Incorporating 3D Mechansims into 2D Dislocation Dynamics

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Outline

1. Discrete Dislocation Plasticity
2. 3D Rules in 2D Framework
3. Work-Hardening
4. Relation to geometric hardening and GNDs
5. **The Stored Energy of Cold Work**

Stored Energy of Cold Work

1. Method of calculation

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2. Unloading

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4. Connection between stored energy, energetic hardening and GNDs

Method of Calculation

$$\int_S \mathbf{t} \cdot \dot{\mathbf{u}} dS = \int_V \dot{\phi} dV + \int_V \zeta dV$$

- small strains and rotations
- quasi-static deformations
- no body forces
- isothermal deformation paths

Method of Calculation

Define

$$\Phi = \int_V \phi dV = \frac{1}{2}\int_V \boldsymbol{\sigma} : \boldsymbol{\epsilon} dV = \frac{1}{2}\int_V (\tilde{\boldsymbol{\sigma}} + \hat{\boldsymbol{\sigma}}) : (\tilde{\boldsymbol{\epsilon}} + \hat{\boldsymbol{\epsilon}}) dV$$

- Exclude region around dislocation cores
- Attribute a finite energy to this region

$$\Phi = \frac{1}{2}\int_V \hat{\boldsymbol{\sigma}} : \hat{\boldsymbol{\epsilon}}\, \mathrm{d}V + \frac{1}{2}\int_V (\hat{\boldsymbol{\sigma}} : \tilde{\boldsymbol{\epsilon}} + \tilde{\boldsymbol{\sigma}} : \hat{\boldsymbol{\epsilon}})\, \mathrm{d}V$$
$$+ \frac{1}{2}\sum_{J \neq K}\sum \int_V \boldsymbol{\sigma}^{(J)} : \boldsymbol{\epsilon}^{(K)}\, \mathrm{d}V$$
$$+ \sum_I \left[\frac{1}{2}\int_{\hat{V}^{(I)}} \boldsymbol{\sigma}^{(I)} : \boldsymbol{\epsilon}^{(I)}\, \mathrm{d}V + \frac{1}{2}\int_{\partial C^{(I)}} \mathbf{t}^{(I)} \cdot \mathbf{u}^{(I)}\, \mathrm{d}S\right] + E_c$$

Plane Strain Specialization

Last two terms in Φ

$$E_l^s = \sum_I \left[\frac{1}{2} \int_{\hat{V}^{(I)}} \boldsymbol{\sigma}^{(I)} : \boldsymbol{\epsilon}^{(I)} \, \mathrm{d}V + \frac{1}{2} \int_{\partial C^{(I)}} \mathbf{t}^{(I)} \cdot \mathbf{u}^{(I)} \, \mathrm{d}S \right] + E_c$$

- Use (isotropic) line tension approximation ($\mathcal{E} = \alpha\mu b^2$: constant line energy/length around loop)
- Assume statistically homogeneous distribution of loops across thickness

$$E_l^{\mathrm{s}} = \sum_{\mathrm{pairs}} (2\mathcal{S}\mathcal{E}) \frac{1}{\mathcal{S}} = 2N_p\mathcal{E} = (\rho + \rho')\, A\, \mathcal{E}$$

ρ': density of “half-loops”

