Enriching gradient-based continuum plasticity theories through discrete dislocation dynamics

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Journée thématique du GDR "Géometrie Différentielle et Mécanique" (GDM)

Outline

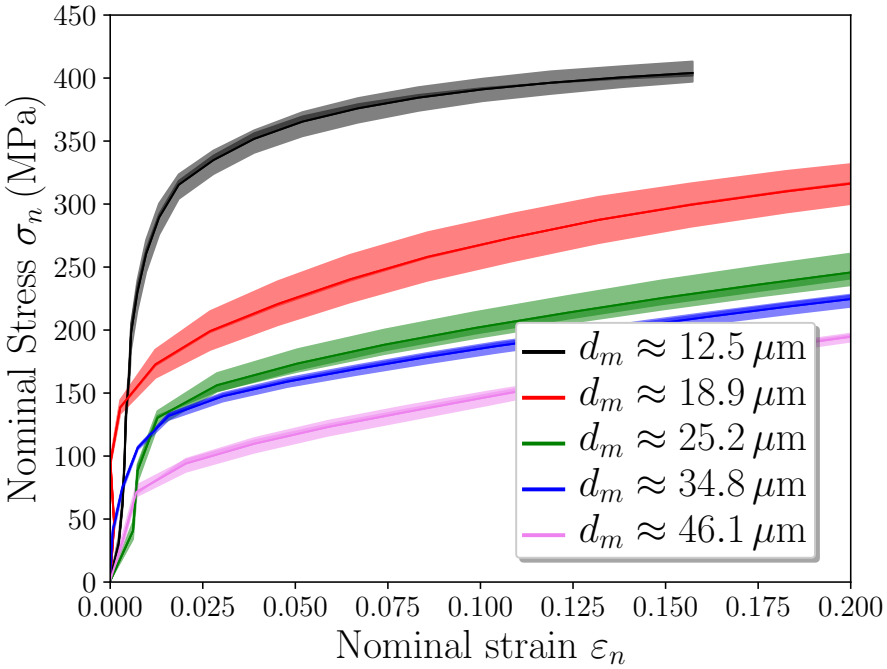
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2. Modeling of size effects with discrete dislocation dynamics
3. Modeling of size effects with strain gradient crystal plasticity
4. Concluding remarks

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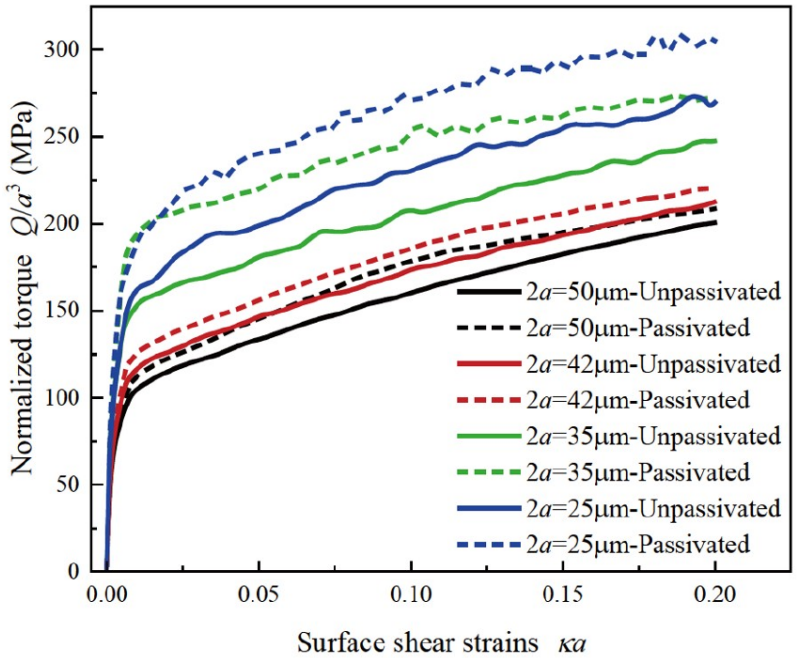
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Size effects in materials

- Experimental evidence of size effects: "smaller is stronger"



Micro-tension tests
[Amouzou-Adoun, 2024]

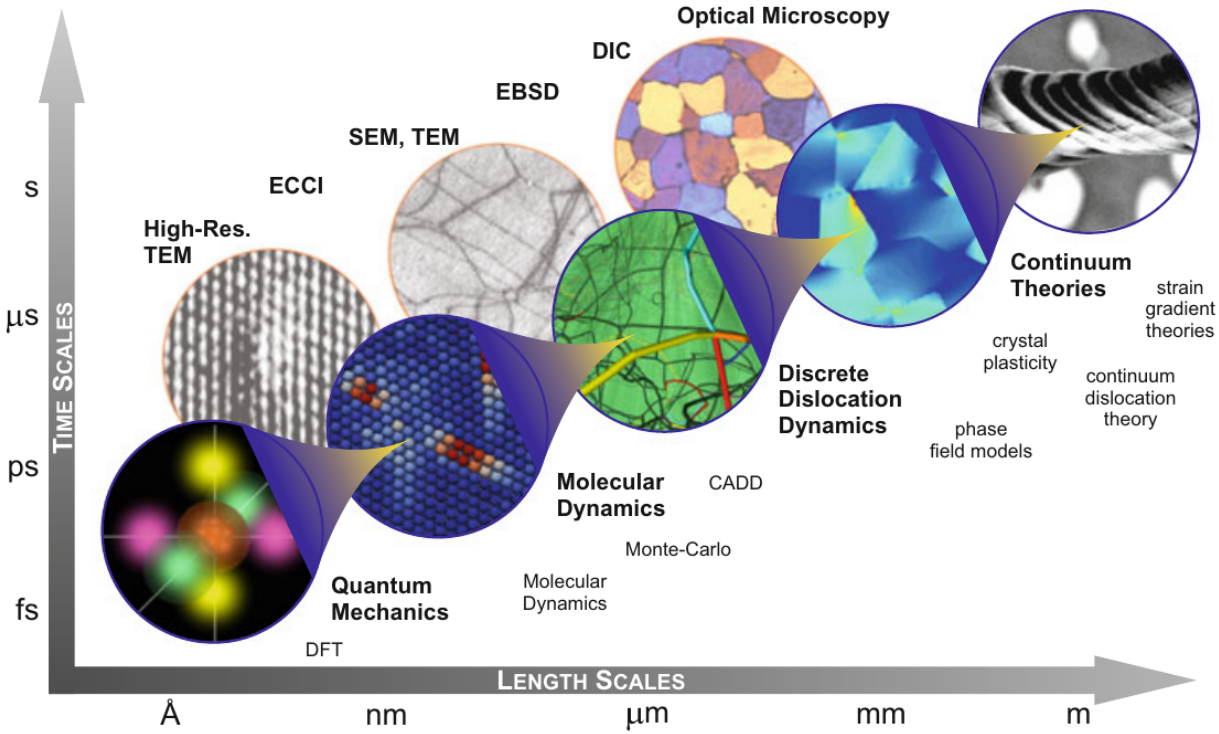


Micro-torsion tests
[Xie et al., 2023]

- Size-dependent strengthening: $\sigma_y \sim h^{-r}$, $r \in [0.2, 1]$ [Dunstan and Bushby, 2014]
- Size-dependent hardening

Modeling of size effects

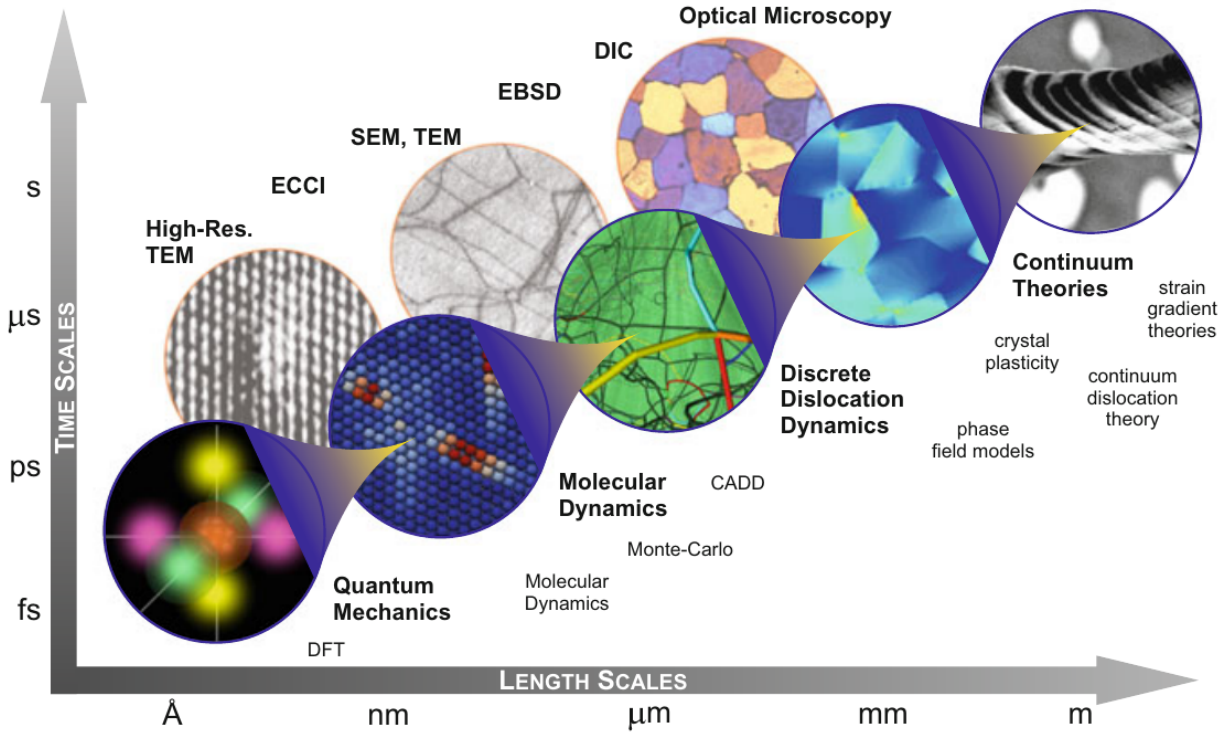
- Modeling approaches across scales: from atomistic to macroscopic scale



Different analysis scales [Kochmann and Amelang, 2016]

Modeling of size effects

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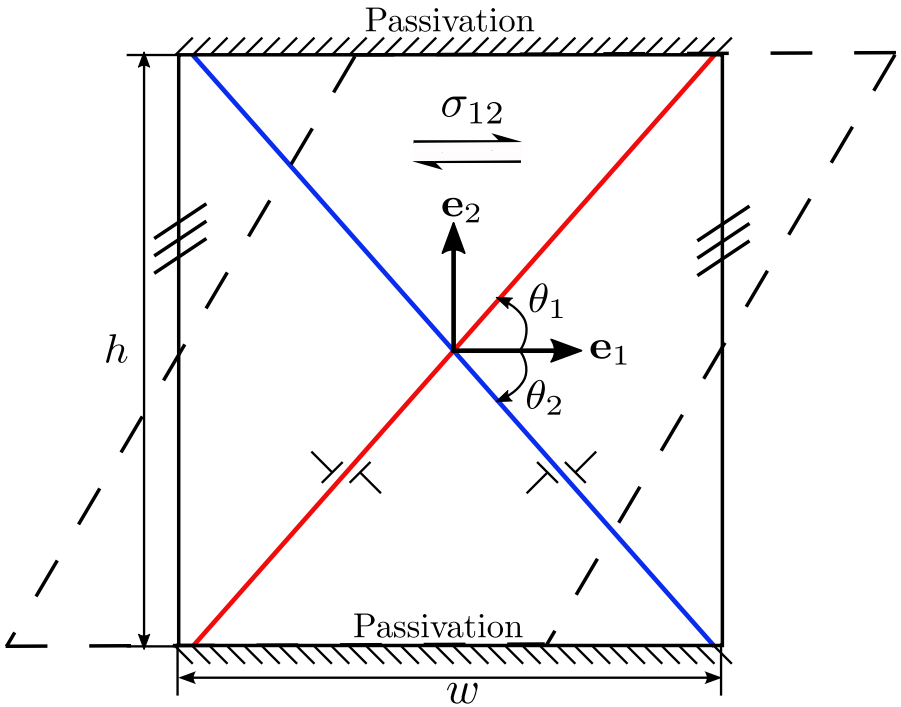


Different analysis scales [Kochmann and Amelang, 2016]

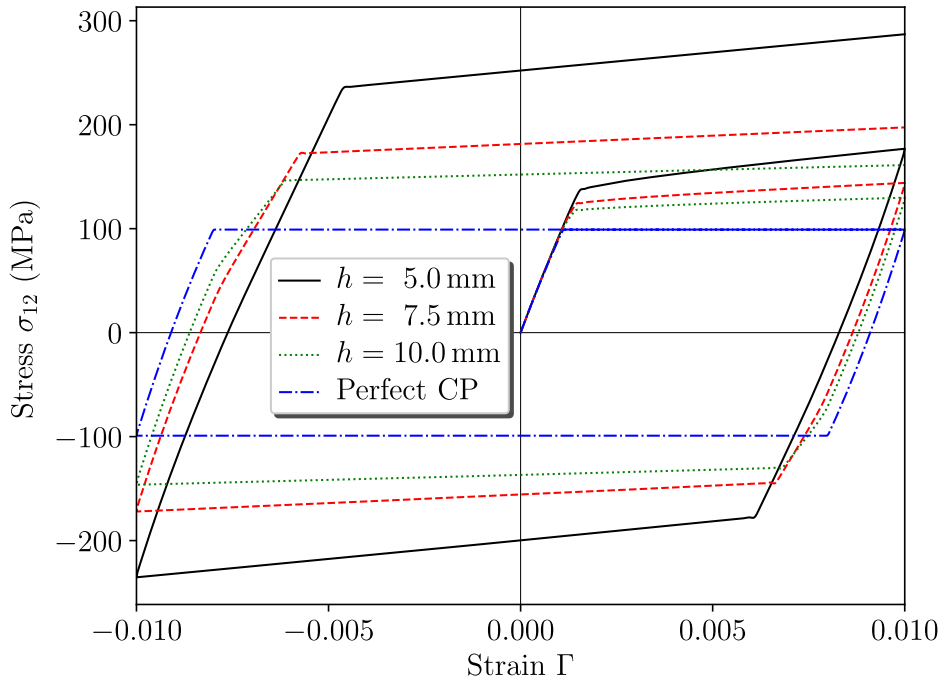
⇒ Gradient-enriched plasticity as a powerful approach to model size effects !

