\tau_s - \tau_0} \dot{\Gamma} \quad \text{with} \quad \dot{\Gamma} = \sum_{s=1}^{12} |\dot{\gamma}^{(s)}|$$

- **Mesoscale FDM crystal plasticity (MFDM-EVP-FFT)**: hardening due to GNDs and SSDs (in a Voce type law) (see e.g. *Djaka et al. 2020*)

$$\dot{\hat{\tau}}_c = \theta_0 \frac{\tau_s - \hat{\tau}_c}{\tau_s - \tau_0} \dot{\Gamma} + k_0 \frac{\eta^2 \mu^2 b}{2(\hat{\tau}_c - \tau_0)} \sum_{s=1}^{12} |\alpha \cdot \mathbf{n}^{(s)}| |\dot{\gamma}^{(s)}| + k_0 \frac{\eta^2 \mu^2 b}{2(\hat{\tau}_c - \tau_0)} \sum_{s=1}^{12} |\alpha \cdot \mathbf{n}^{(s)}| |\alpha \times \mathbf{V}|$$

$$\text{with } \dot{\Gamma} = |\alpha \times \mathbf{V}| + \sum_{s=1}^{12} |\dot{\gamma}^{(s)}| \quad \text{and} \quad L_g = \frac{1}{k_0 |\alpha \cdot \mathbf{n}^{(s)}|} \quad \begin{array}{l} \text{« geometric » (physical)} \\ \text{mean free path} \end{array}$$

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EVP-FFT formulation with Augmented Lagrangian scheme

- **Elasto-viscoplastic constitutive law (implicit backward Euler time integration)**

$$\boldsymbol{\varepsilon}^{t+\Delta t} = \mathbf{C}^{-1} : \mathbf{T}^{t+\Delta t} + \boldsymbol{\varepsilon}^{p,t} + \dot{\boldsymbol{\varepsilon}}^{p,t+\Delta t} (\mathbf{T}^{t+\Delta t}) \Delta t$$

- **Lippmann-Schwinger integral equation**

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \mathbf{E} - \left(\Gamma^0 * \boldsymbol{\tau} \right)(\mathbf{x}) \quad \text{with} \quad \begin{cases} \tau_{ij} = \delta C_{ijkl} \varepsilon_{kl} & : \text{stress polarization tensor} \\ \Gamma_{ijkl}^0 & : \text{modified Green tensor} \end{cases} \quad \text{Lebensohn et al. IJP (2012)}$$

FFT

$$\Rightarrow \quad \tilde{\boldsymbol{\varepsilon}}(\boldsymbol{\xi}) = -\Gamma^0(\boldsymbol{\xi}) : \boldsymbol{\tau}(\boldsymbol{\xi}) \quad \text{and} \quad \tilde{\boldsymbol{\varepsilon}}(0) = \mathbf{E}$$

- **Solved by Augmented Lagrangian formulation (non linear)**
- **Finite difference schemes together with DFT** to avoid spurious oscillations *Willot (2015)*
- **Spectral resolution of GND density transport:**

Hyperbolic transport equation Exponential spectral filter (*Djaka et al, MSMSE 2015*)

$$\tilde{\alpha}_{ij}^{t+\Delta t} = \sigma(\eta) \left(\tilde{\alpha}_{ij}^t - \Delta t \, i \, \xi_k \left(\widetilde{(\alpha_{ij} v_k)^t} - \widetilde{(\tilde{\alpha}_{ik} \tilde{v}_j)^t} \right) \right) - \Delta t \, i \, \xi_k \, e_{jkl} \left(\widetilde{L_{il}^p} \right)^t$$

$$\sigma\left(\frac{k_1}{N_1}, \frac{k_2}{N_2}, \frac{k_3}{N_3}\right) = \exp\left(-\beta\left(\left(\frac{k_1}{N_1}\right)^{2p} + \left(\frac{k_2}{N_2}\right)^{2p} + \left(\frac{k_3}{N_3}\right)^{2p}\right)\right) \quad \text{with} \quad \begin{cases} \beta = -\log \varepsilon_M : \text{« damping » parameter} \\ \varepsilon_M : \text{relatively small value} \\ \eta : \text{discrete frequencies} \\ 2p : \text{filter order} \end{cases}$$

EVP-FFT formulation with Augmented Lagrangian scheme

- **Elasto-viscoplastic constitutive law (implicit backward Euler time integration)**

$$\boldsymbol{\varepsilon}^{t+\Delta t} = \mathbf{C}^{-1} : \mathbf{T}^{t+\Delta t} + \boldsymbol{\varepsilon}^{p,t} + \dot{\boldsymbol{\varepsilon}}^{p,t+\Delta t}(\mathbf{T}^{t+\Delta t})\Delta t \quad \text{Lebensohn, et al. IJP 2012}$$

- **Lippmann-Schwinger integral equation**

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \mathbf{E} - (\Gamma^0 * \boldsymbol{\tau})(\mathbf{x}) \quad \text{with} \quad \left\{ \begin{array}{l} \tau_{ij} = \delta C_{ijkl} \varepsilon_{kl} : \text{stress polarization tensor} \\ \Gamma^0_{ijkl} : \text{modified Green tensor} \end{array} \right.$$

FT  $\tilde{\boldsymbol{\varepsilon}}(\boldsymbol{\xi}) = -\Gamma^0(\boldsymbol{\xi}) : \boldsymbol{\tau}(\boldsymbol{\xi}) \quad \text{and} \quad \tilde{\boldsymbol{\varepsilon}}(0) = \mathbf{E}$

- **Solved by Augmented Lagrangian formulation (non linear)**

$$\tau_{ij}^{(n)} = \lambda_{ij}^{(n)} - C_{ijkl}^0 e_{kl}^{(n)} \quad \text{Michel et al. (2001)}$$

$$\mathbf{R}_{ij}^{es}(\mathbf{T}^{(n+1)}) = T_{ij}^{(n+1)} + C_{ijmn}^0 \varepsilon_{mn}^{(n+1)}(\mathbf{T}^{(n+1)}) - \lambda_{ij}^{(n)} - C_{ijmn}^0 e_{mn}^{(n+1)} = 0$$

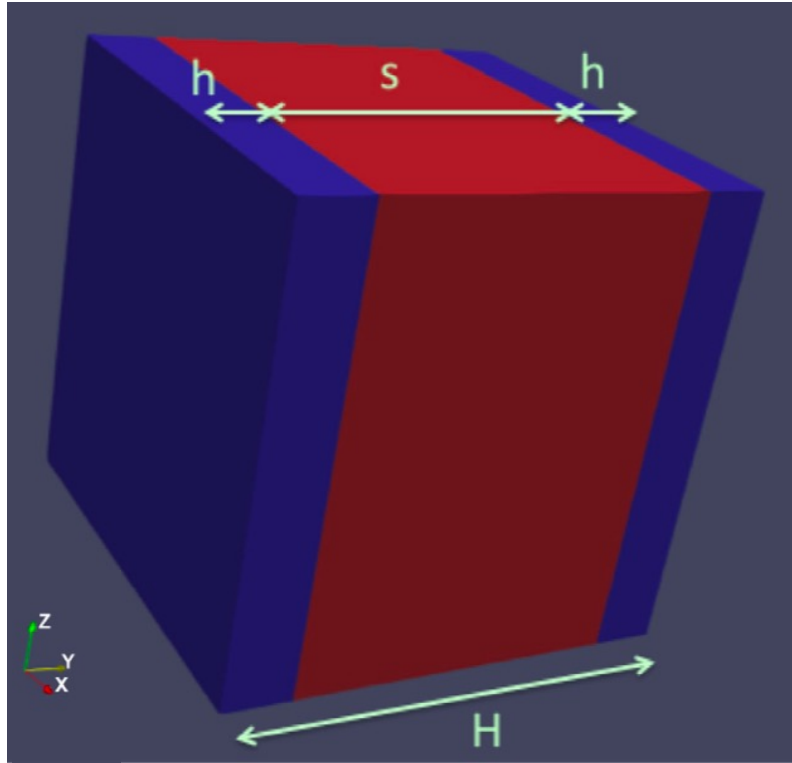
$$T_{ij}^{(n+1,p+1)} = T_{ij}^{(n+1,p)} - \left(\left(\partial R_{ij}^{es} / \partial T_{mn} \right)_{\mathbf{T}^{(n+1,p)}} \right)^{-1} R_{mn}^{es}(\mathbf{T}^{(n+1,p)})$$

$$\left(\partial R_{ij}^{es} / \partial T_{mn} \right)_{\mathbf{T}^{(n+1,p)}} = \delta_{im} \delta_{jn} + C_{ijkl}^0 C_{klmn}^{-1} + \Delta t C_{ijkl}^0 \left(\partial \dot{\varepsilon}_{kl}^p / \partial T_{mn} \right)_{\mathbf{T}^{(n+1,p)}}$$

$$\boldsymbol{\lambda}^{(n+1)} = \boldsymbol{\lambda}^{(n)} + \mathbf{C}^0 : (\mathbf{e}^{(n+1)} - \boldsymbol{\varepsilon}^{(n+1)}) \quad (\text{new guess, Uzawa descent algorithm})$$