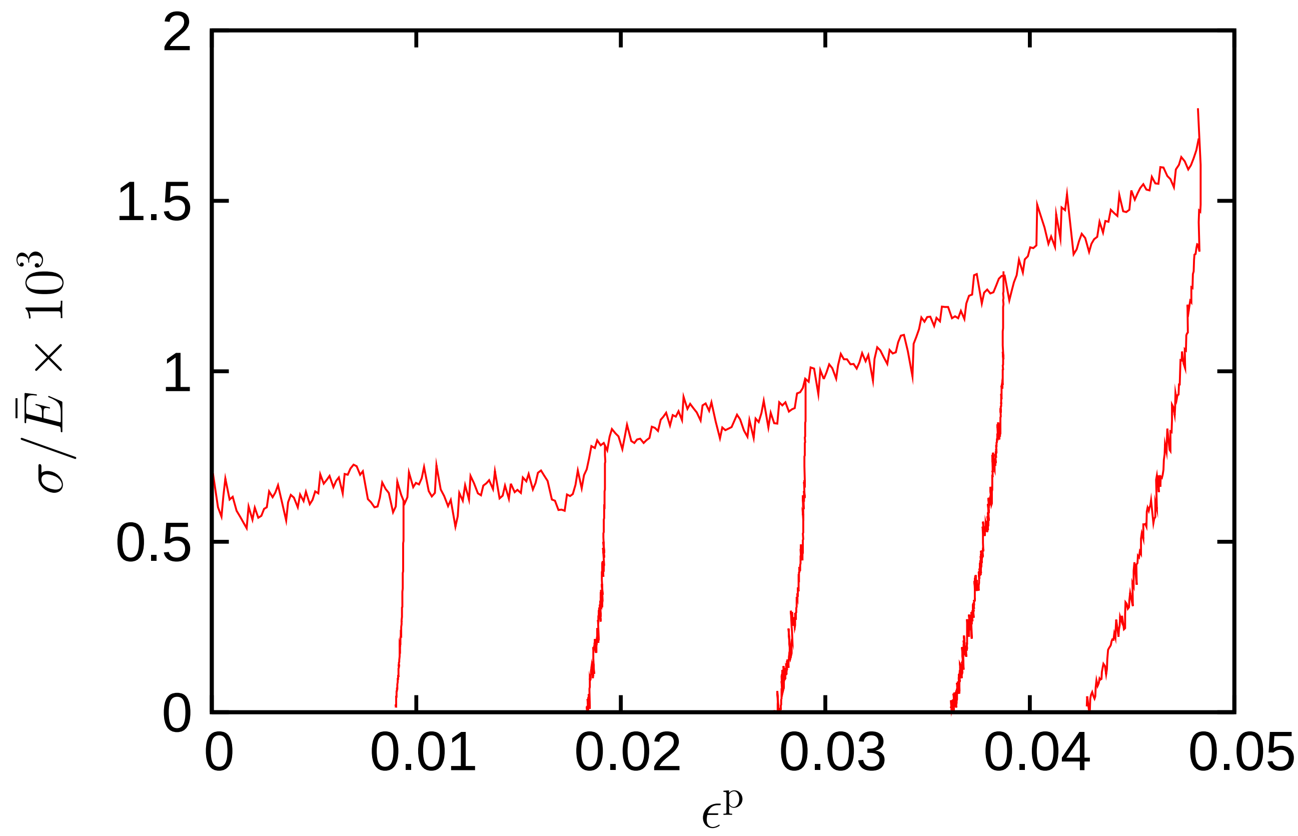
Method of Calculation

Consider loading program from initial $t = 0$ (stress-free state) to time t:

$$\int_0^t \dot{\mathcal{W}} dt = \Phi(t) + \int_0^t \mathcal{D} dt$$

Tension	Bending
$\mathcal{W} = A \int_0^t \Sigma \dot{\varepsilon} dt$	$\mathcal{W} = \int_0^t M \dot{\Theta} dt$
$E^{\mathrm{s}}(t) = \Phi(t) - \frac{A}{2\bar{E}} \Sigma^2$	$E^{\mathrm{s}}(t) = \Phi(t) - \frac{L}{2D} M^2$

Unloading (tension)