Gradient-enriched plasticity theories: strengths

⇒ Able to naturally capture size-dependent strengthening and hardening



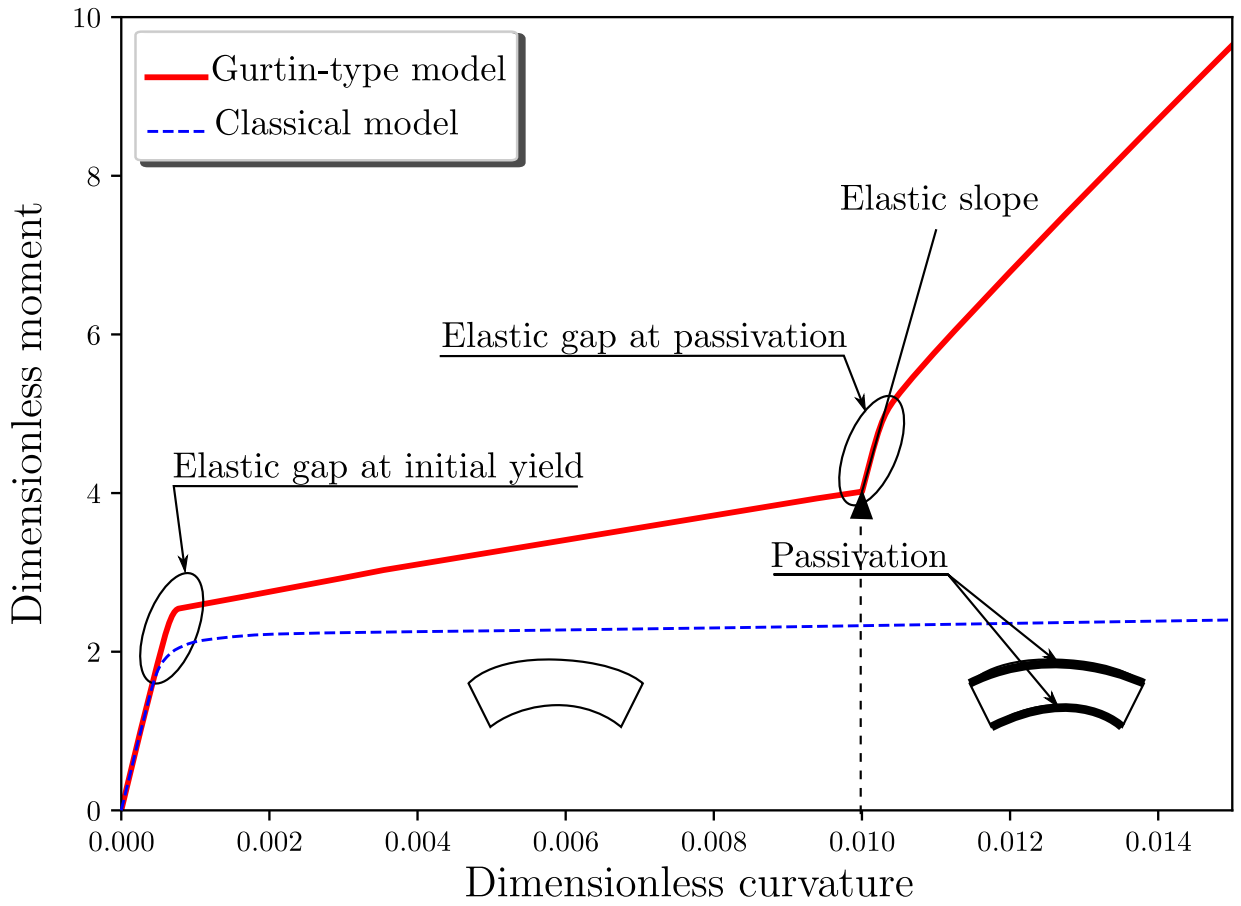
Constrained shear test with two symmetric slip systems



Macroscopic response [Jebahi and Forest, 2023]

Gradient-enriched plasticity theories: limitations

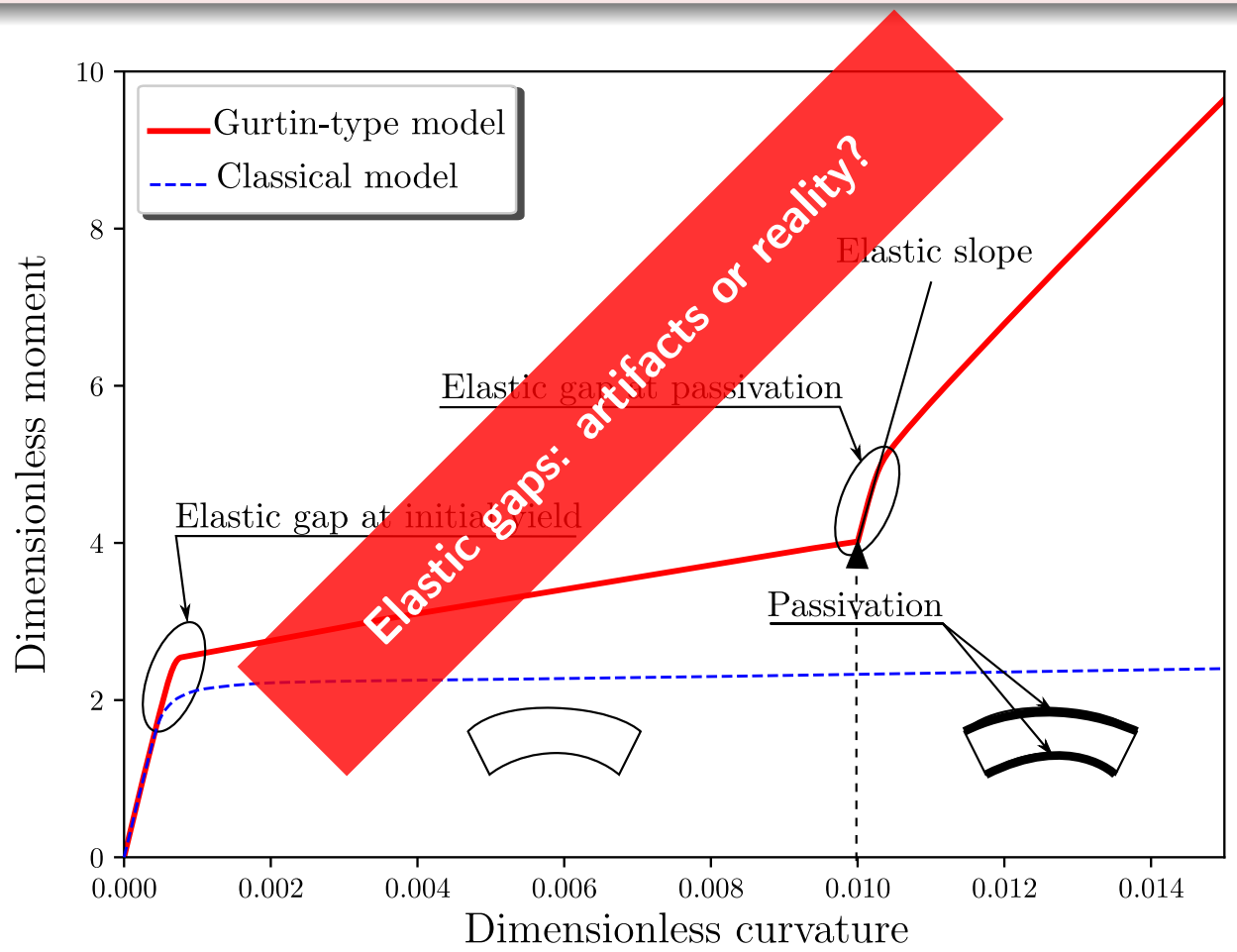
⇒ Limitations in predicting **quantitatively** size effects
⇒ Prediction of uncommon size effects under certain loading conditions: **elastic gaps** !



Constrained bending response at small scales [Amouzou-Adoun et al., 2023]

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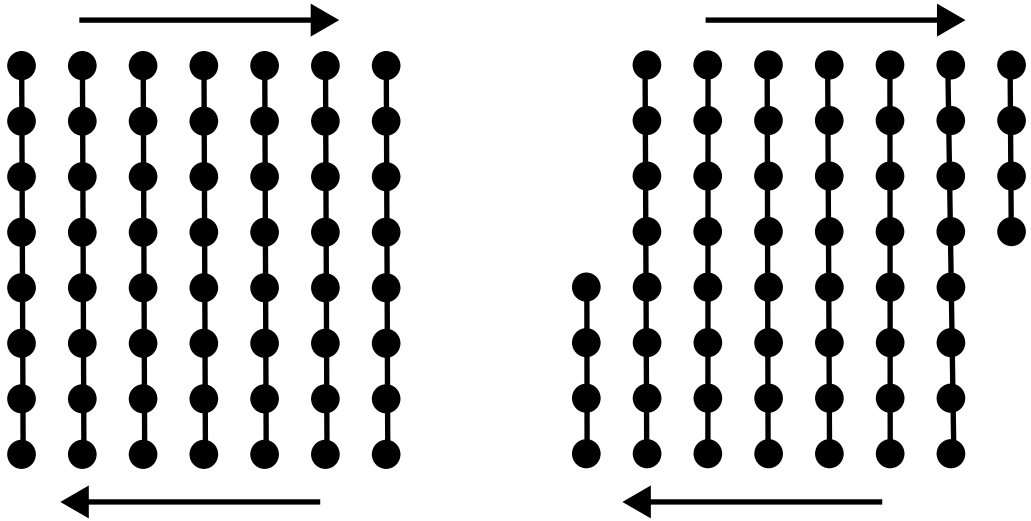


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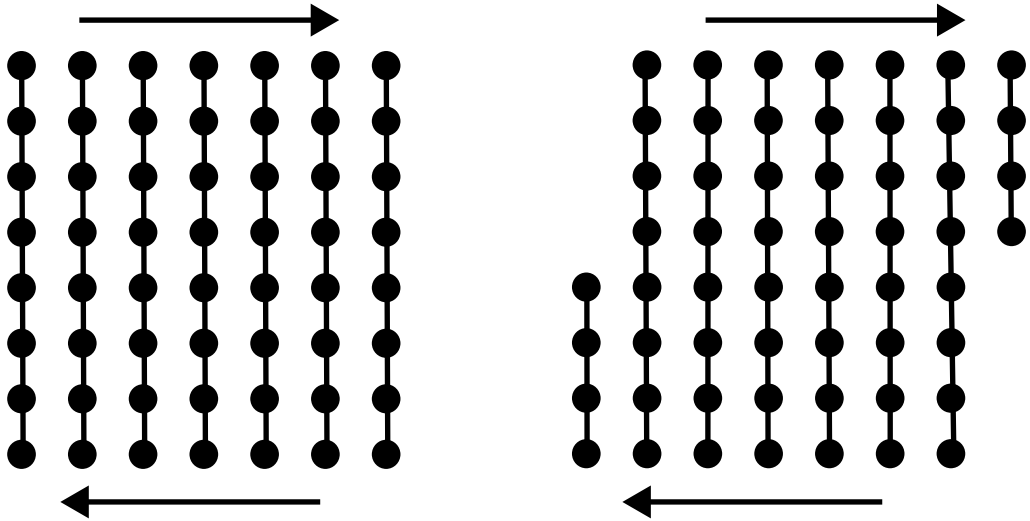
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Concept of dislocations to solve the mystery of deformation