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Application 1: Two-phase laminate structures



$\Phi 1 (^{\circ})$	$\Phi (^{\circ})$	$\Phi 2 (^{\circ})$
300.	54.7356	45

- Specific parameters for GND density transport equation c: for Courant condition , exponential filter parameters)

$p=1$	$\varepsilon_M=0.2$	$c=0.25$	$\Delta t(\text{CFL}) = \mathbf{c} \cdot \Delta \mathbf{x} / \max(\mathbf{v})$
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- Simulation parameters

Constant Volume fraction of elastic precipitates: $f=0.3125$ or $f=0.125$

Period: $H=2h+s$

s : channel size

- Materials parameters (Al)

Isotropic elasticity:

$E = 69\text{GPa}$ ($\mu=25.9\text{GPa}$) $\nu = 0.33$

Hardening and flow rule

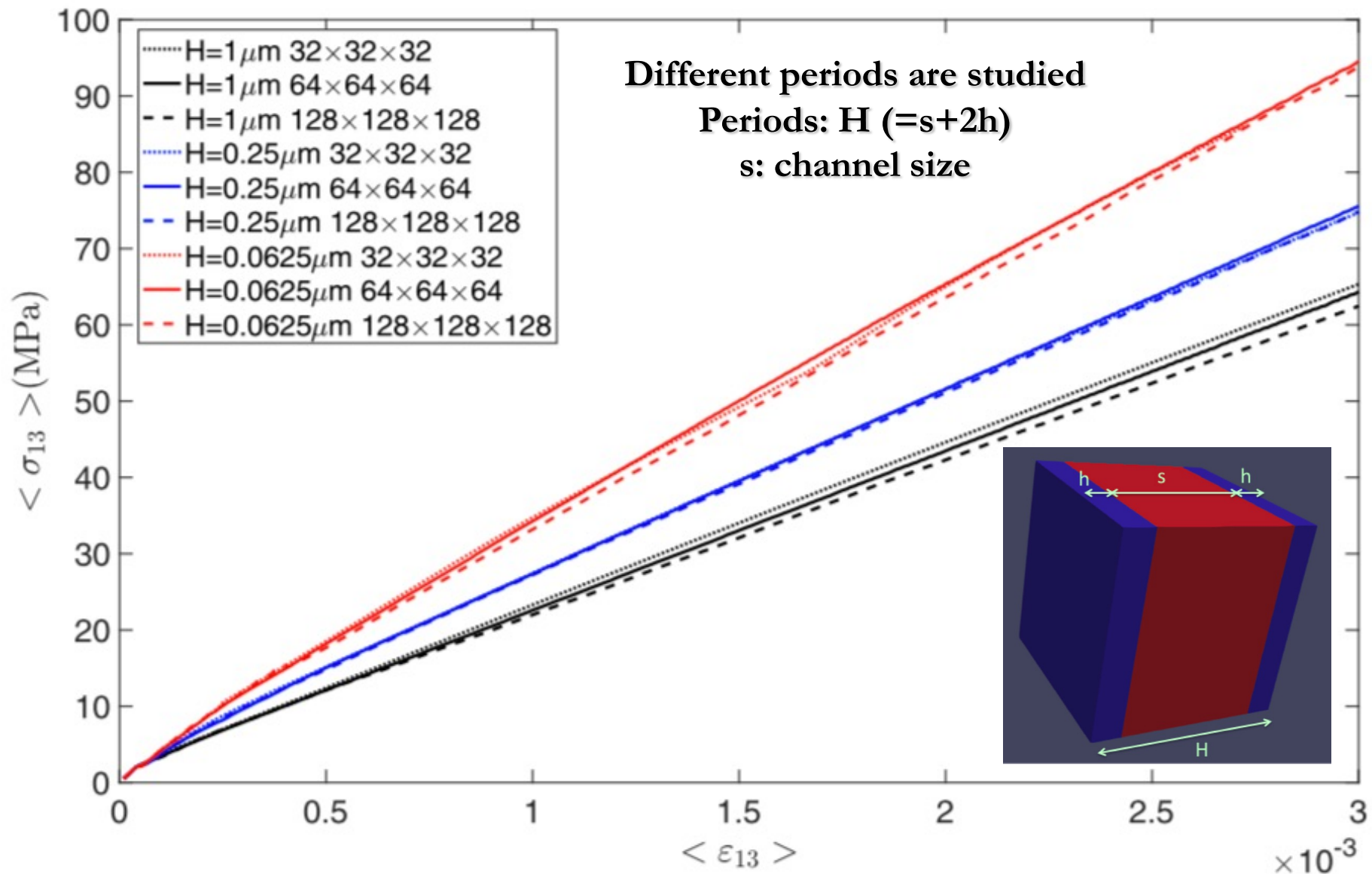
$\tau_0 = 3\text{MPa}$ $\theta_0 = 150\text{MPa}$ $\tau_s = 12\text{MPa}$ $k_0 = 20 \text{ or } 500$ $b = 2.86 \times 10^{-10} \text{m}$ $\eta = 0.33$ $\dot{\gamma}_0 = 1\text{s}^{-1}$ $m = 0.05$
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- Boundary conditions: Pure shear test

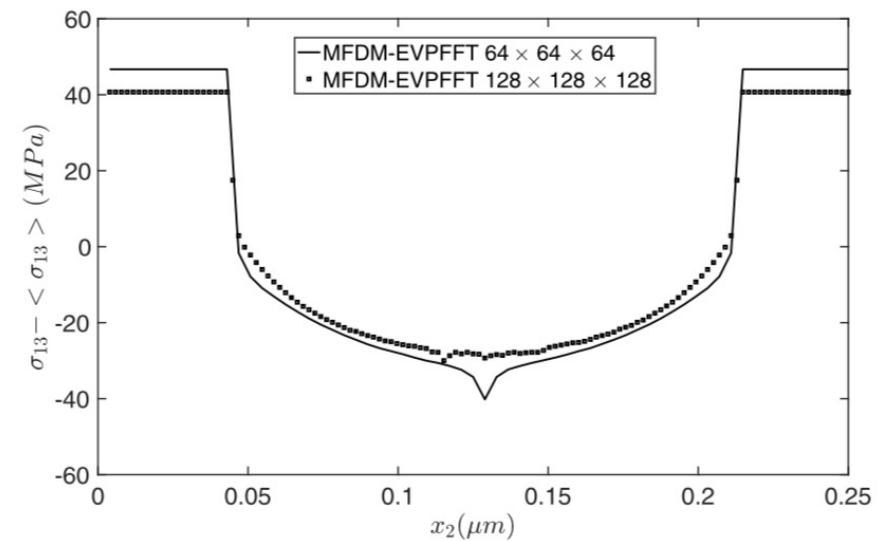
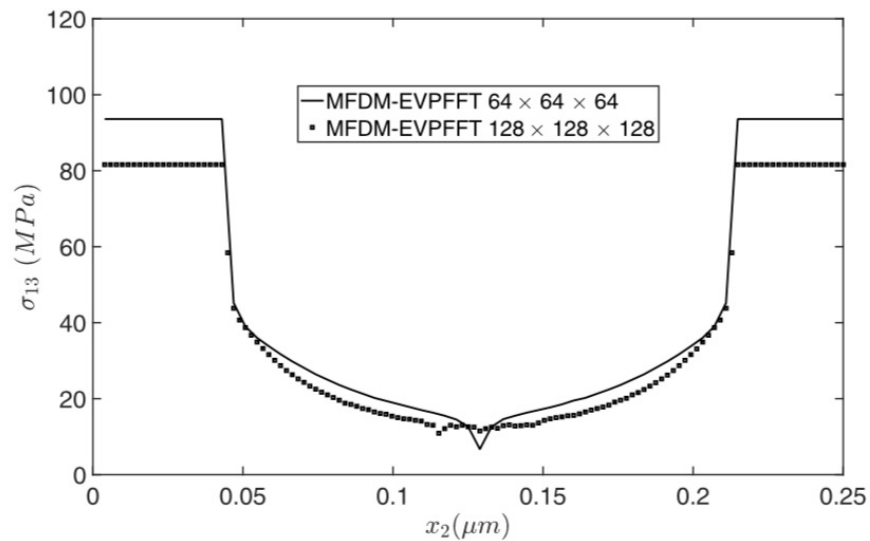
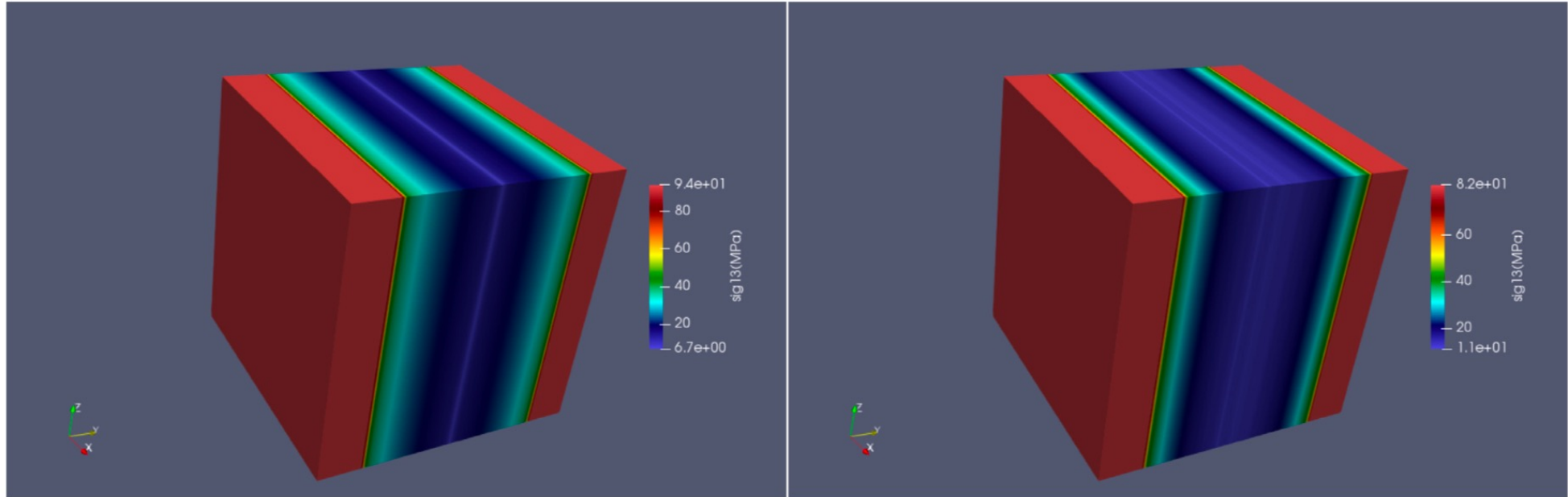
$$\dot{E}_{13} = \dot{E}_{31} = 0.001\text{s}^{-1}$$