Junctions are not destroyed by annihilation

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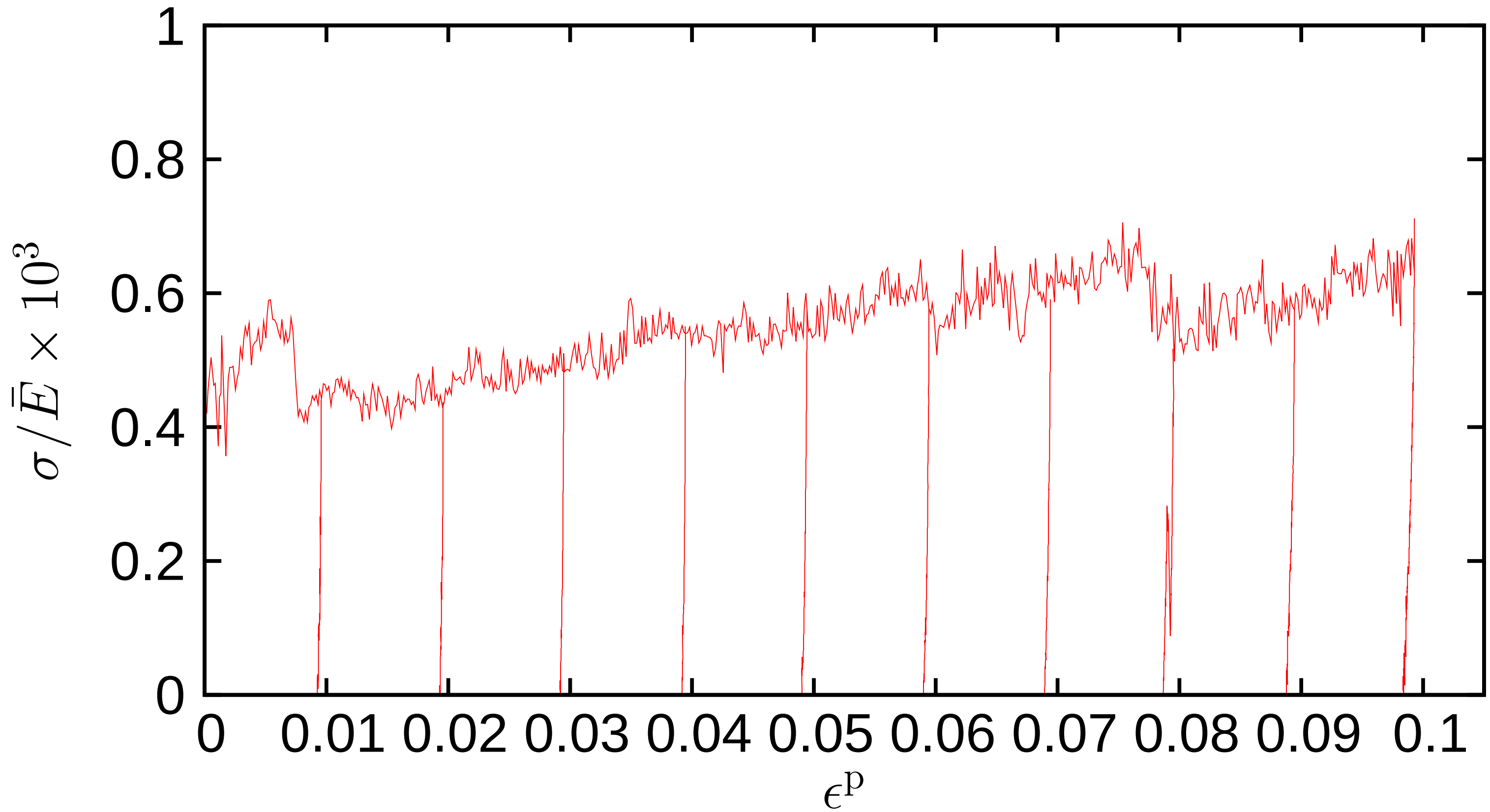

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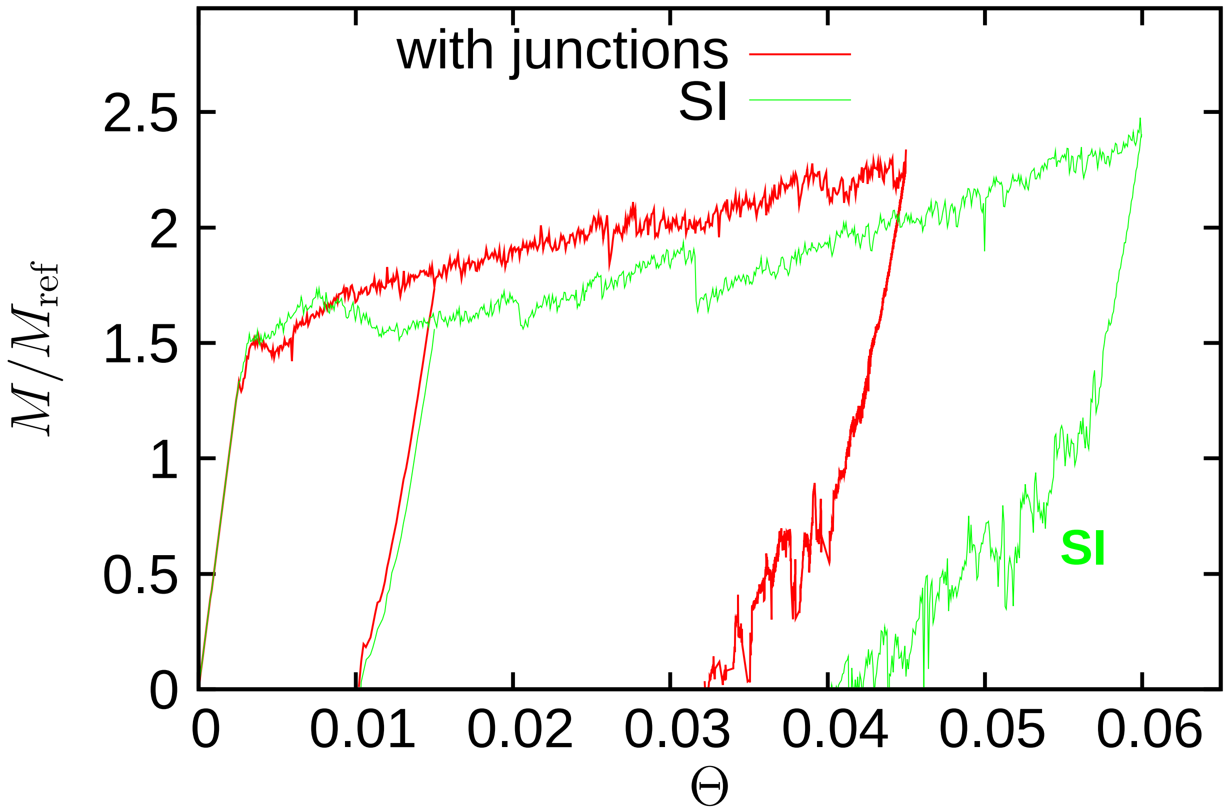