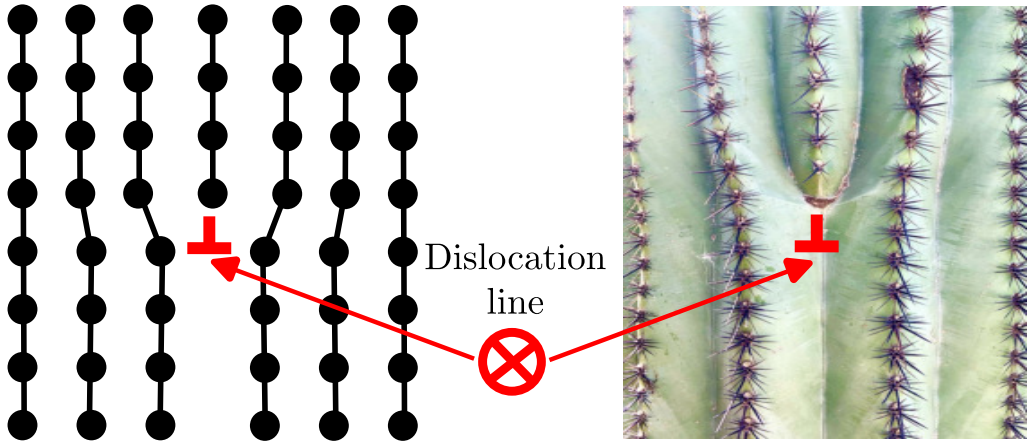


Critical shear stress to permanently deform the lattice: $\tau_e^{th} \approx \mu/2\pi \gg \tau_e^{exp}$

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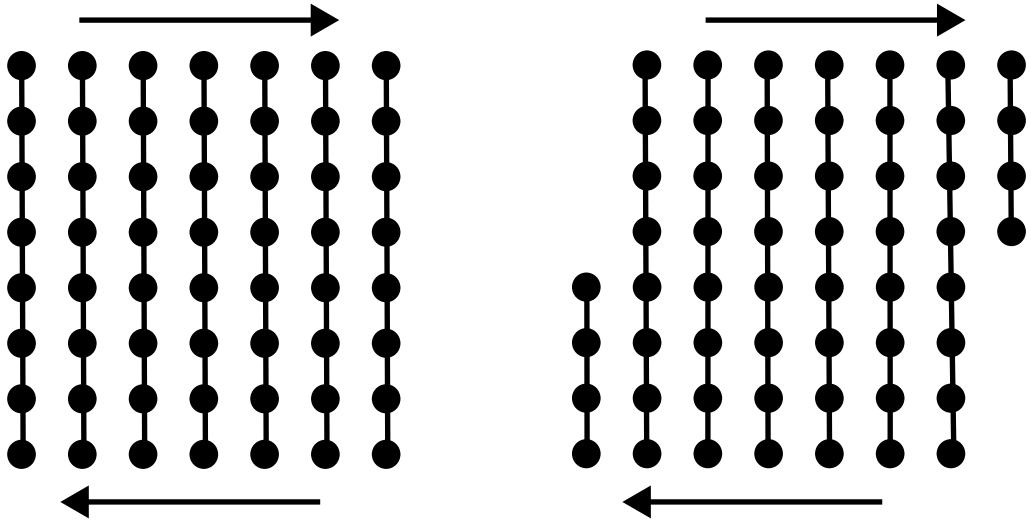


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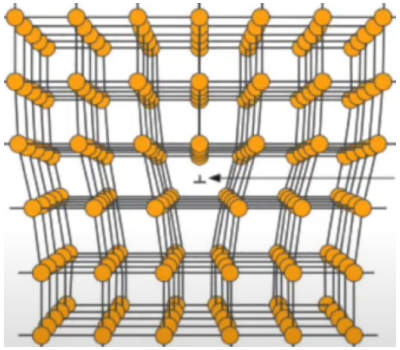


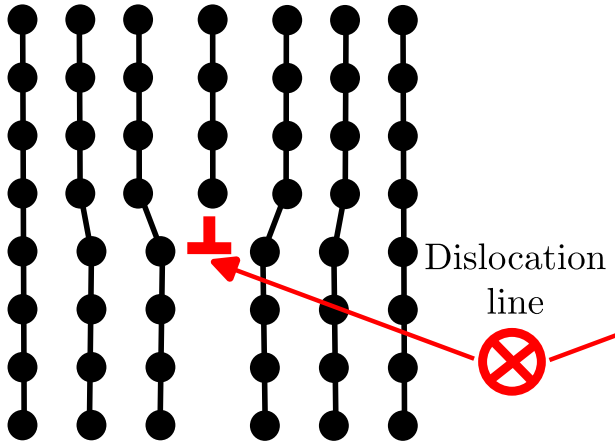
Linear crystallographic defects : dislocations [Volterra, 1907]

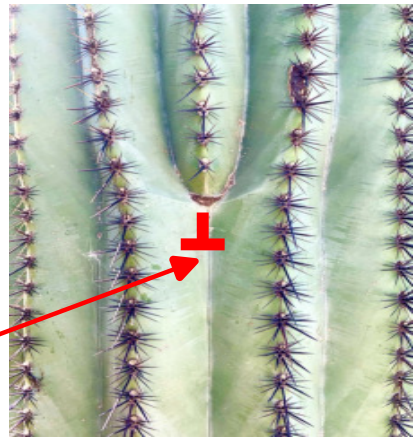
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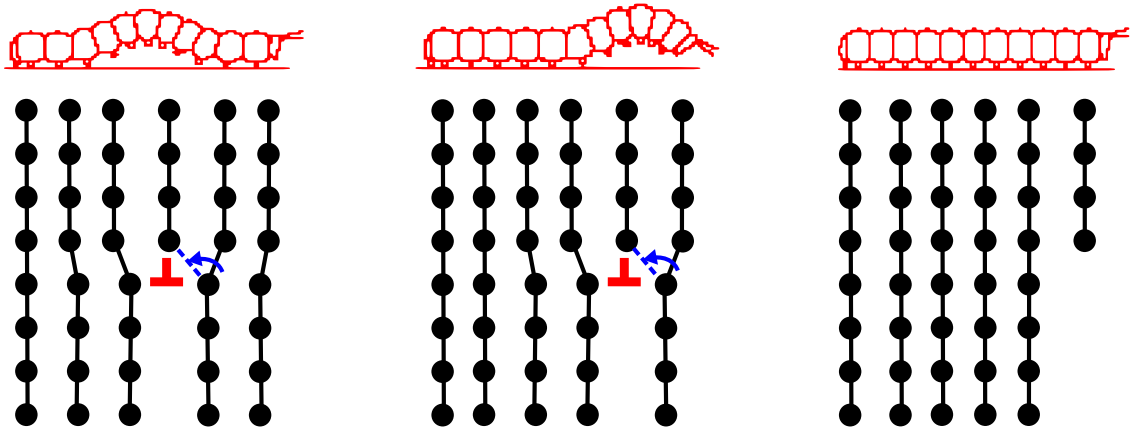






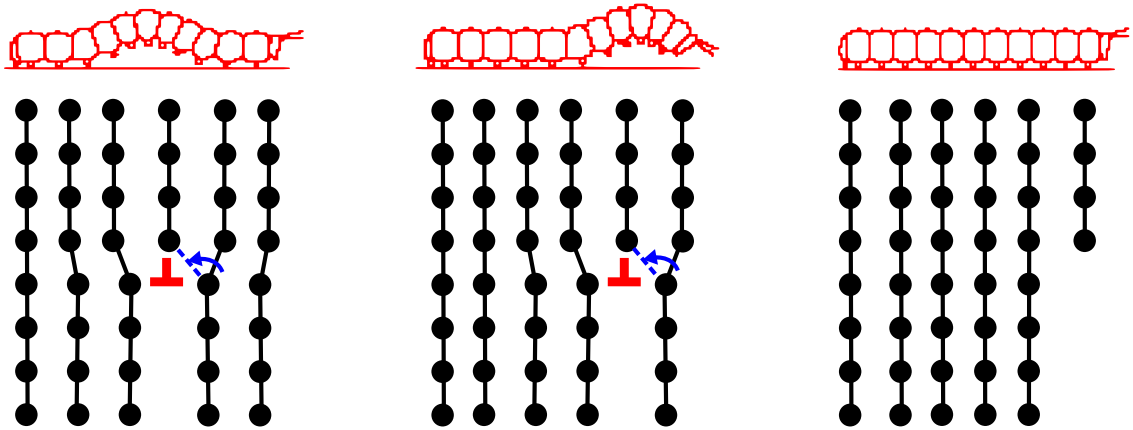
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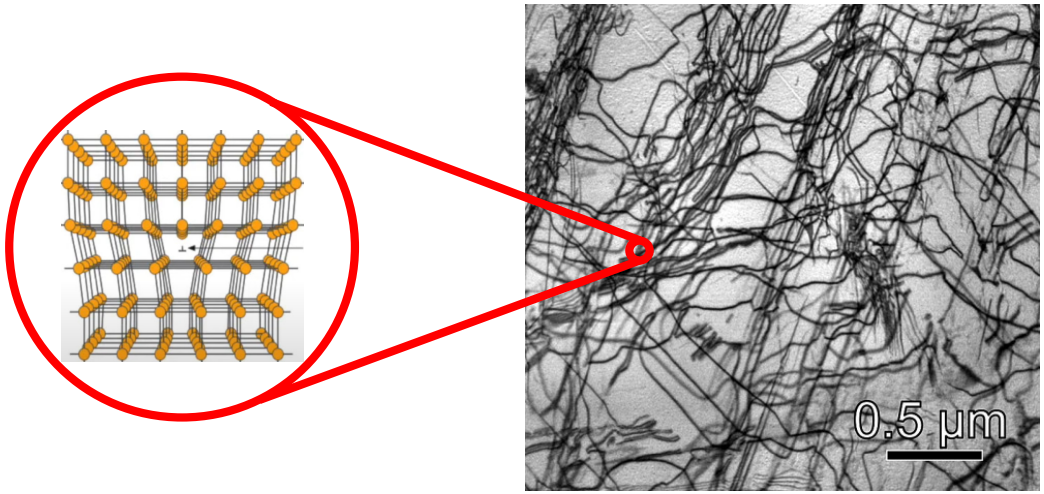


Small scale mechanisms of permanent deformation (plasticity): movement of dislocations ([Orowan, 1934], [Taylor, 1934] and [Polanyi, 1934])

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Transmission electron microscopy observation of dislocation structure in a metallic alloy [Xu et al., 2018]

Discrete dislocation dynamics: general principle

Description of plasticity through the movement of dislocations:

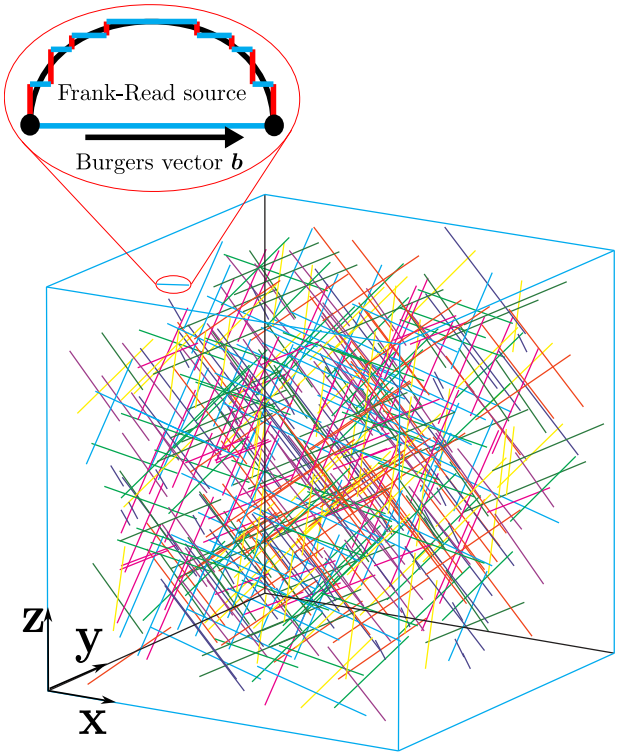
- Edge-screw discretization
- Dislocation velocity

$$v = \frac{\tau_{\text{eff}}}{B} b$$

$$\begin{cases} \tau_{\text{eff}} = \left(|\tau^*| - \tau_{\text{Peierls}} \right)^+ \text{sign}(\tau^*) \\ \tau^* = \left[\left(\frac{1}{b} [\hat{\boldsymbol{\sigma}} + \tilde{\boldsymbol{\sigma}}] \mathbf{b} \right) \times \mathbf{l} \right] \cdot \mathbf{g} + \tau_{\text{lt}} \end{cases}$$

- Local interaction rules
- Plastic strain computation

$$\dot{\boldsymbol{\varepsilon}}^p = \sum_{\alpha=1}^{q} \frac{\dot{\gamma}^\alpha}{2} \left(\mathbf{b}^\alpha \otimes \mathbf{n}^\alpha + \mathbf{n}^\alpha \otimes \mathbf{b}^\alpha \right)$$