$$\Delta t(\text{init}) = 0.01\text{s} \quad \Delta t = \min(\Delta t(\text{init}), \Delta t(\text{CFL}))$$

Mesh size convergence

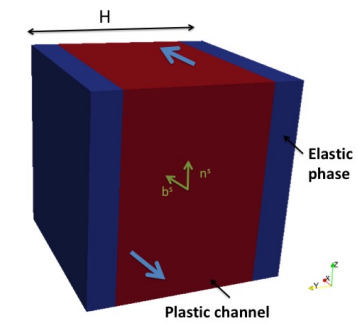


Stress profiles $\rightarrow$ spatial gradients



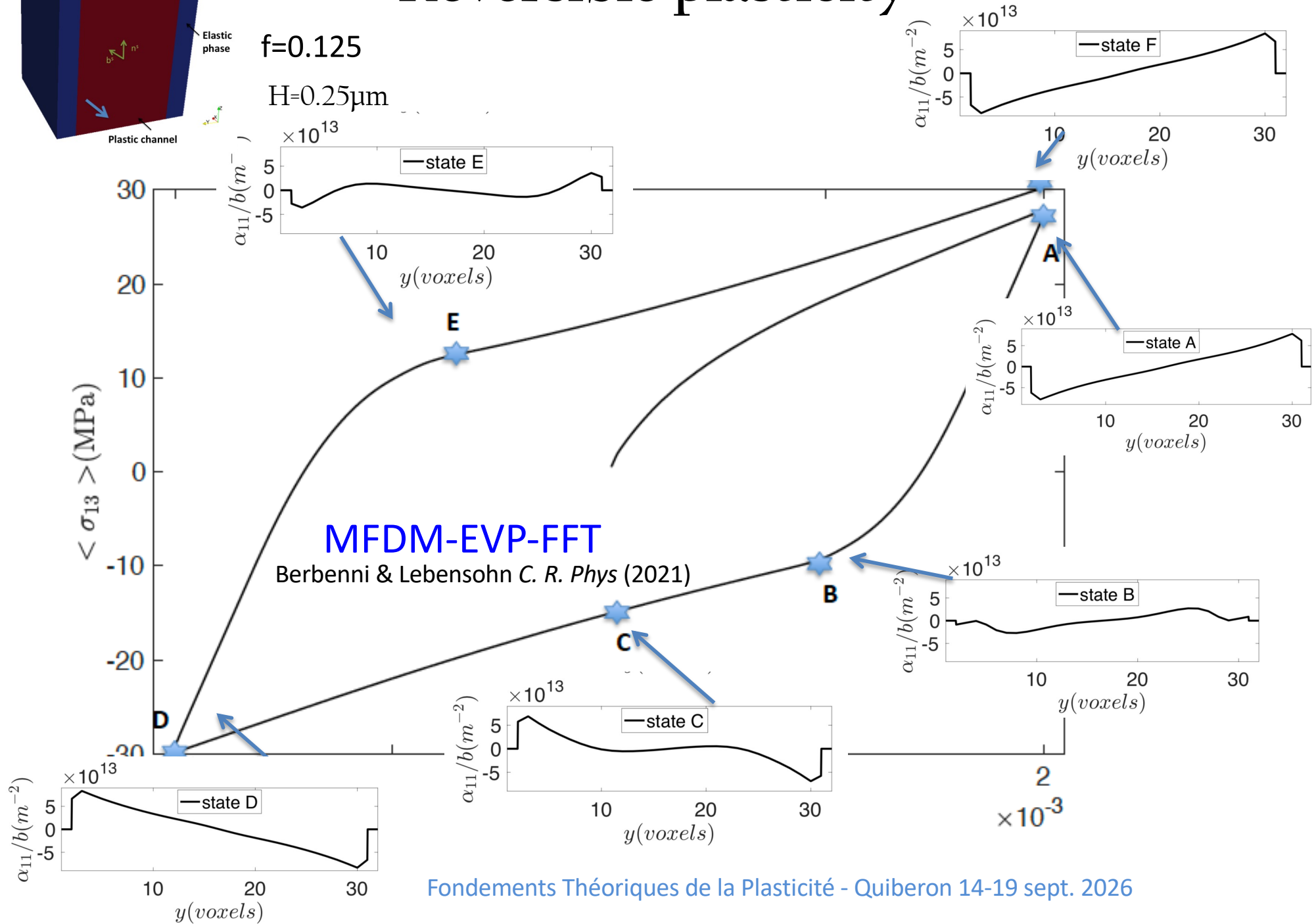
K.S. Djaka, S. Berbenni, V. Taupin, R. A. Lebensohn *Int. J. Solids Struct.* 184 (2020) 136–152