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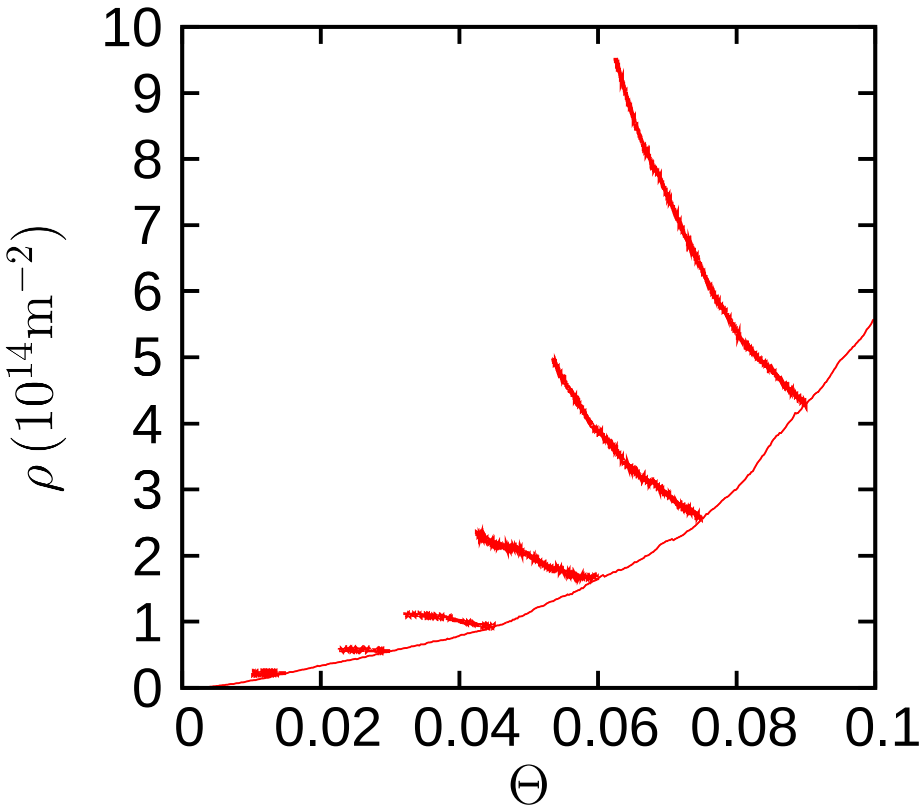
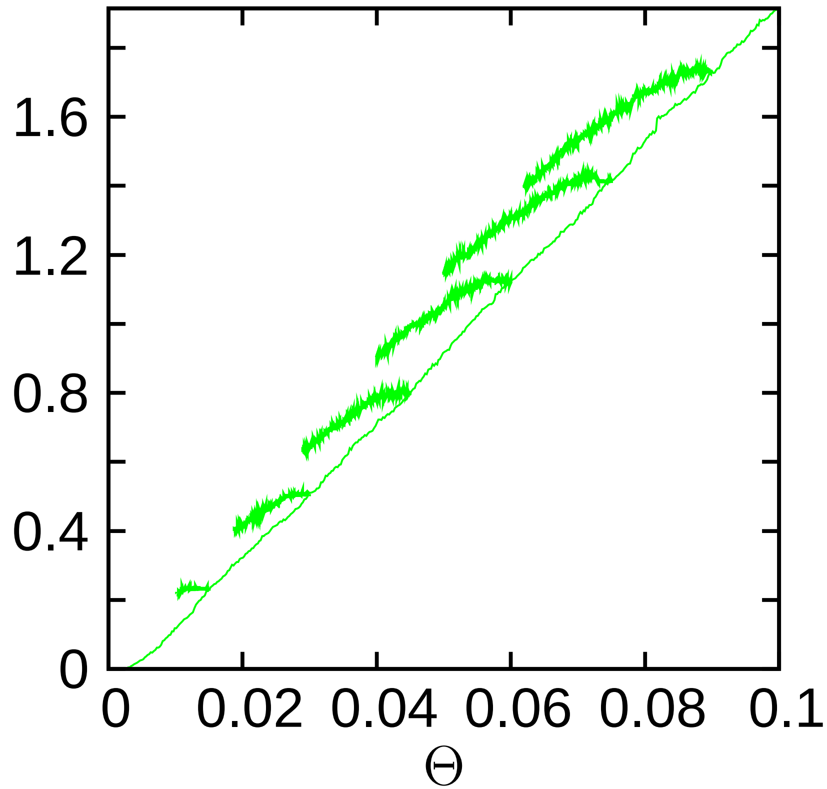
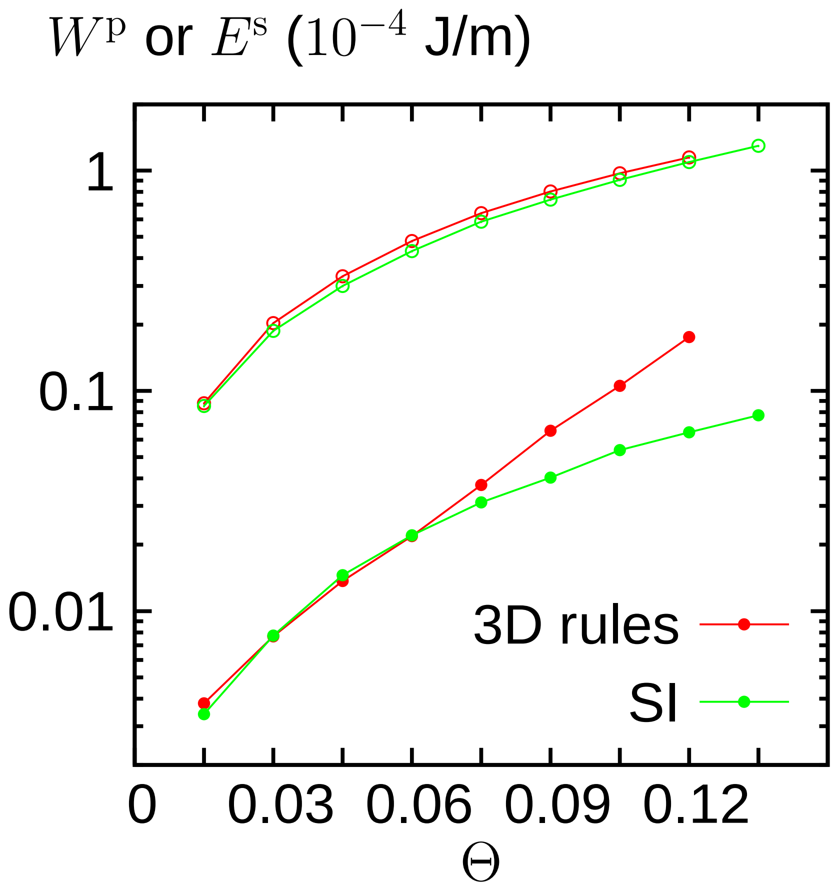