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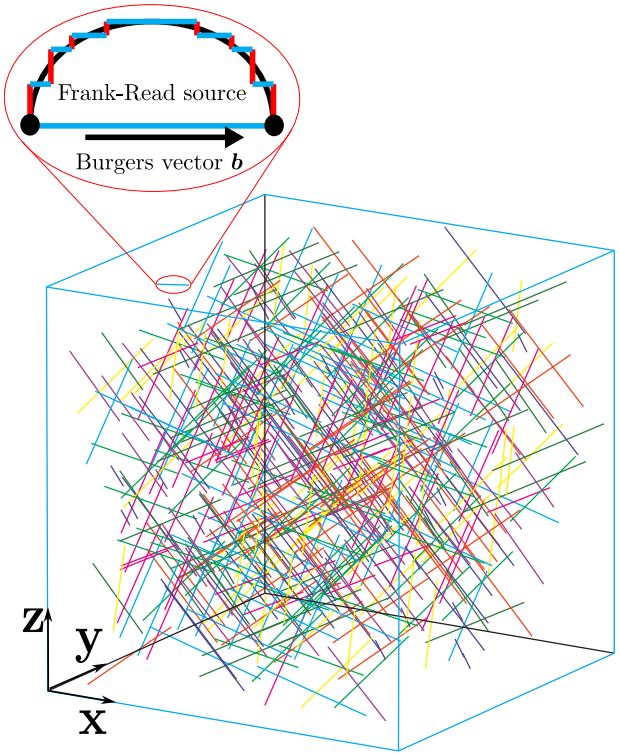
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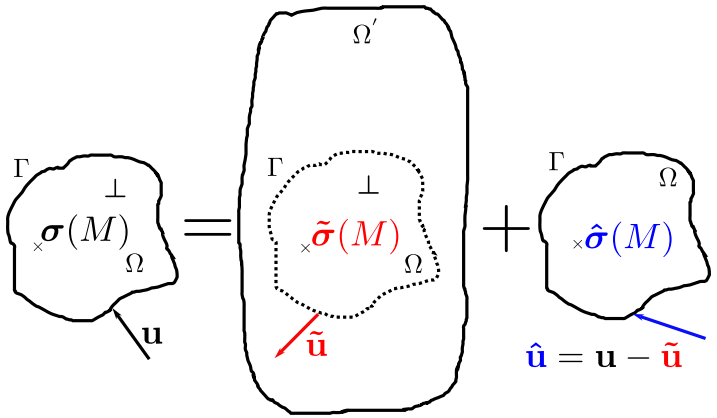
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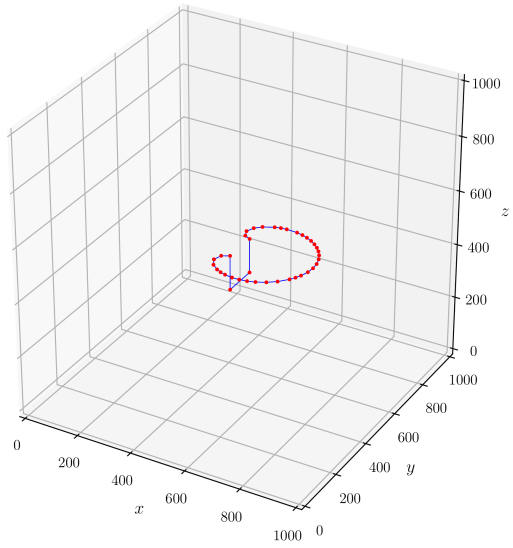
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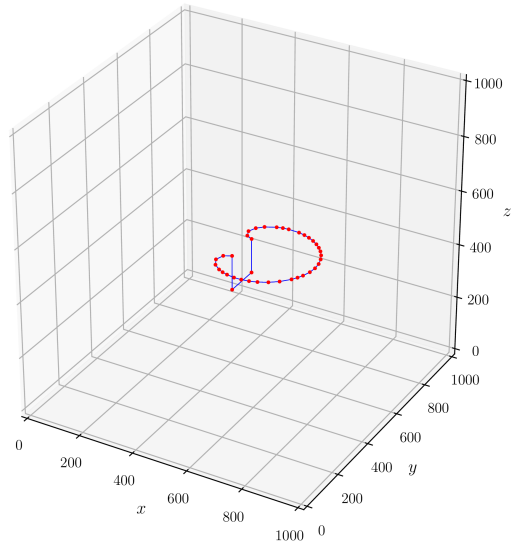
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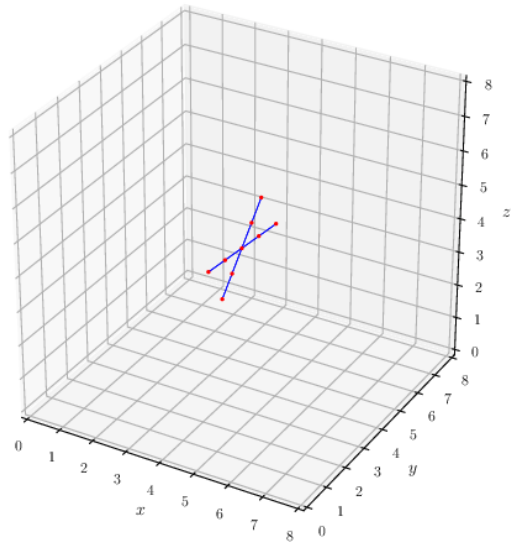
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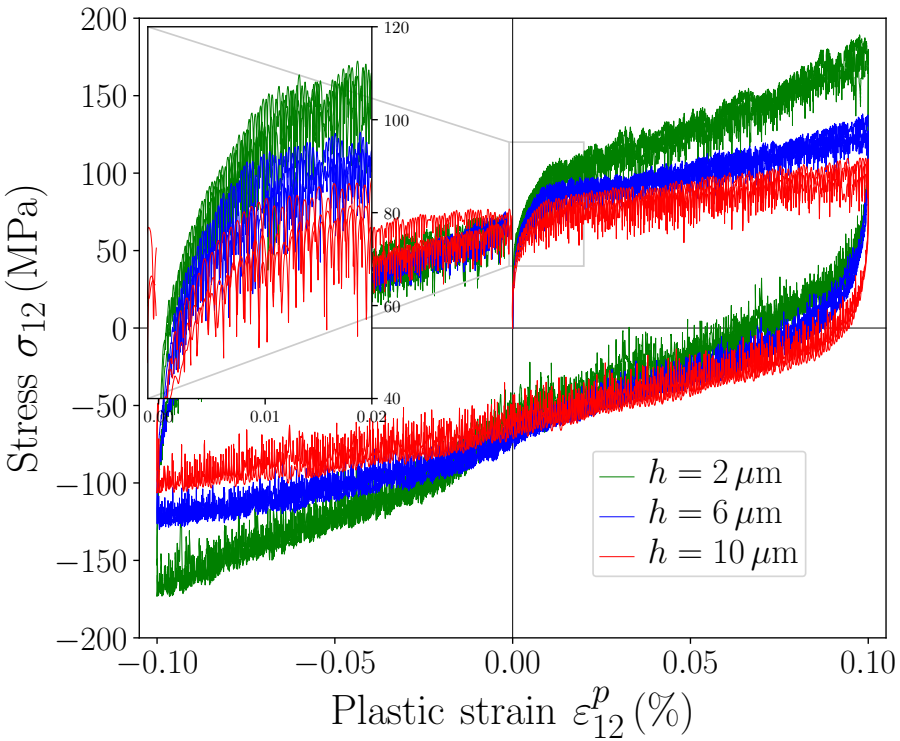
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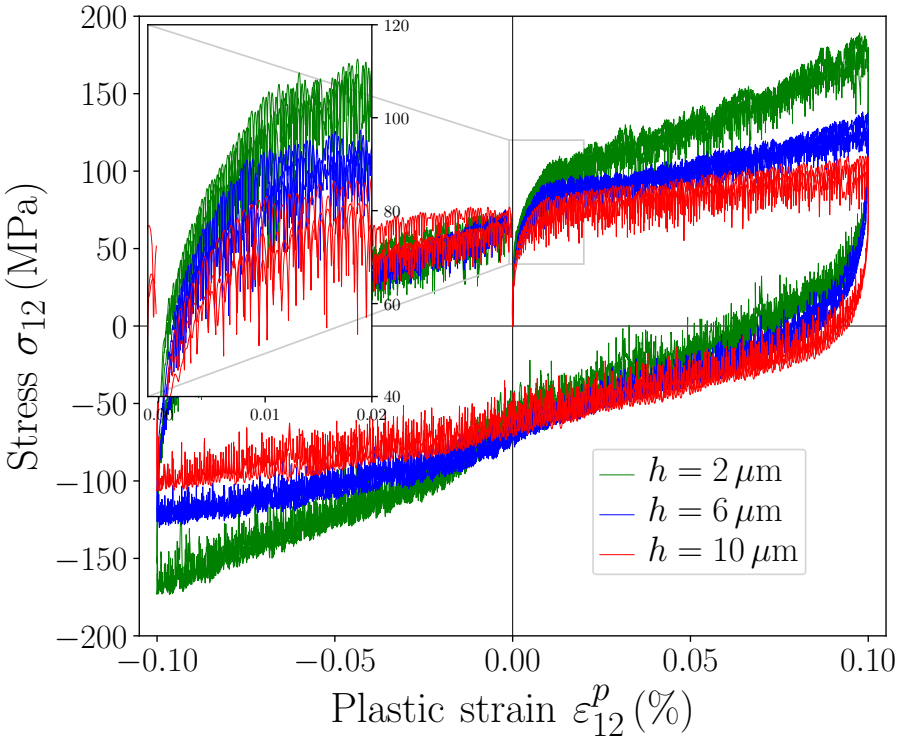
Size effects with discrete dislocation dynamics

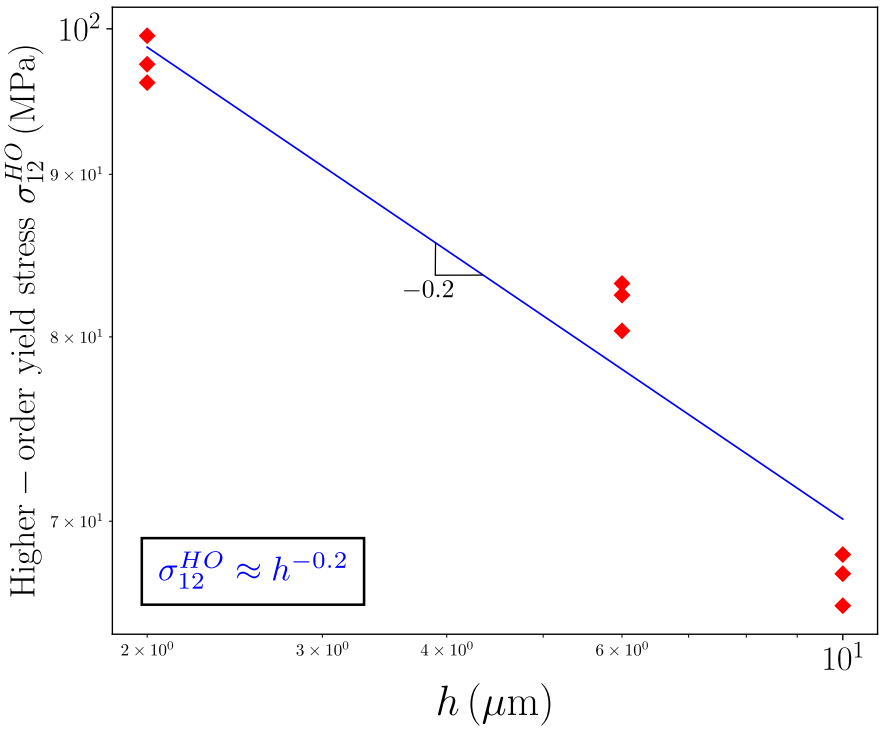
- Cyclic shear responses of passivated plate for different thicknesses h (2 symmetric slip systems, initial dislocation density $\rho_0 = 3 \times 10^{12}\,\mathrm{m}^{-2}$).