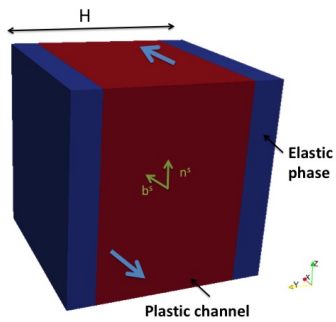
Reversible plasticity



$$f=0.125$$

$$H=0.25\mu\text{m}$$



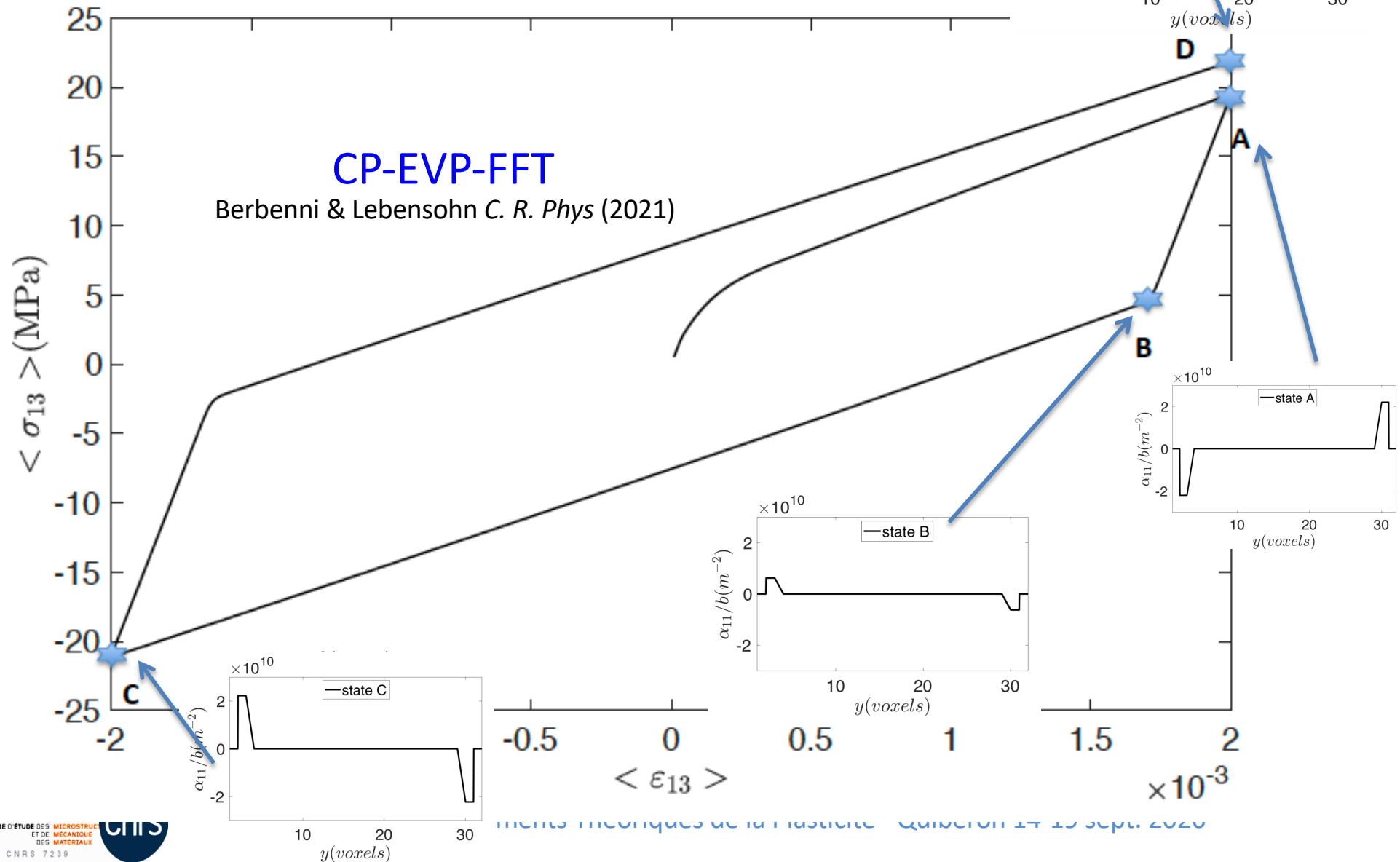


Reversible plasticity

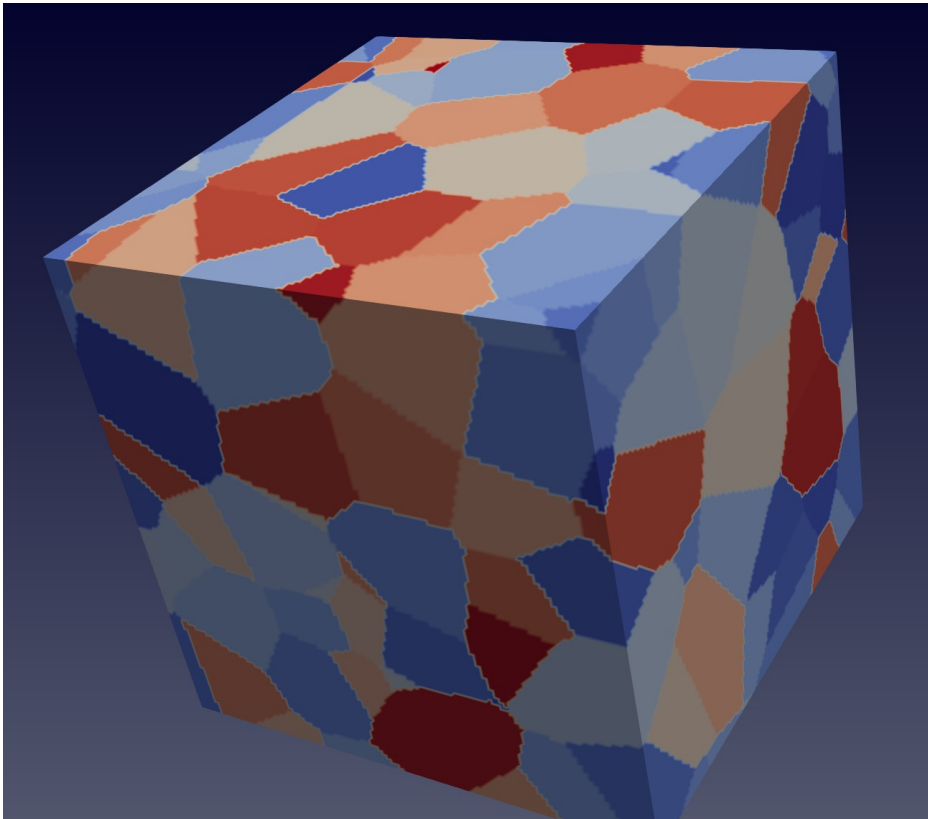
$f=0.125$

Bauschinger effect due to composite effect only (see Mughrabi, 1988) (no size effect)

$H=0.25\mu\text{m}$



- Application 2: F.C.C. polycrystals



Ex: 100 grains ($128 \times 128 \times 128$)

- **Specific parameters for GND density transport equation c: for Courant condition , exponential filter parameters)**

$$p=1 \quad \varepsilon_M=0.2 \quad c=0.25 \quad \Delta t(\text{CFL}) = \mathbf{c} \cdot \Delta \mathbf{x} / \max(\mathbf{v})$$

- **Simulation parameters**

Periodic unit cell: Al polycrystal

Random texture

27 grains, Average grain size from $0.083 \mu\text{m}$ to $125.54 \mu\text{m}$ ($H/\sqrt[3]{27}$)

100 grains, Average grain size from $0.1 \mu\text{m}$ to $100 \mu\text{m}$ ($H/\sqrt[3]{100}$)

- **Materials parameters (Al)**

Isotropic elasticity $E = 69\text{GPa}$ ($\mu=25.9\text{GPa}$)
 $\nu = 0.33$

Hardening and flow rule

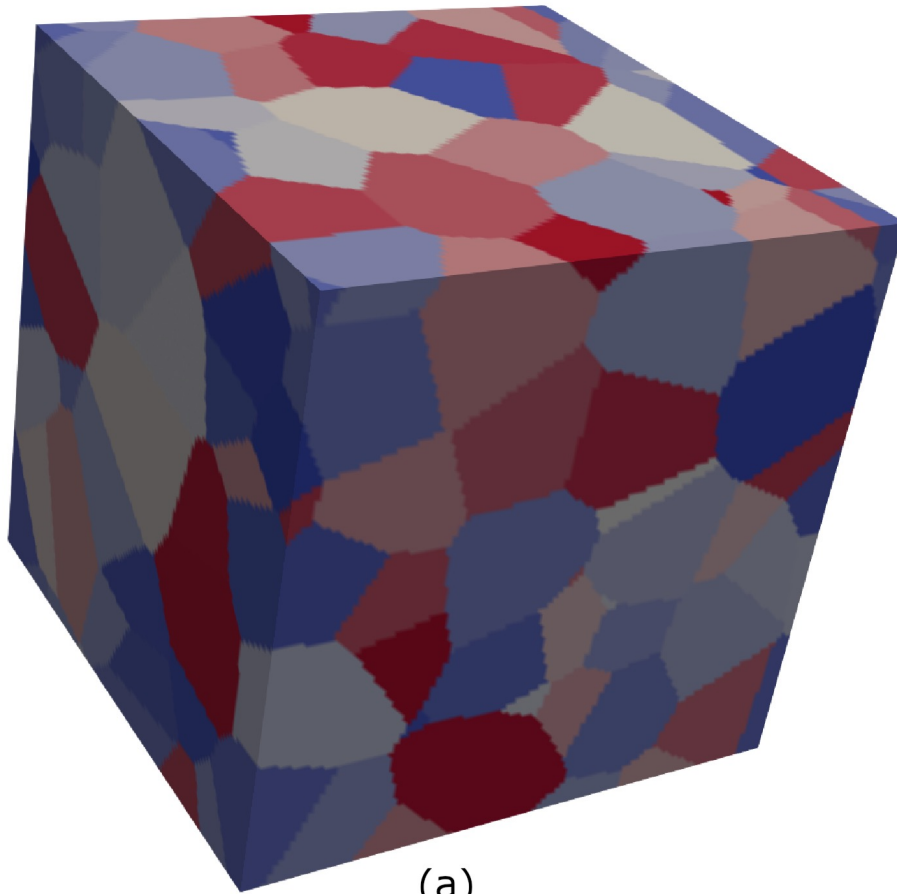
$$\begin{aligned} \tau_0 &= 3\text{MPa} & \theta_0 &= 150\text{MPa} \\ \tau_s &= 12\text{MPa} & k_0 &= 20 \\ b &= 2.86 \times 10^{-10} \text{m} & \eta &= 0.33 \\ \dot{\gamma}_0 &= 1\text{s}^{-1} & m &= 0.05 \end{aligned}$$