3D Rules



2D Rules (SI)

Energy stored in bending



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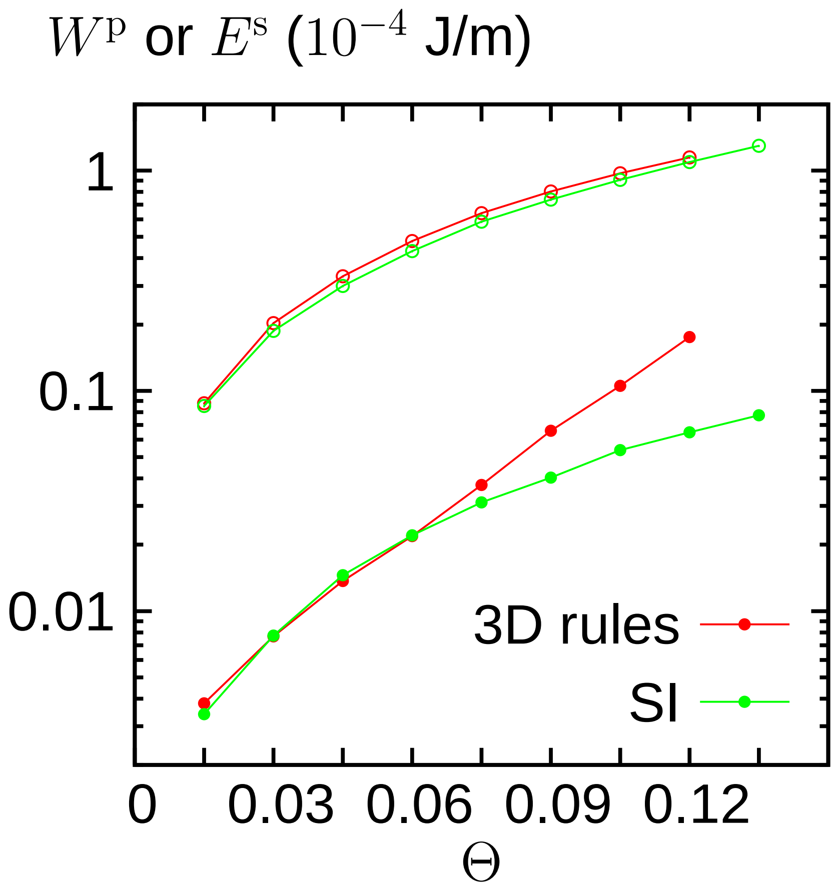
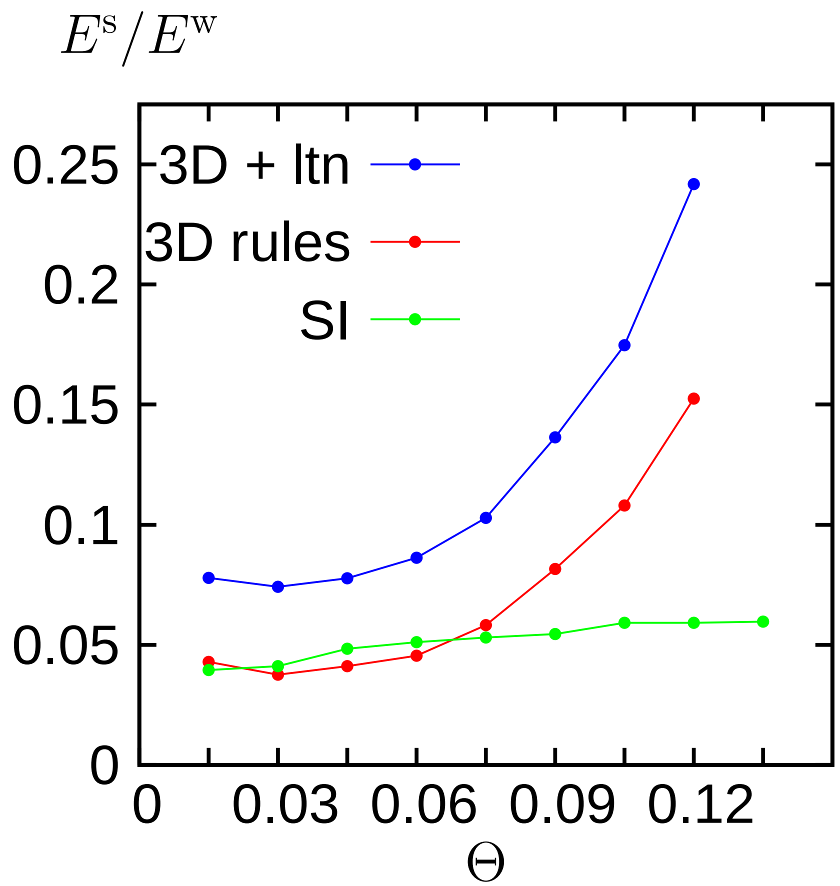
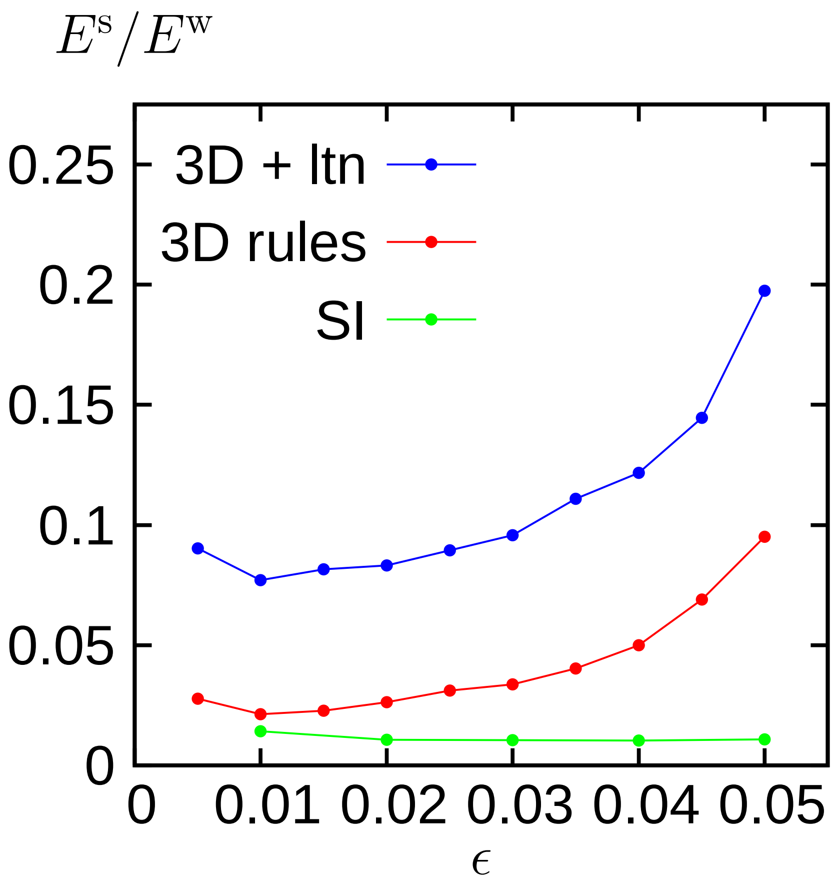