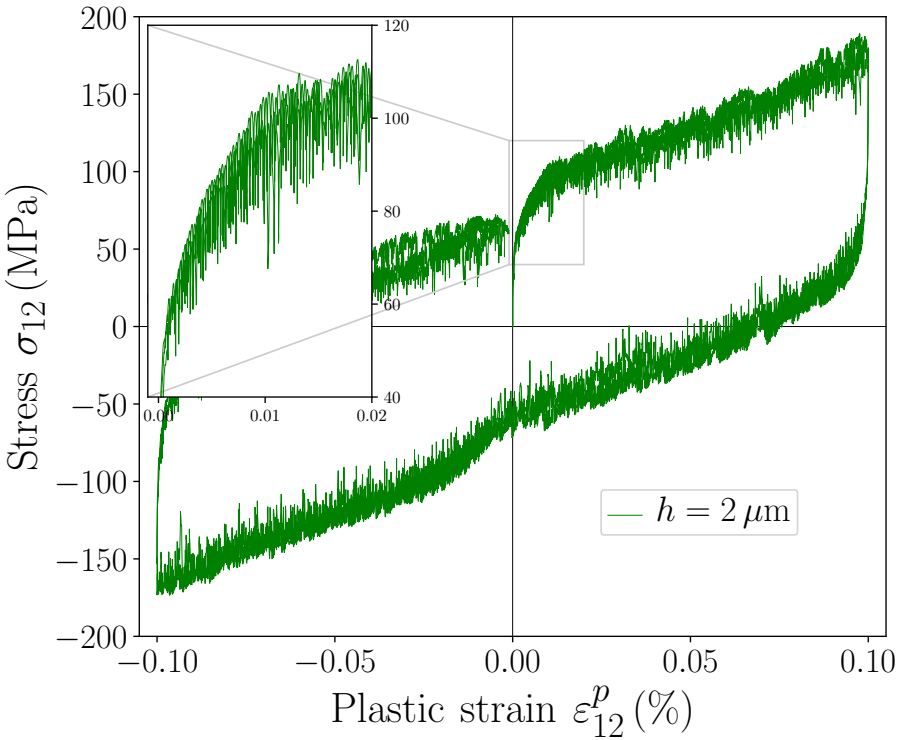
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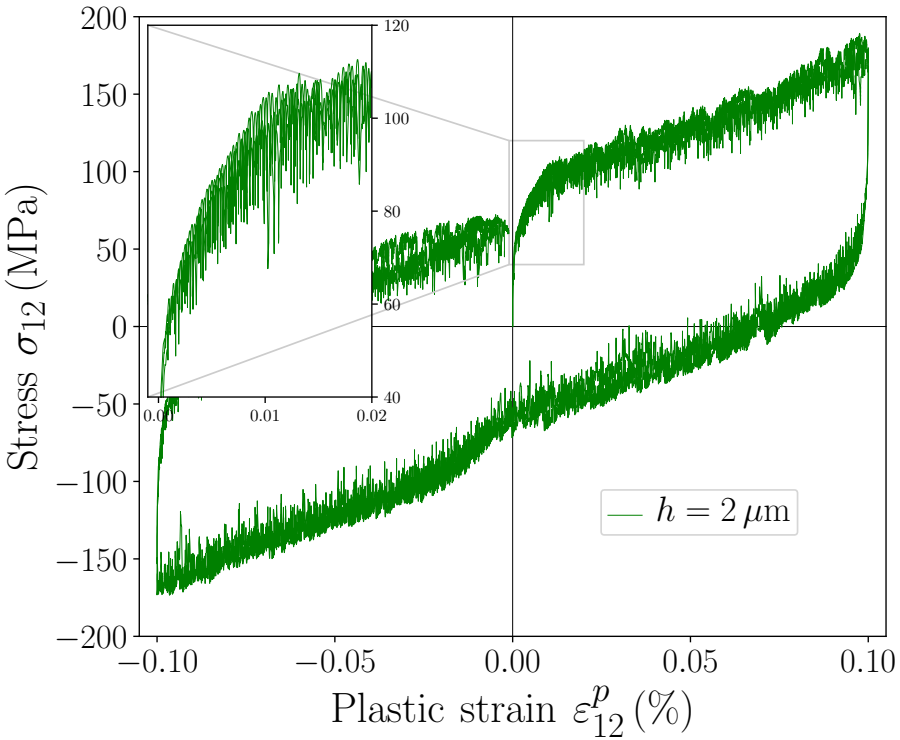


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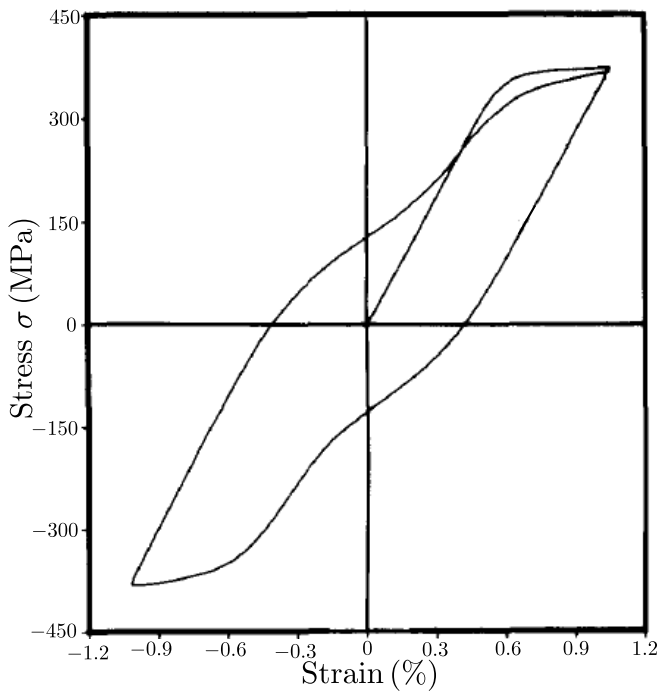


DDD response for $h = 2\,\mu$m: nonlinear kinematic hardening

Size effects with discrete dislocation dynamics

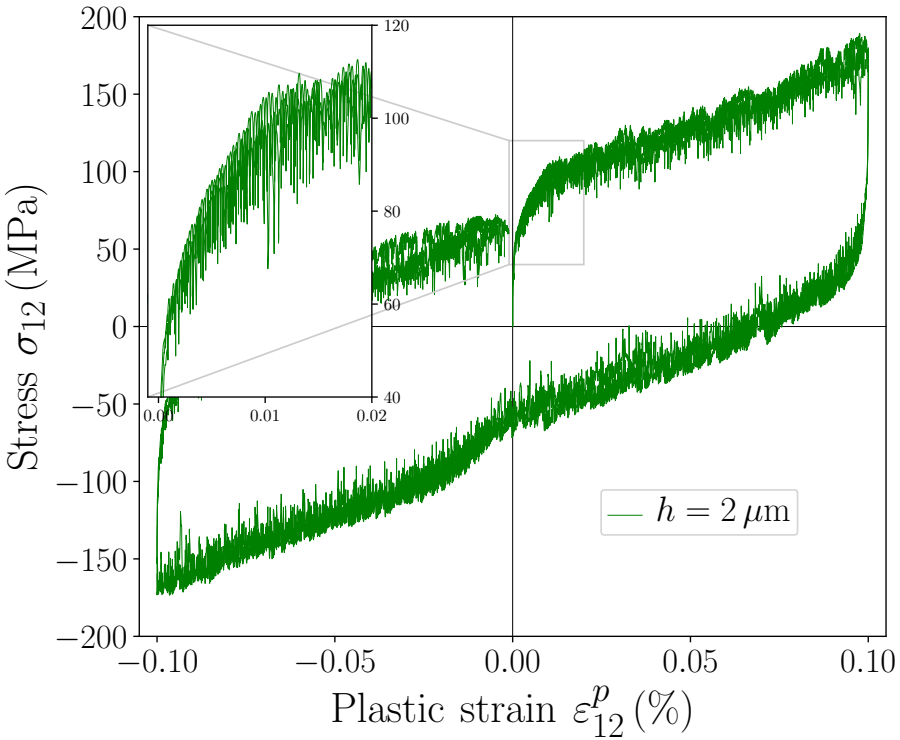


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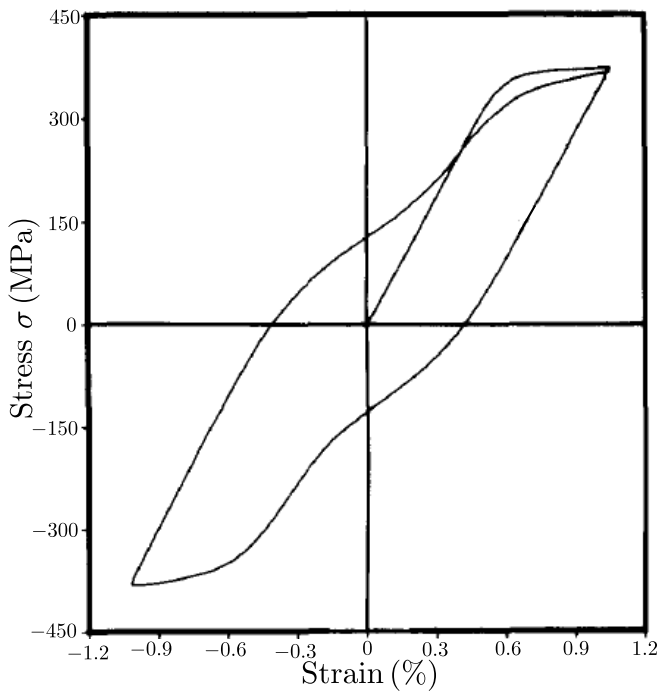


KIII kinematic hardening of [Asaro, 1975] (taken from [Hidayetoglu et al., 1985]).

Size effects with discrete dislocation dynamics



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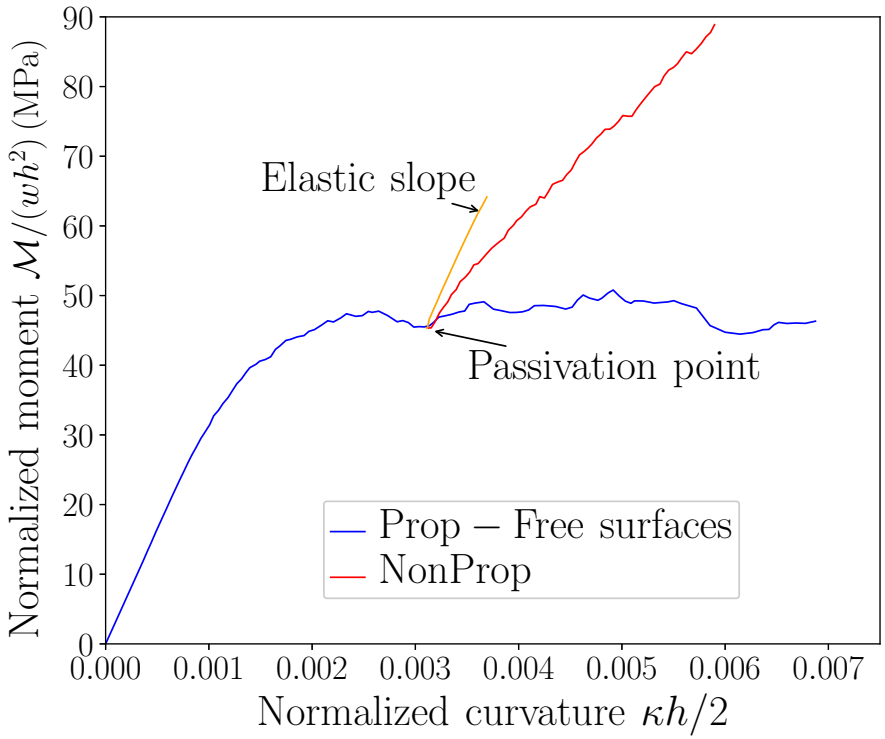


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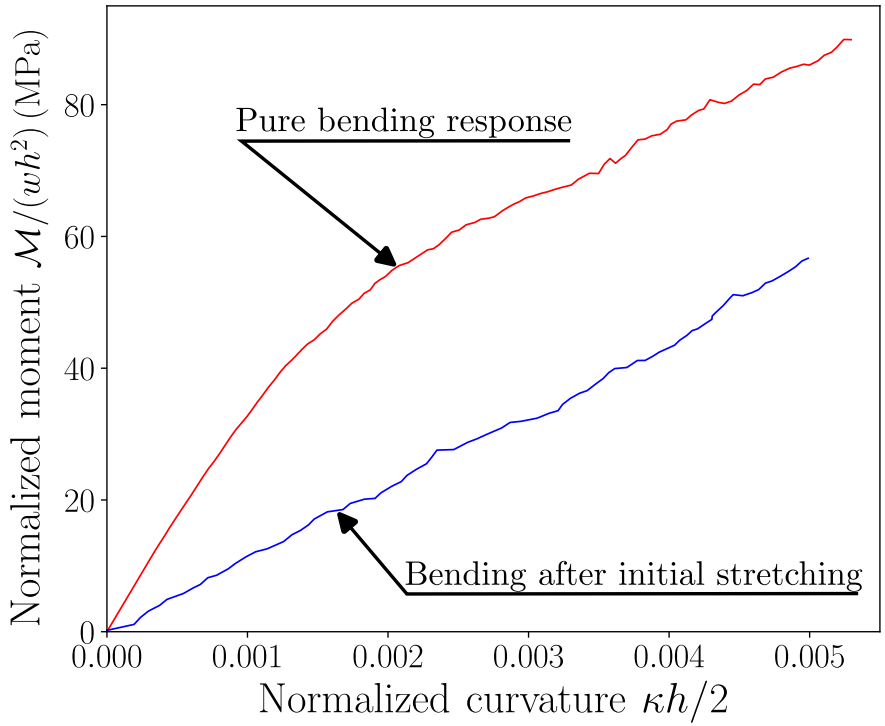
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Size effects with discrete dislocation dynamics

On the hunt for elastic gaps !