- **Boundary conditions: Pure tensile test**

$$\dot{E}_{33} = \dot{\varepsilon}_{33} = 0.001\text{s}^{-1}$$

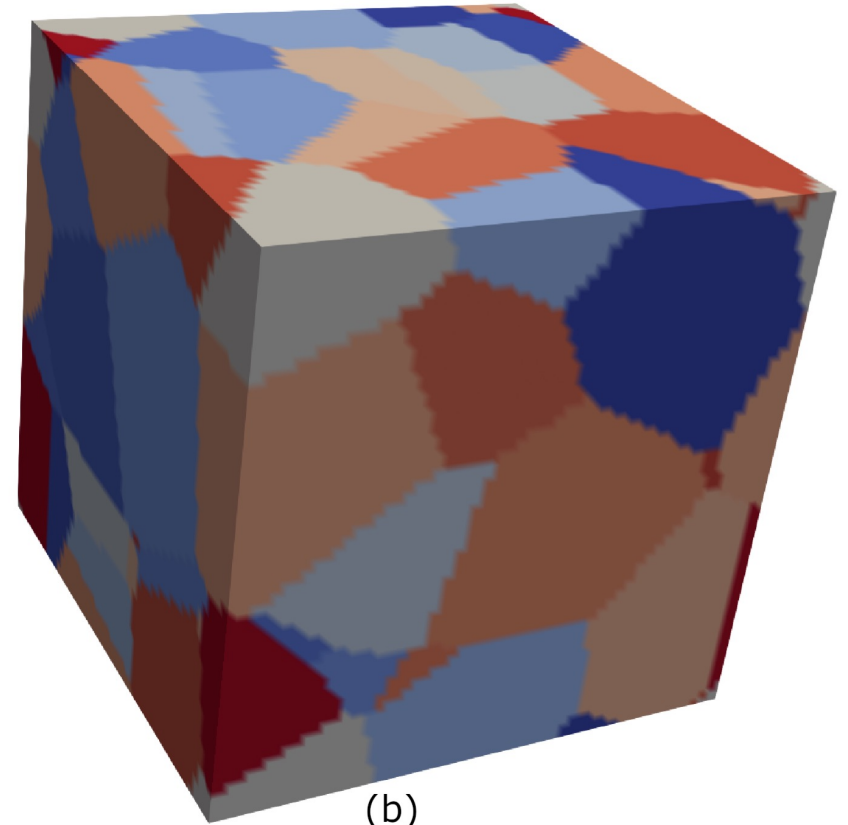
$$\Delta t(\text{init}) = 0.01\text{s} \quad \Delta t = \min(\Delta t(\text{init}), \Delta t(\text{CFL}))$$

Periodic Voronoi tessellated F.C.C. polycrystals



(a)

100 grains ($128 \times 128 \times 128$)

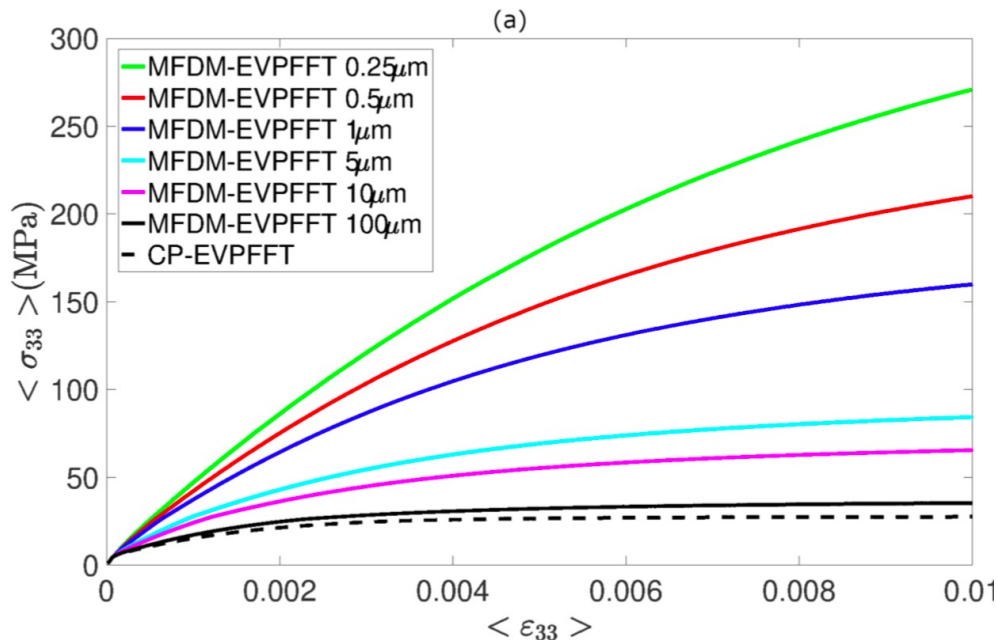


(b)

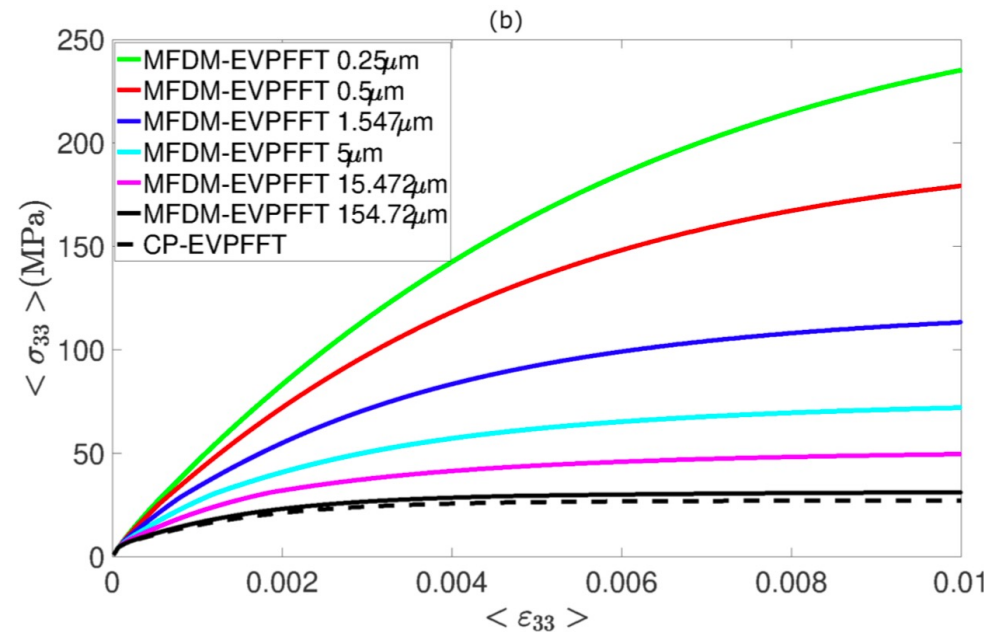
27 grains ($64 \times 64 \times 64$)

S. Berbenni, V. Taupin, R. A. Lebensohn. *Journal of the Mechanics and Physics of Solids* 135 (2020) 103808

Macroscopic tensile stress/strain: Grain size (d) effect (27grains/100 grains in the unit cell)



27 grains ($64 \times 64 \times 64$)