Tension vs Bending



Tension

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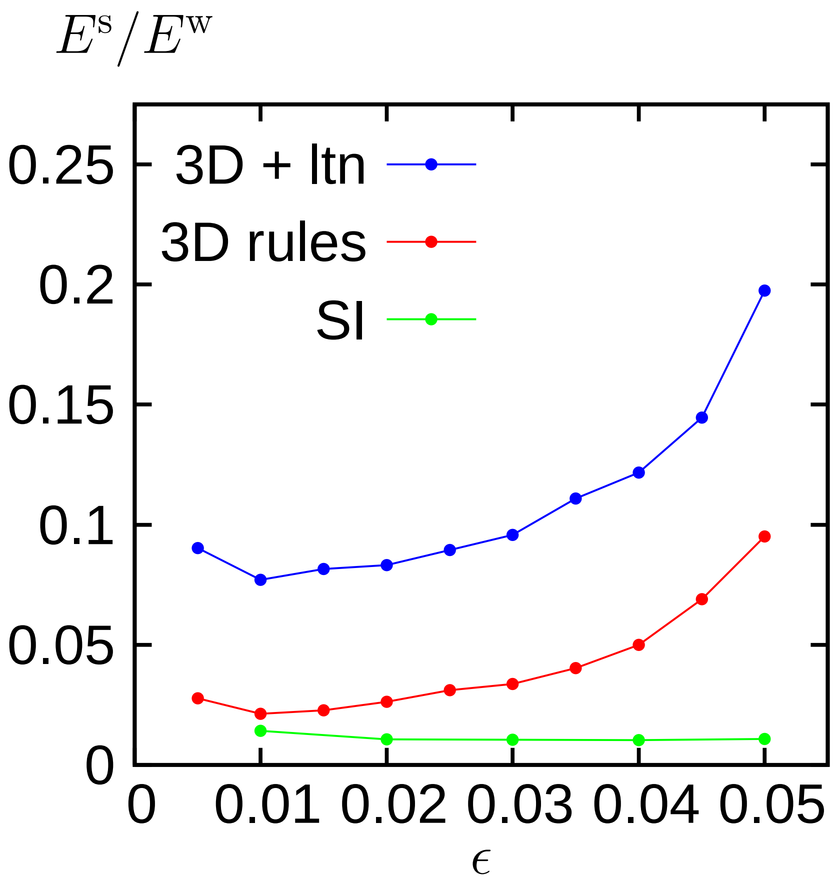

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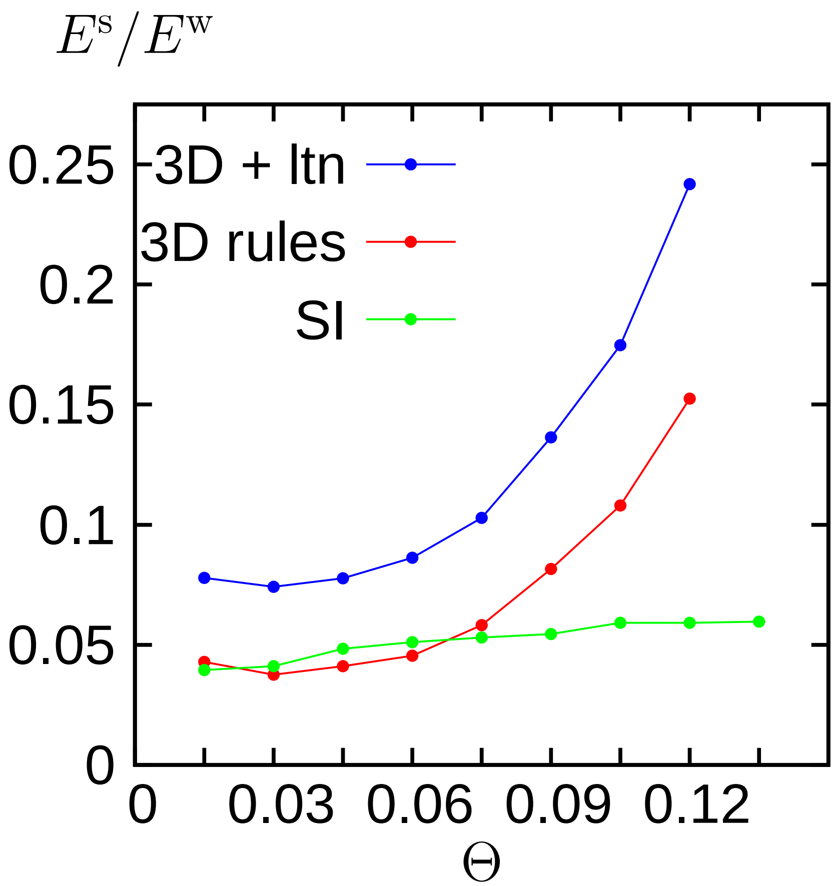