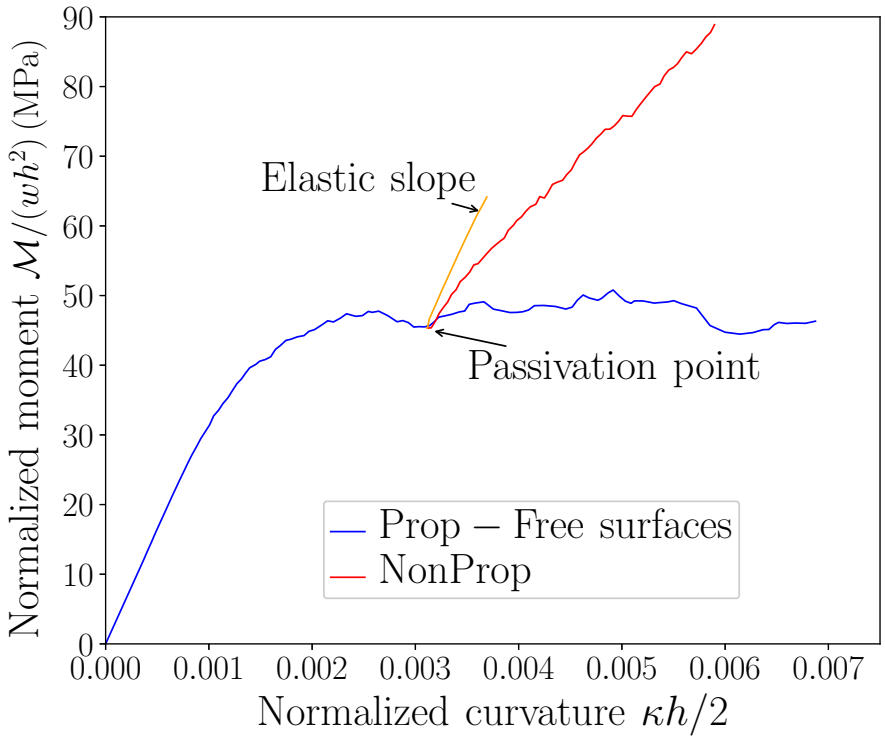
Bending-Passivation response



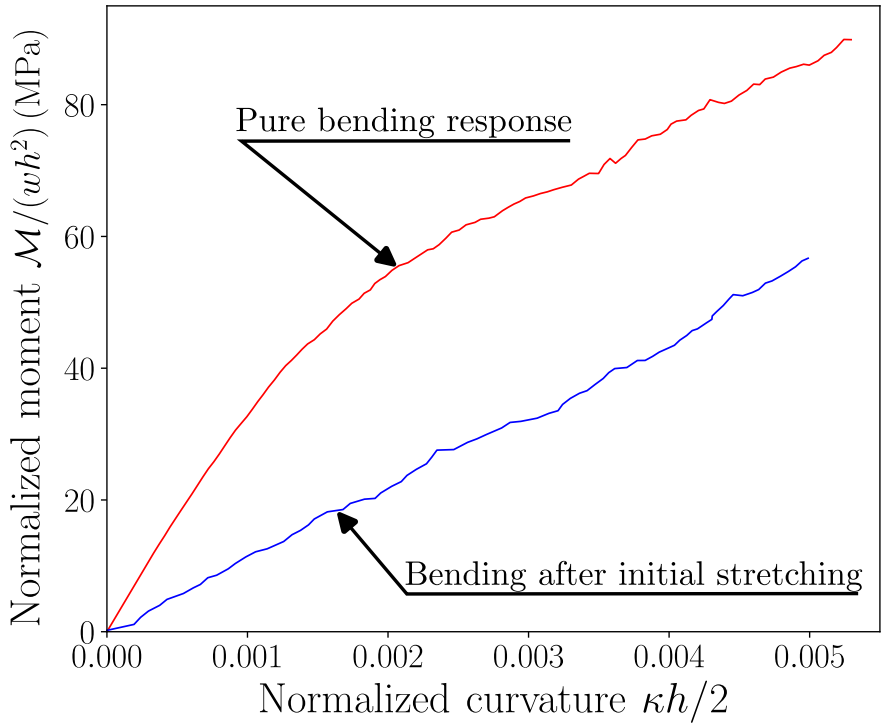
Tension-Bending response

Size effects with discrete dislocation dynamics

On the hunt for elastic gaps !



Bending-Passivation response



Tension-Bending response

$\Rightarrow$ No traces of elastic gaps are captured with DDD

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Multi-kinematic SGCP approach

Internal and external virtual powers:

$$\mathrm{DOF} = \{\mathbf{u}, \gamma^\alpha\} \Rightarrow \begin{cases} \mathcal{P}_{int} = \displaystyle\int_{\mathcal{V}} \boldsymbol{\sigma} : \delta\dot{\boldsymbol{\varepsilon}}^e \,\mathrm{dv} + \sum_{\alpha=1}^{q} \int_{\mathcal{V}} \pi^\alpha \delta\dot{\gamma}^\alpha \,\mathrm{dv} + \sum_{\alpha=1}^{q} \int_{\mathcal{V}} \boldsymbol{\xi}^{\boldsymbol{\alpha}} \cdot \delta\boldsymbol{\nabla}\dot{\gamma}^\alpha \,\mathrm{dv} \\ \mathcal{P}_{ext} = \displaystyle\int_{\mathcal{S}} \mathbf{t} \cdot \delta\dot{\mathbf{u}} \,\mathrm{ds} + \sum_{\alpha=1}^{q} \int_{\mathcal{S}} \chi^\alpha \delta\dot{\gamma}^\alpha \,\mathrm{ds} \end{cases}$$

with γ^α is plastic slip associated with slip system α

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Balance equations (from the principle of virtual power $\mathcal{P}_{int} = \mathcal{P}_{ext}$):

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$$\text{Microscopic:} \begin{cases} \tau^\alpha + \boldsymbol{\nabla} \cdot \boldsymbol{\xi}^\alpha - \pi^\alpha = 0 & \text{in} \quad \mathcal{V} \\ \boldsymbol{\xi}^\alpha \cdot \mathbf{n} = \chi^\alpha & \text{on} \quad \mathcal{S} \end{cases}$$

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$$\text{Microscopic:} \begin{cases} \tau^\alpha + \boldsymbol{\nabla} \cdot \boldsymbol{\xi}^\alpha - \pi^\alpha = 0 & \text{in} \quad \mathcal{V} \\ \boldsymbol{\xi}^\alpha \cdot \mathbf{n} = \chi^\alpha & \text{on} \quad \mathcal{S} \end{cases}$$

2^{nd} law of thermodynamic:

$$\overline{\int_{\mathcal{V}} \psi \,\mathrm{dv}}^{\cdot} \leq \mathcal{P}_{ext} = \mathcal{P}_{int} \quad \Longleftrightarrow \quad \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^e + \sum_{\alpha=1}^{q} \pi^\alpha \dot{\gamma}^\alpha + \boldsymbol{\xi}^{\boldsymbol{\alpha}} \cdot \delta\boldsymbol{\nabla}\dot{\gamma}^\alpha - \dot{\psi} \geq 0$$

Higher-order kinematic hardening modeling

From parallel (stress) to series (kinematic) decomposition:

$$\boldsymbol{\xi}^{\alpha} = \boldsymbol{\xi}_r^{\alpha} + \boldsymbol{\xi}_d^{\alpha} \qquad \Rightarrow \qquad \boldsymbol{\nabla}\gamma^{\alpha} = \boldsymbol{\kappa}_r^{\alpha} + \boldsymbol{\kappa}_d^{\alpha}$$

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Chaboche-type kinematic hardening model [Chaboche, 1989, Besson et al., 2010]

$$\tau^{\alpha} \quad - \quad \underbrace{(-\boldsymbol{\nabla}\cdot\boldsymbol{\xi}^{\alpha})} \quad = \quad \pi^{\alpha}$$

$$\text{Backstress } \mathbf{Z} = \sum_{i=1}^{D} \mathbf{Z}_i$$

$$\boldsymbol{\xi}^{\alpha} = \sum_{i=1}^{D} \boldsymbol{\xi}_i^{\alpha}, \qquad \boldsymbol{\xi}_i^{\alpha} = \frac{\partial \psi_p}{\partial \boldsymbol{\kappa}_r^{\alpha\, i}}, \qquad \boldsymbol{\kappa}^{\alpha} = \boldsymbol{\nabla}\gamma^{\alpha} = \boldsymbol{\kappa}_r^{\alpha\, i} + \boldsymbol{\kappa}_d^{\alpha\, i}$$

$$\psi_p = \sum_{i=1}^{D} \frac{1}{n_i} X_0\, l_{eni}^{n_i} \sum_{\alpha=1}^{q} \left(\left| \mathbf{s}^{\alpha} \cdot \boldsymbol{\kappa}_r^{\alpha\, i} \right|^{n_i} + \left| \mathbf{l}^{\alpha} \cdot \boldsymbol{\kappa}_r^{\alpha\, i} \right|^{n_i} \right)$$

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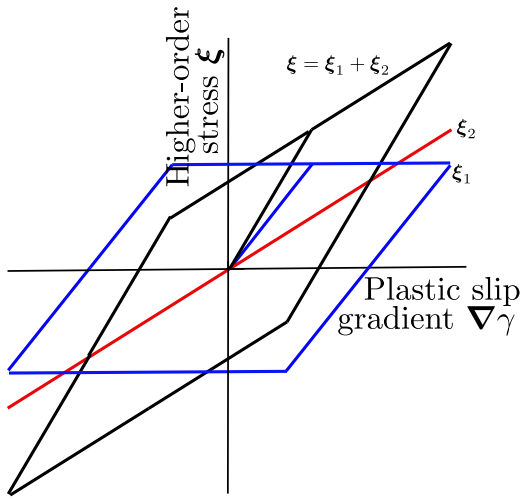
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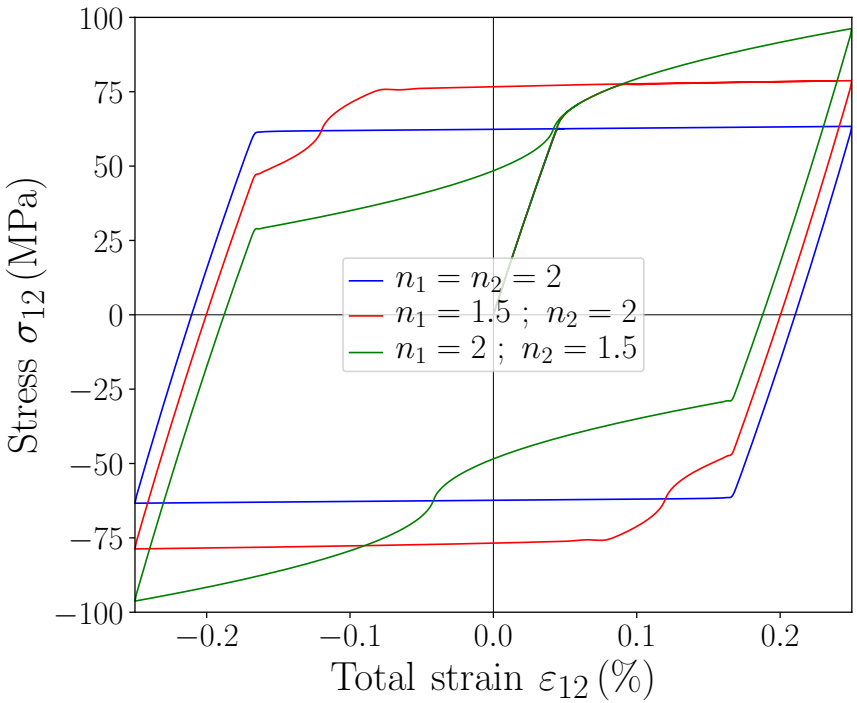
$$\psi_p = \sum_{i=1}^{D} \frac{1}{n_i} X_0\, l_{eni}^{n_i} \sum_{\alpha=1}^{q} \left(\left| \mathbf{s}^{\alpha} \cdot \boldsymbol{\kappa}_r^{\alpha\, i} \right|^{n_i} + \left| \mathbf{l}^{\alpha} \cdot \boldsymbol{\kappa}_r^{\alpha\, i} \right|^{n_i} \right)$$

Based on DDD results (two-stage plasticity):

- Two decompositions of $\boldsymbol{\kappa}^{\alpha} = \boldsymbol{\nabla}\gamma^{\alpha}$ $(D = 2)$.