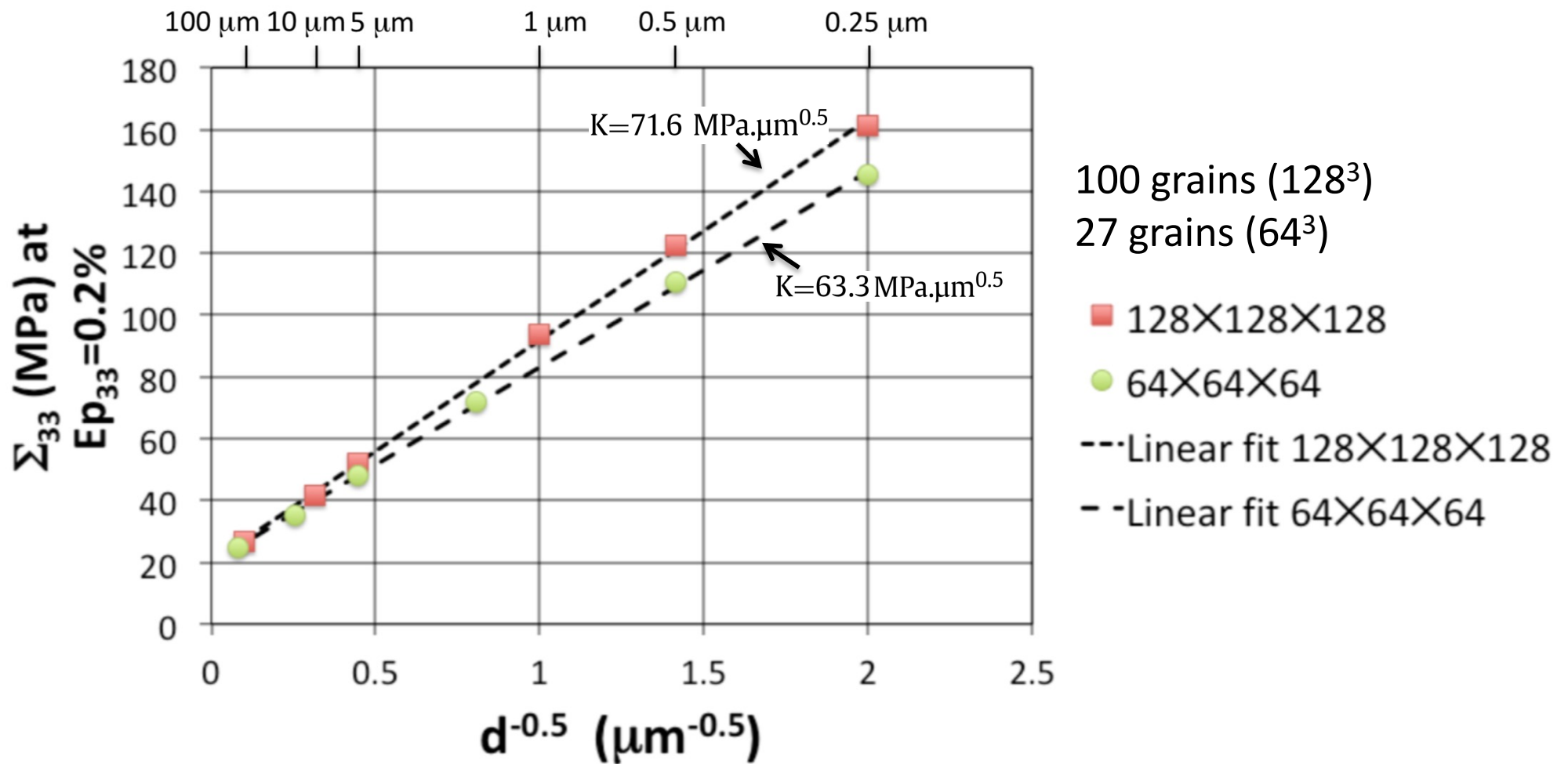


100 grains ($128 \times 128 \times 128$)

MFDM-EVP-FFT -> grain size effect

CP-EVP-FFT -> grain size independent

Hall-Petch diagrams (MFDM-EVP-FFT)



$$\langle \sigma_{33} \rangle = \langle \sigma_{33}^{\infty} \rangle + K d^{-0.5} \quad \text{with} \quad n = -0.5 \quad \langle \sigma_{33}^{\infty} \rangle = 19.8 \text{ MPa}$$

S. Berbenni, V. Taupin, R. A. Lebensohn. *Journal of the Mechanics and Physics of Solids* 135 (2020) 103808

Mesocale Field Dislocation Mechanics in EVP-FFT

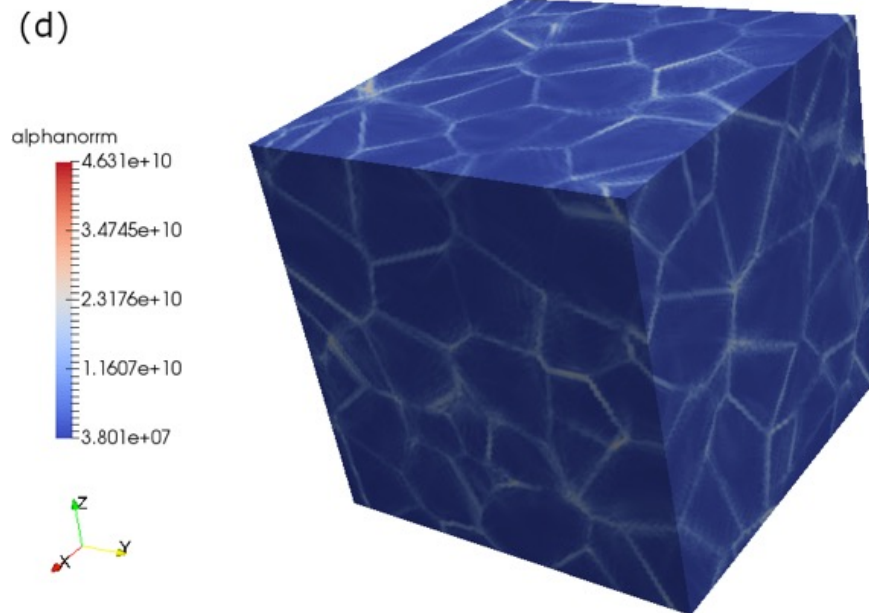
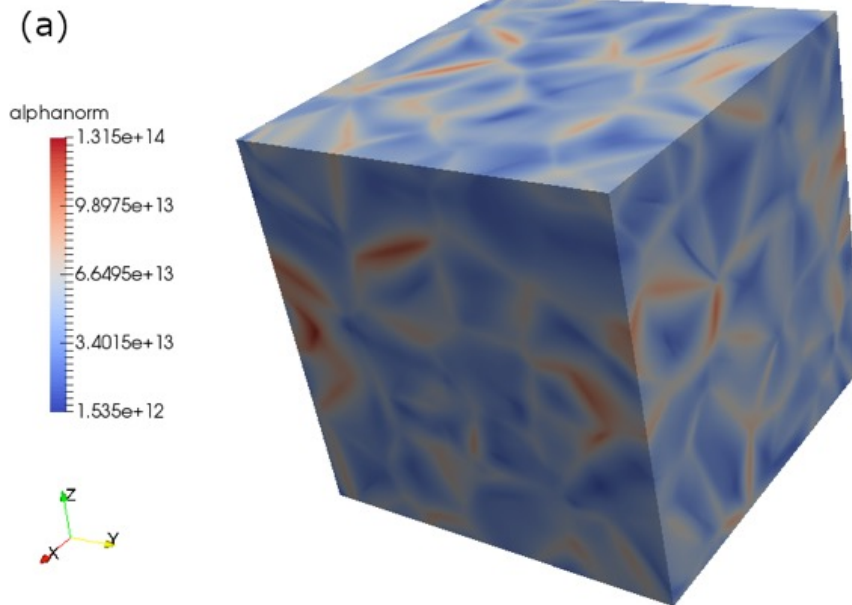
MFDM-EVP-FFT
(grain size effect)

$d=0.25\mu\text{m}$

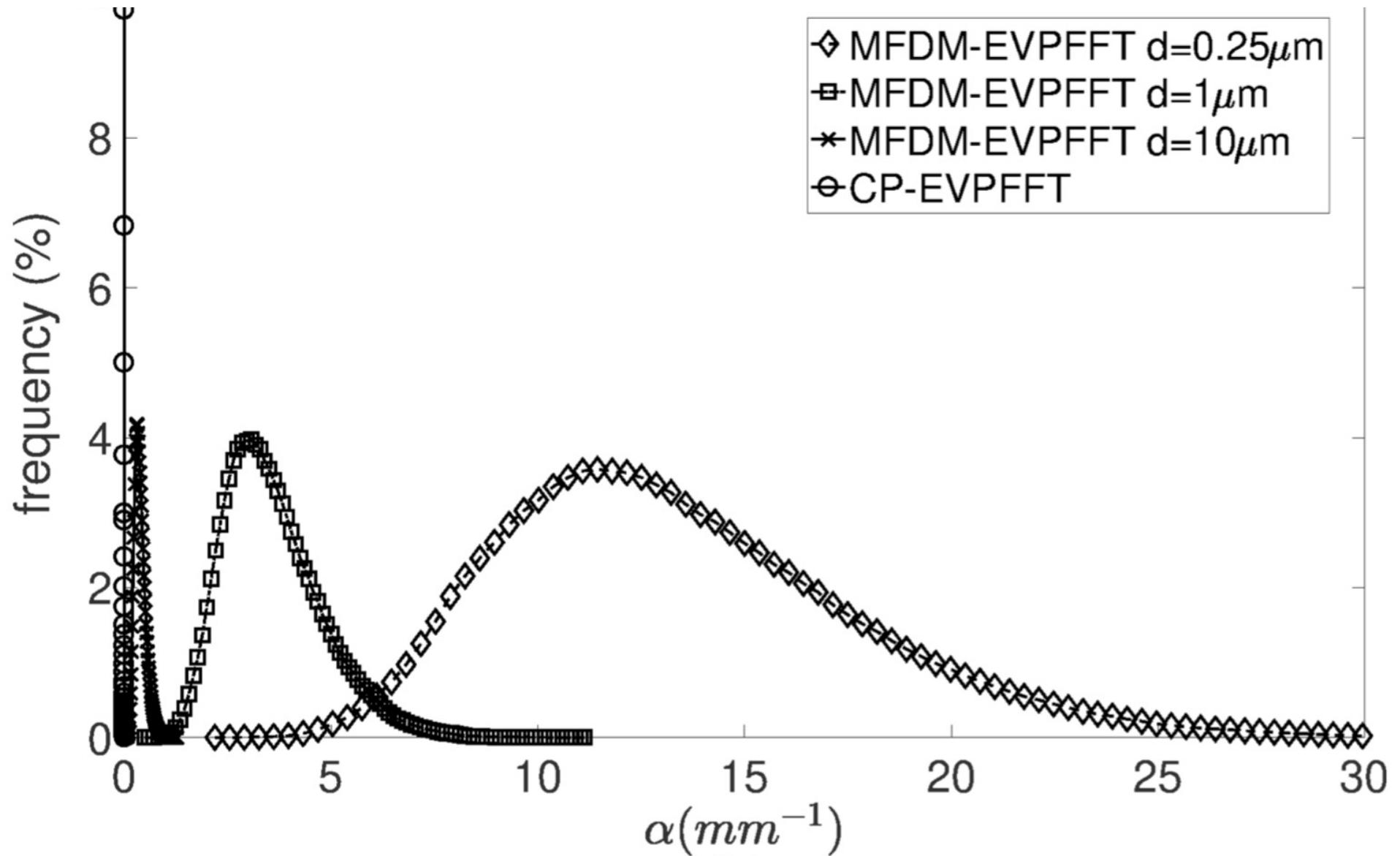
GND density distributions

$$\rho_{\text{GND}} = \|\alpha\| / b = \sqrt{\alpha : \alpha} / b$$

CP-EVP-FFT
(no grain size effect)



Field Histogram

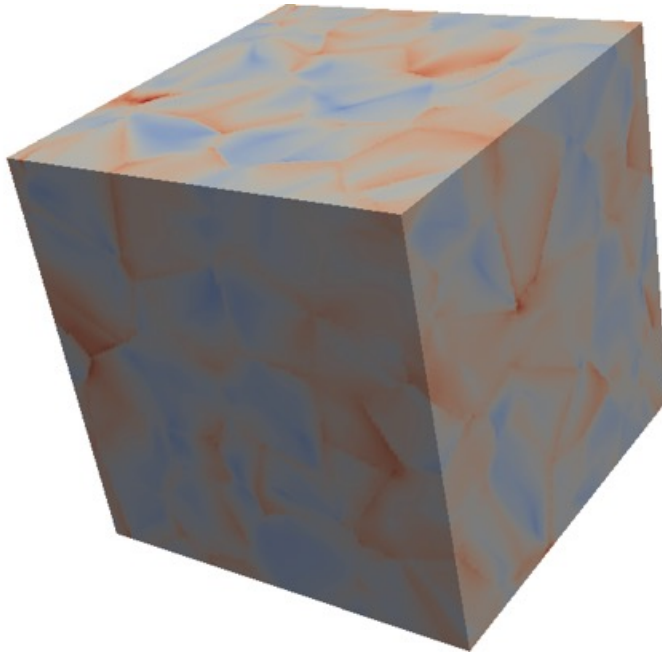
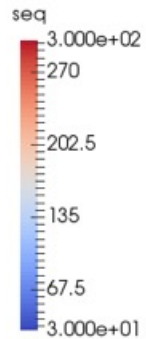


Mesocale Field Dislocation Mechanics in EVP-FFT

MFDM-EVP-FFT
(grain size effect)

$d=0.25\mu\text{m}$

(a)

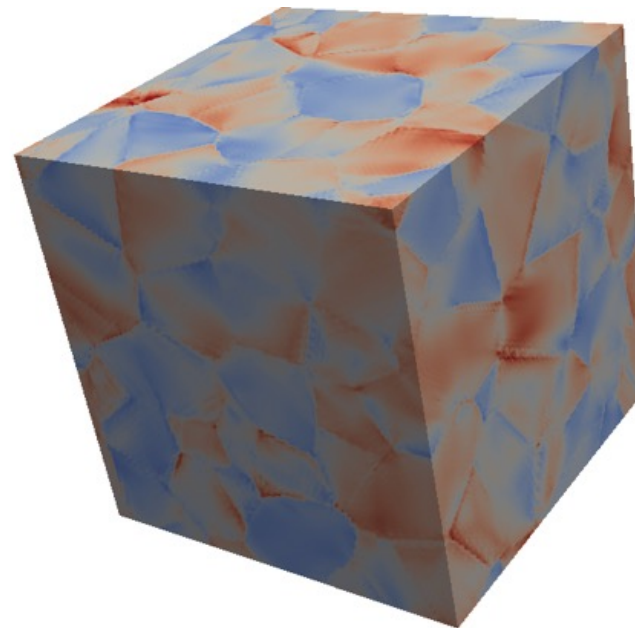
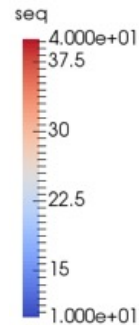


Equivalent Von Mises stress

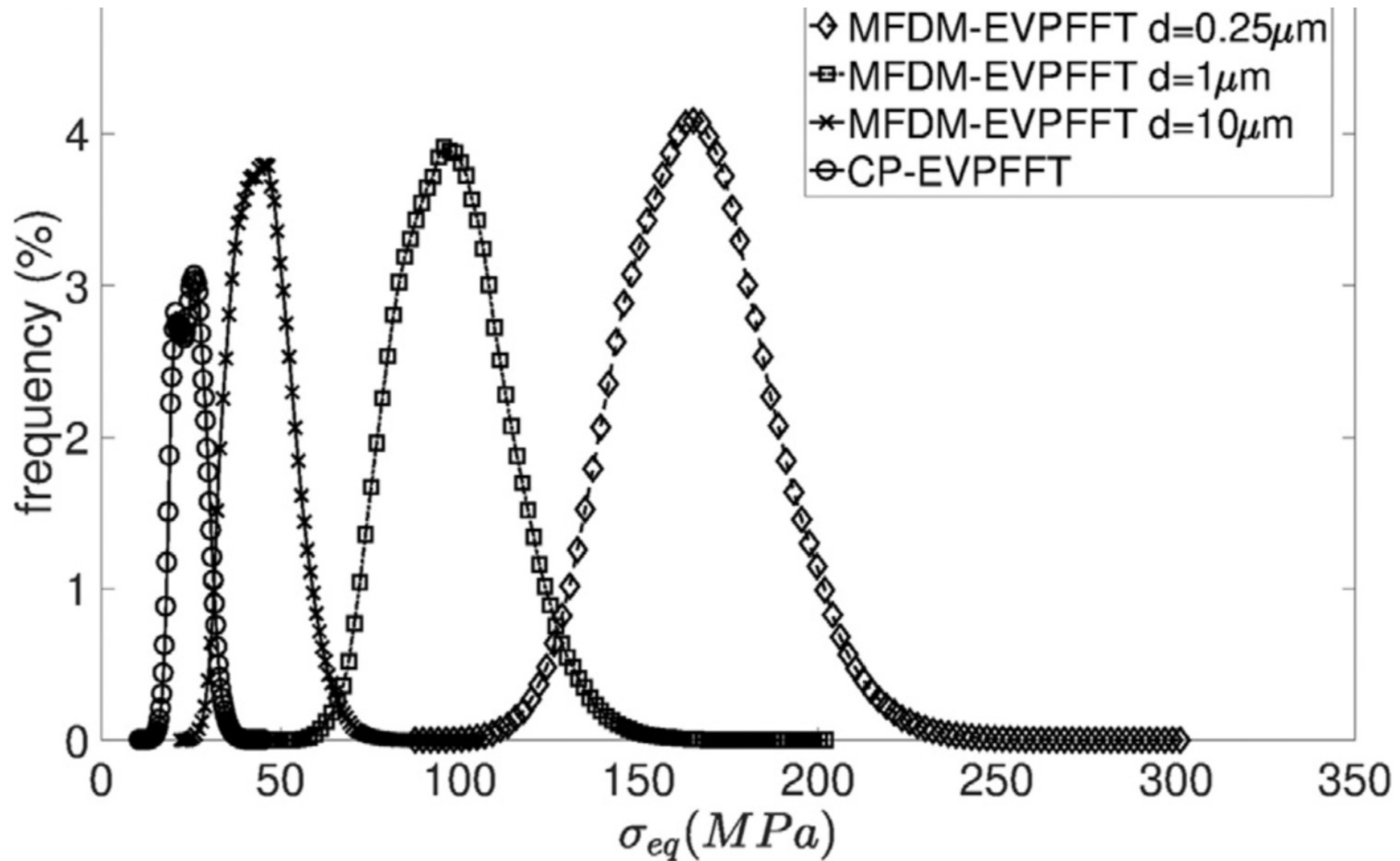
$$\sigma_{eq} = \sqrt{\frac{3}{2} \mathbf{s} : \mathbf{s}}$$