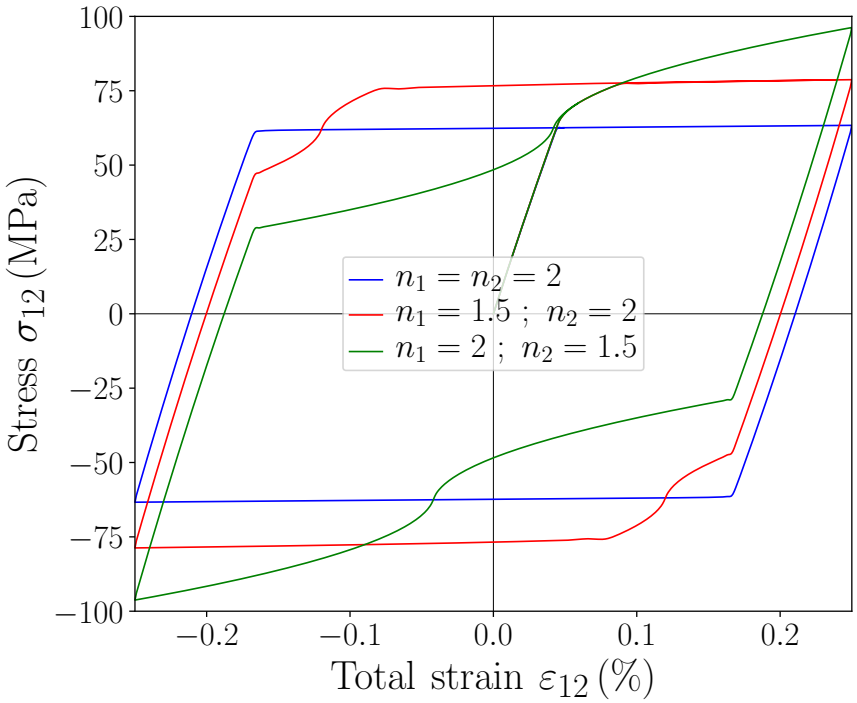


Discussion: Capabilities of the proposed model

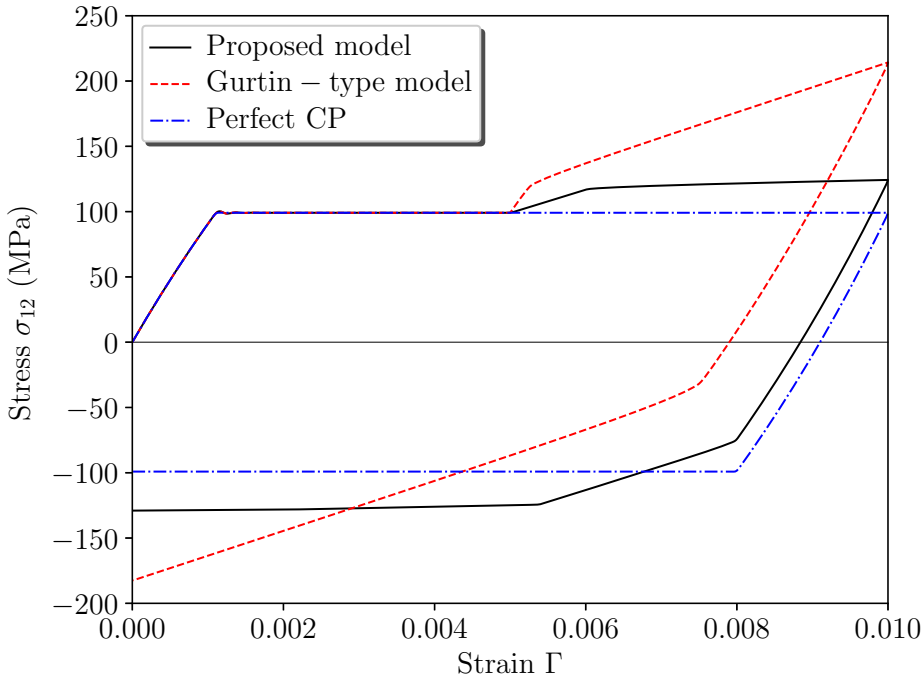


Evidence of the non-linear kinematic hardening

Discussion: Capabilities of the proposed model

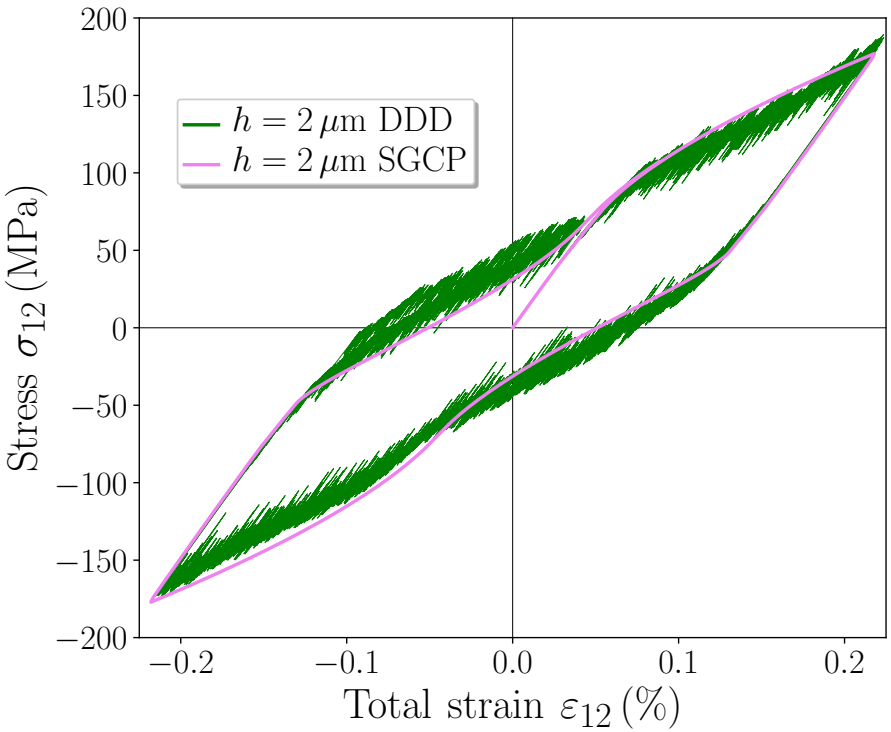


Evidence of the non-linear kinematic hardening



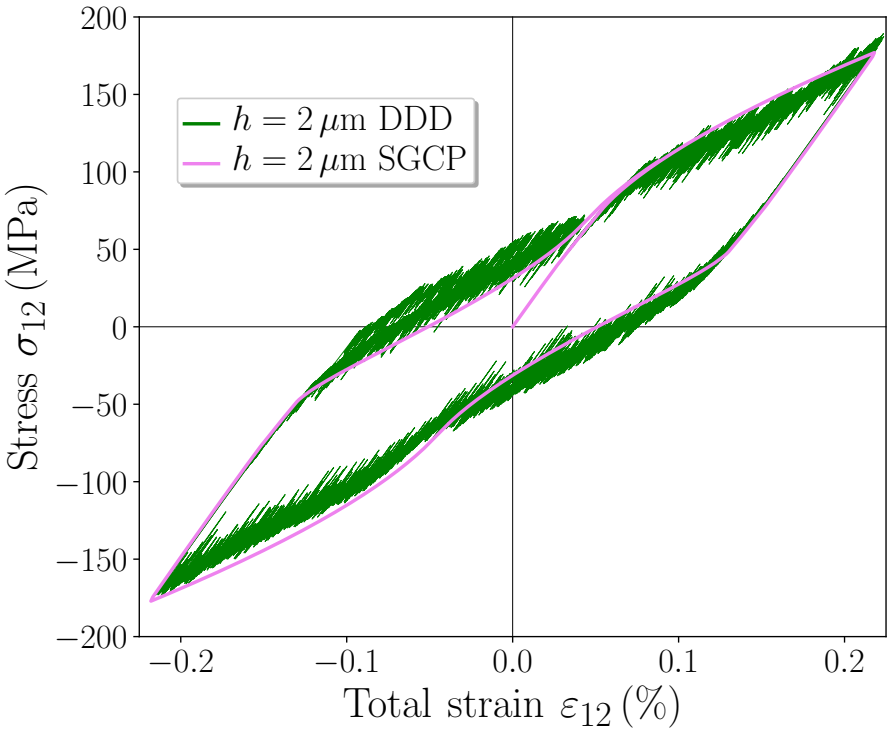
Study of elastic gaps under non-proportional shear conditions

Discussion: comparison with DDD

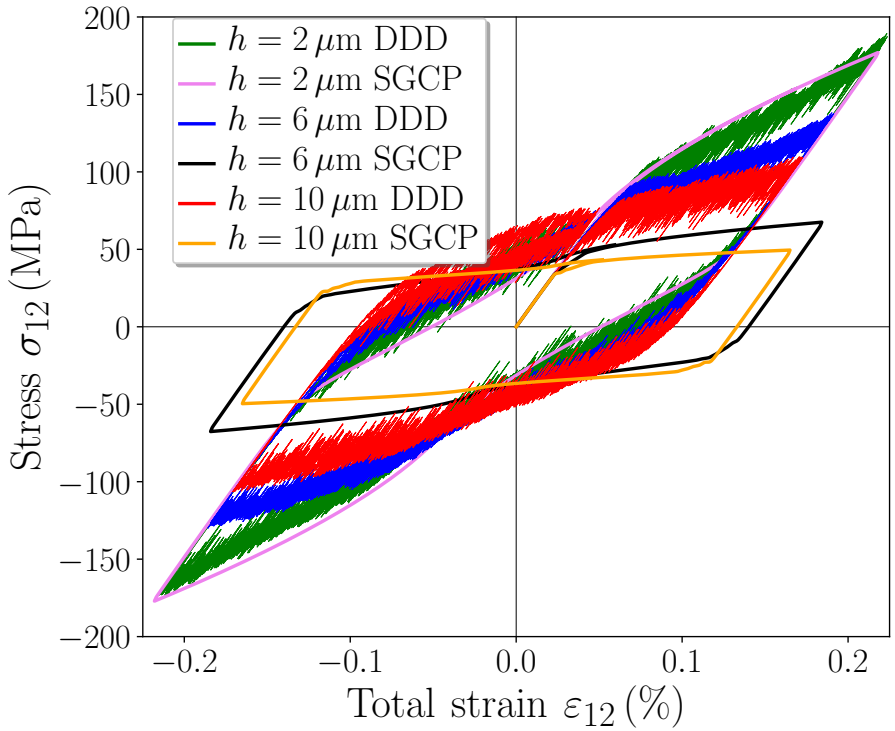


Comparison with DDD results for $h = 2\mu$m.

Discussion: comparison with DDD

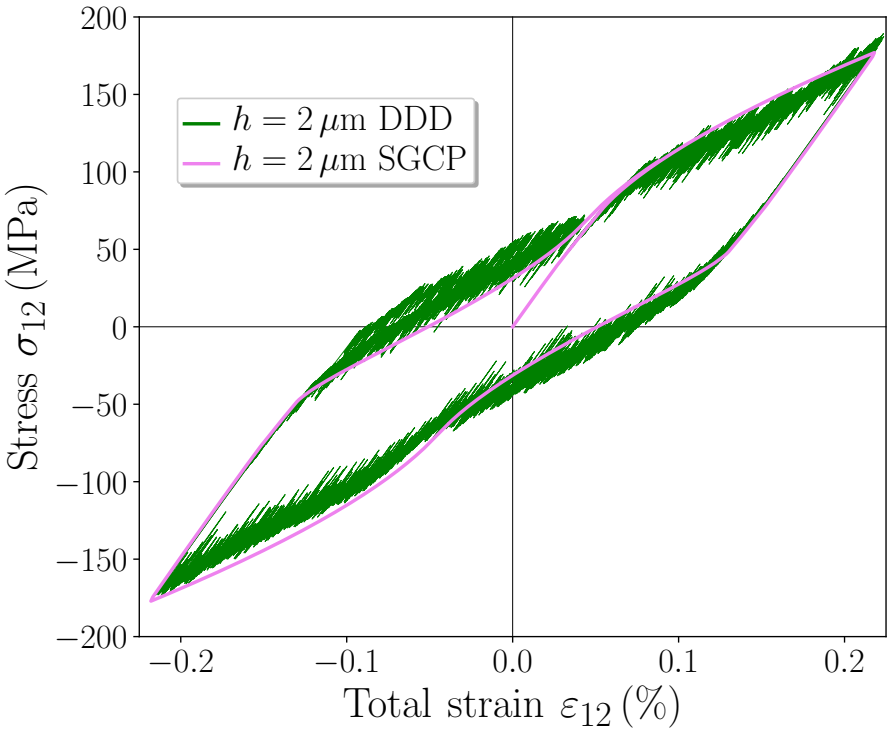


Comparison with DDD results for $h = 2\mu$m.

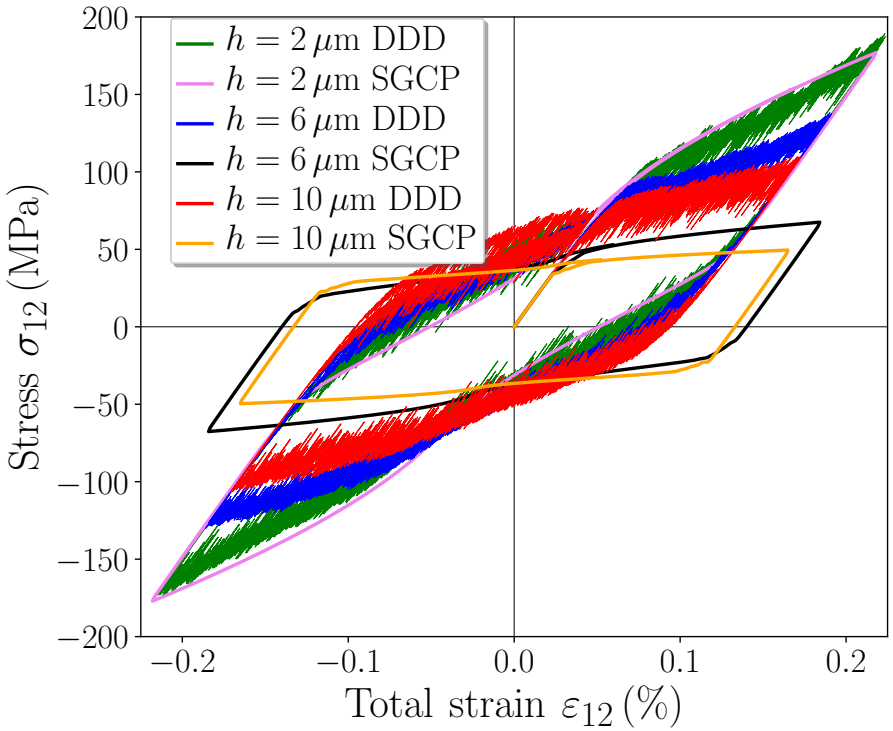


Macroscopic shear for different h: DDD vs. SGCP

Discussion: comparison with DDD



Comparison with DDD results for $h = 2\mu$m.