CP-EVP-FFT
(no grain size effect)

(d)



Field Histogram

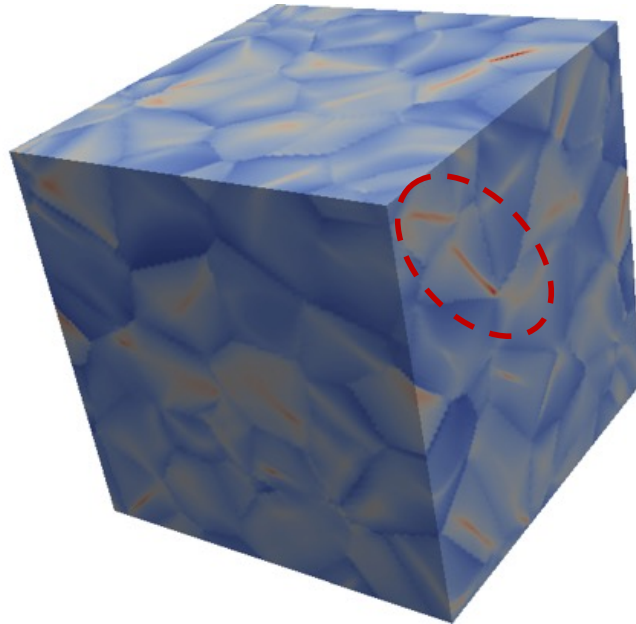
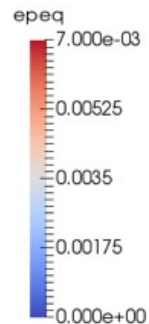


Mesocale Field Dislocation Mechanics in EVP-FFT

MFDM-EVP-FFT
(grain size effect)

$d=0.25\mu\text{m}$

(a)

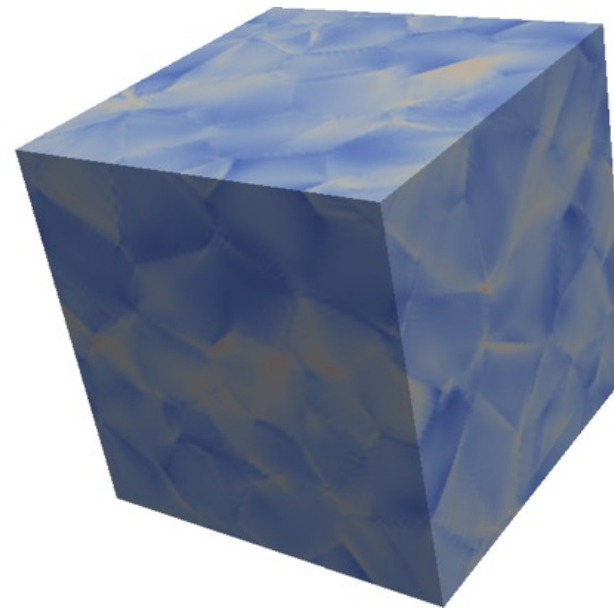
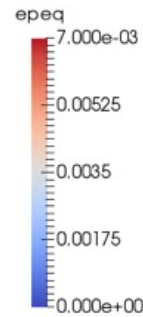


Equivalent Plastic strain

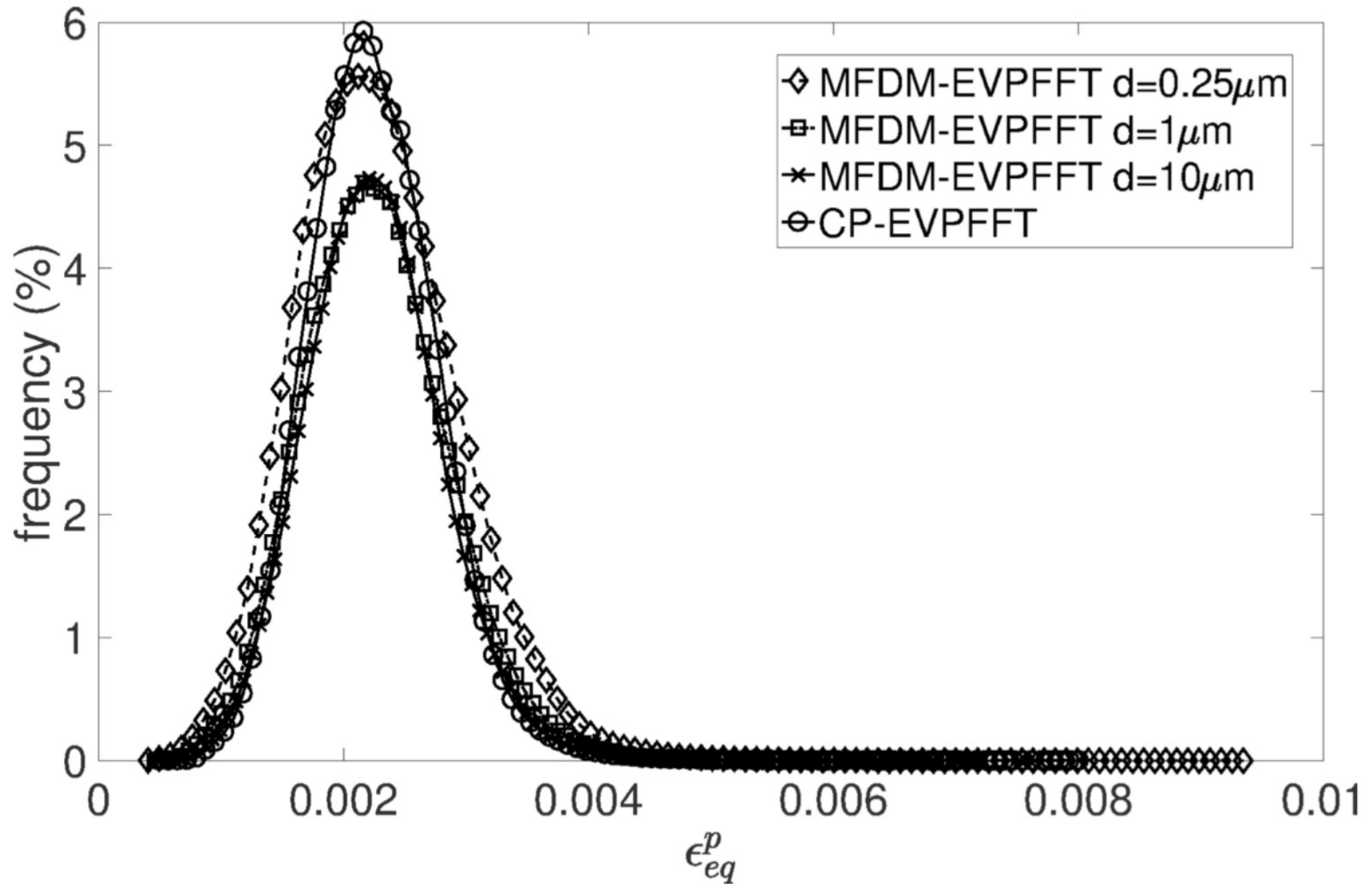
$$p = \varepsilon_p^{\text{eq}} = \int_0^t \sqrt{\frac{2}{3} \dot{\varepsilon}^p : \dot{\varepsilon}^p} dt$$

CP-EVP-FFT
(no grain size effect)

(d)



Field Histogram



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- **References**

References I

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References II

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