Macroscopic shear for different h: DDD vs. SGCP

- Strengthening: $\sigma_{12}^{HO} \sim h^{-1}$ (Orawan law) $\neq$ DDD results $\sigma_{12}^{HO} \sim h^{-0.2}$.

Micromorphic multi-kinematic SGCP approach

$$\text{DOF}: \ \{\mathbf{u}, \gamma^{\alpha}\} \Rightarrow \{\mathbf{u}, \boldsymbol{\chi}^{p}\}, \qquad \boldsymbol{\nabla} \cdot \boldsymbol{\xi}^{\alpha} \Rightarrow \operatorname{curl} \boldsymbol{\chi}^{\mathbf{P}}, \qquad \boldsymbol{\chi}^{p} \underset{\text{Penalty}}{\overset{H_{\chi}}{\Longleftrightarrow}} \mathbf{H}^{p} (\text{Plastic distorsion})$$

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Macroscopic equilibrium:
$$\begin{cases} \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} = \mathbf{0} & \text{in} \quad \mathcal{V} \\ \boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t} & \text{on} \quad \mathcal{S} \end{cases}$$

Microscopic equilibrium:
$$\begin{cases} \mathbf{s} + \operatorname{curl} \mathbf{M} = \mathbf{0} & \text{in} \quad \mathcal{V} \\ \mathbf{M} \cdot \boldsymbol{\epsilon} \cdot \mathbf{n} = \mathbf{m} & \text{on} \quad \mathcal{S} \end{cases}$$

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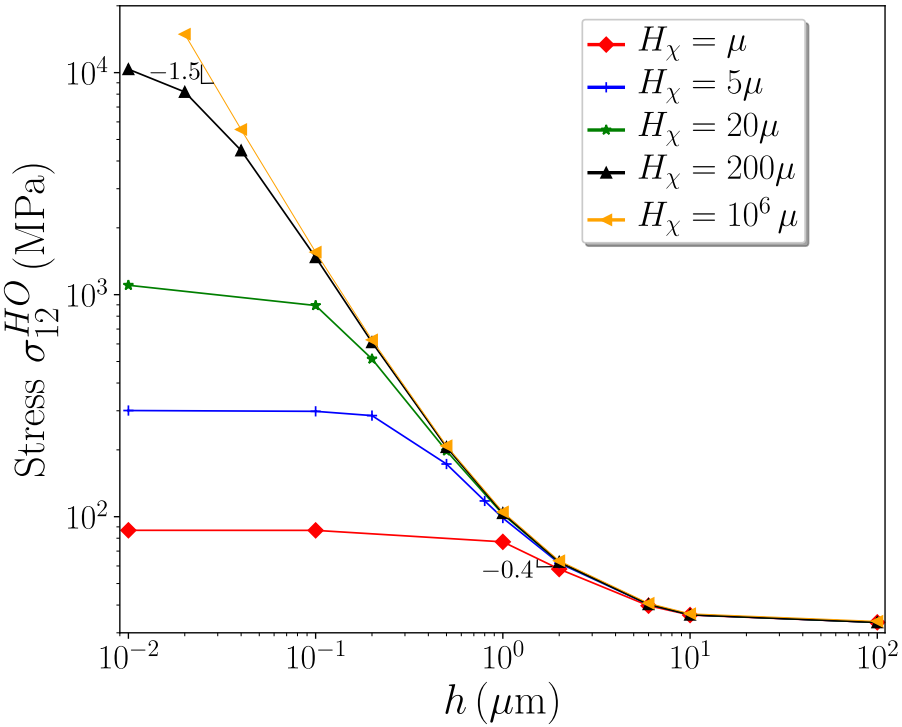
Chaboche-type kinematic hardening model [Chaboche, 1989, Besson et al., 2010]

$$\mathbf{s} - \left(- \sum_{i=1}^{D} \operatorname{curl} \mathbf{M}_i \right) = \mathbf{0}$$

$$\mathbf{M} = \sum_{i=1}^{D} \mathbf{M}_i, \qquad \operatorname{curl} \boldsymbol{\chi}^{p} = \boldsymbol{\kappa}_r^i + \boldsymbol{\kappa}_d^i, \qquad \mathbf{M}_i = \frac{\partial \psi_p}{\partial \boldsymbol{\kappa}_r^i}, \qquad \mathbf{s} = \frac{\partial \psi_p}{\partial \boldsymbol{\chi}^{p}}$$

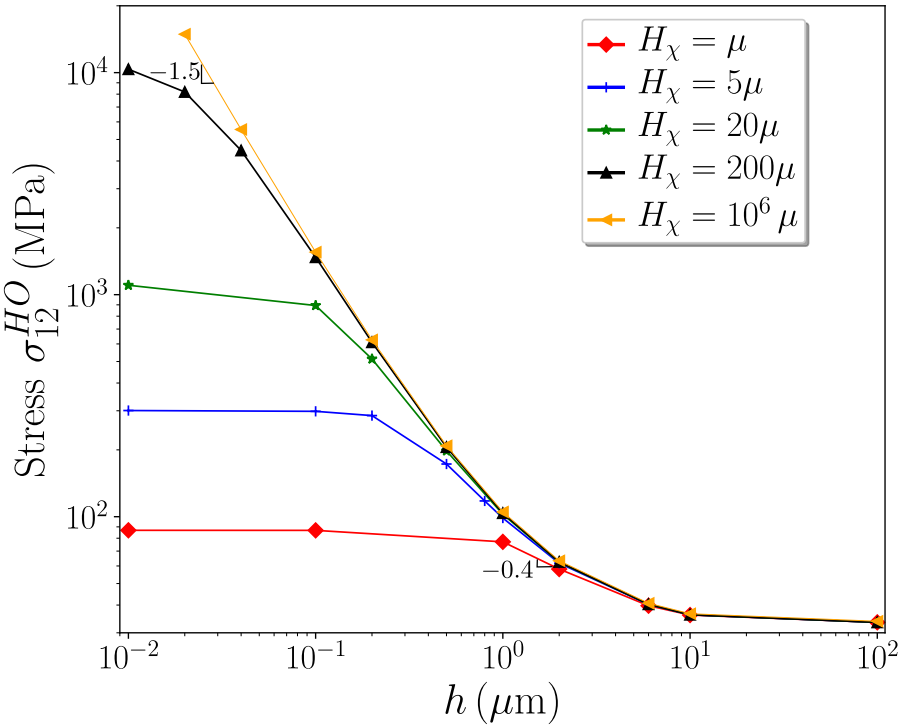
$$\psi_p = \sum_{i=1}^{D} \frac{1}{n_i} X_0 \, l_{eni}^{n_i} \left\| \boldsymbol{\kappa}_r^i \right\|^{n_i} + \frac{1}{2} H_{\chi} \left\| \mathbf{H}^{p} - \boldsymbol{\chi}^{p} \right\|^2$$

Discussion: comparison with DDD

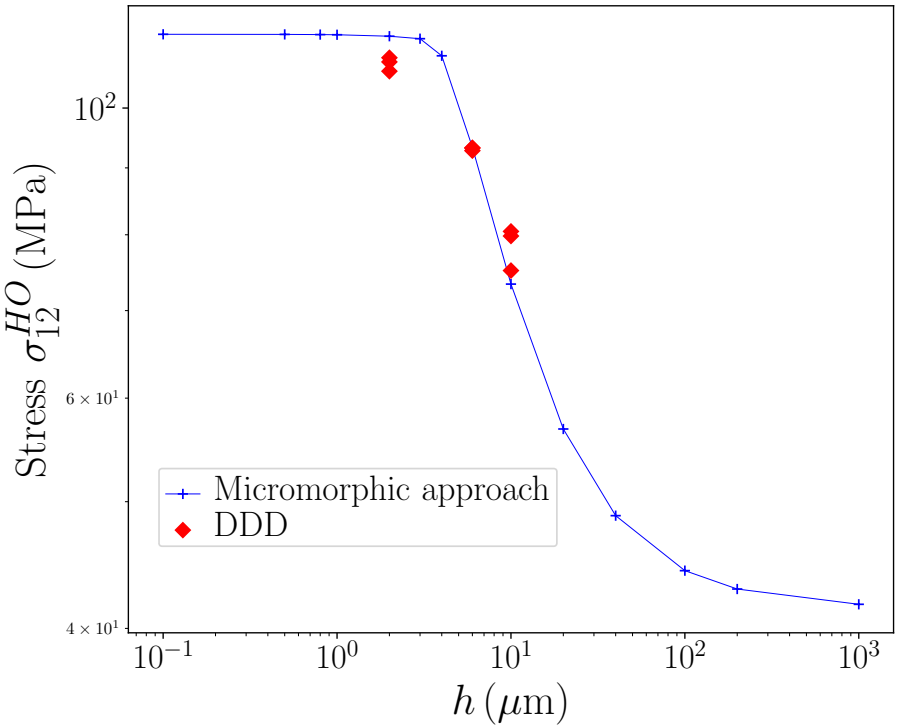


Scaling relationship from micromorphic results: effect of penalty parameter H_χ

Discussion: comparison with DDD



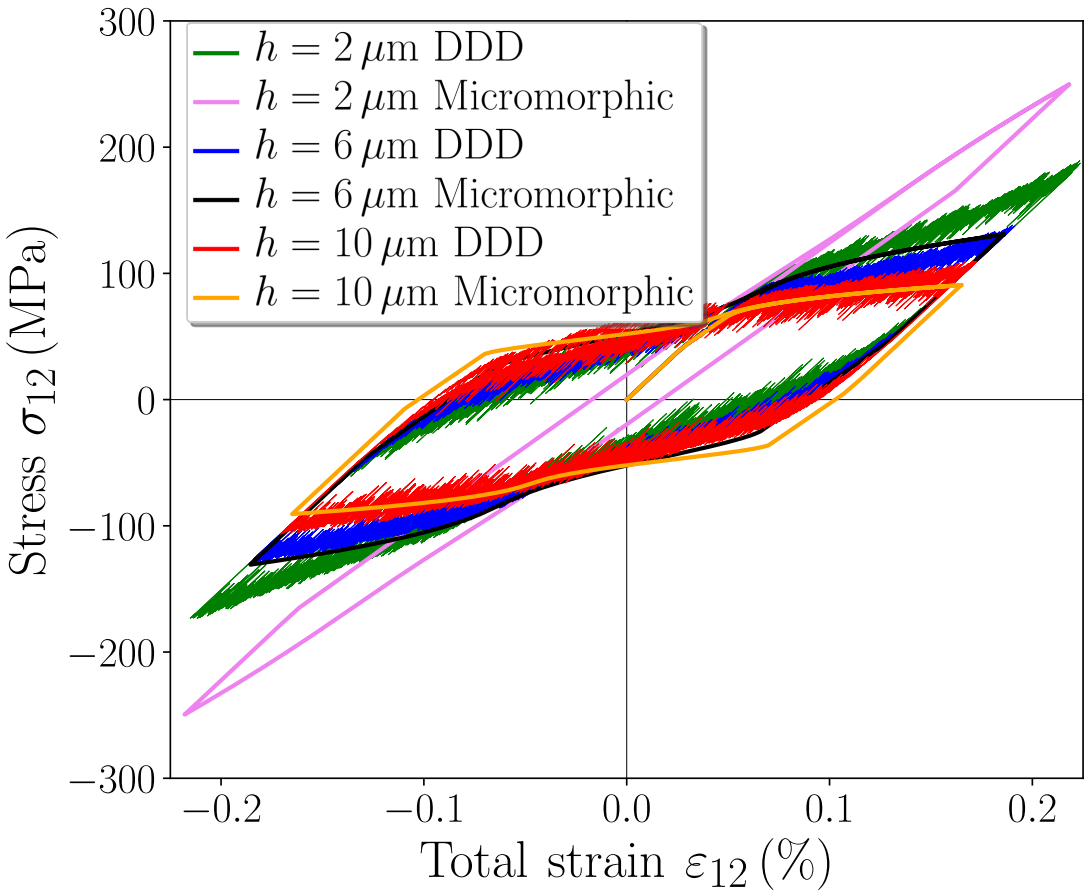
Scaling relationship from micromorphic results: effect of penalty parameter H_χ



Comparison with DDD after H_χ identification

- Good (quantitative) prediction of the scaling factor by the micromorphic SGCP model.

Discussion: comparison with DDD



- Good (quantitative) prediction of the overall shear response within a range of geometrical sizes.

Outline

1. Context and motivation: need for modeling of size effects
2. Modeling of size effects with discrete dislocation dynamics
3. Modeling of size effects with strain gradient crystal plasticity
4. Concluding remarks

Conclusions

Discrete Dislocation Dynamics (DDD) Modeling

- Evidence of size-dependent strengthening ($\sigma_y \sim h^{-0.2}$ in the case constrained shear conditions).
- Evidence of size-dependent kinematic hardening with clear inflection points, consistent with Asaro's type III behavior.
- New insights into small scale plasticity mechanisms: more physical interpretation of strengthening and hardening.

Gradient-Enhanced Continuum Modeling

- A refined SGCP framework based on a multi-kinematic decomposition of gradient terms into energetic and dissipative parts.
- Current challenges include limited flexibility in capturing lower than one scaling factors.
- A micromorphic formulation successfully extends the approach, enabling accurate control of the scaling factor within the physical range between 0 and 2.

Thank you for your attention!

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