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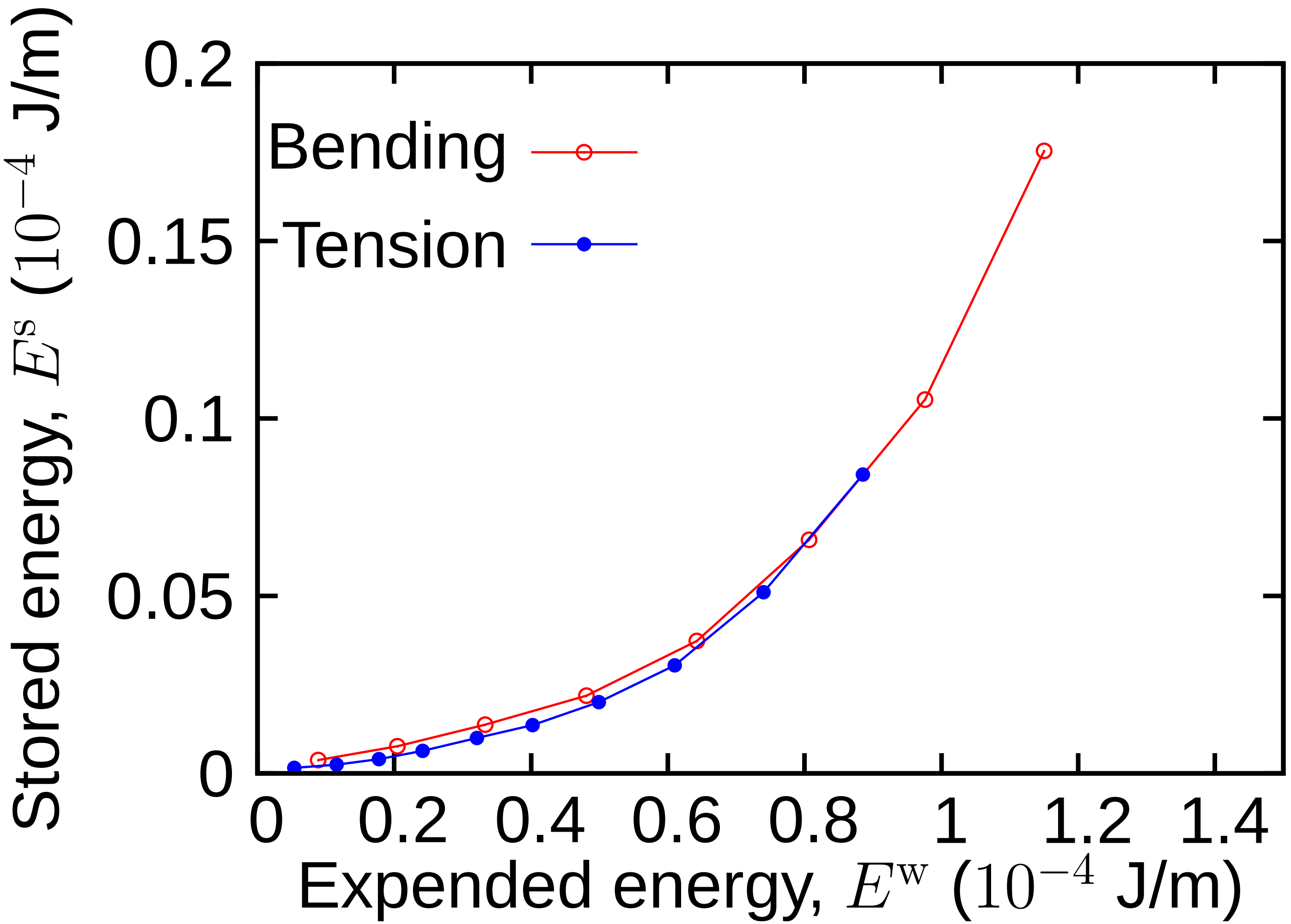

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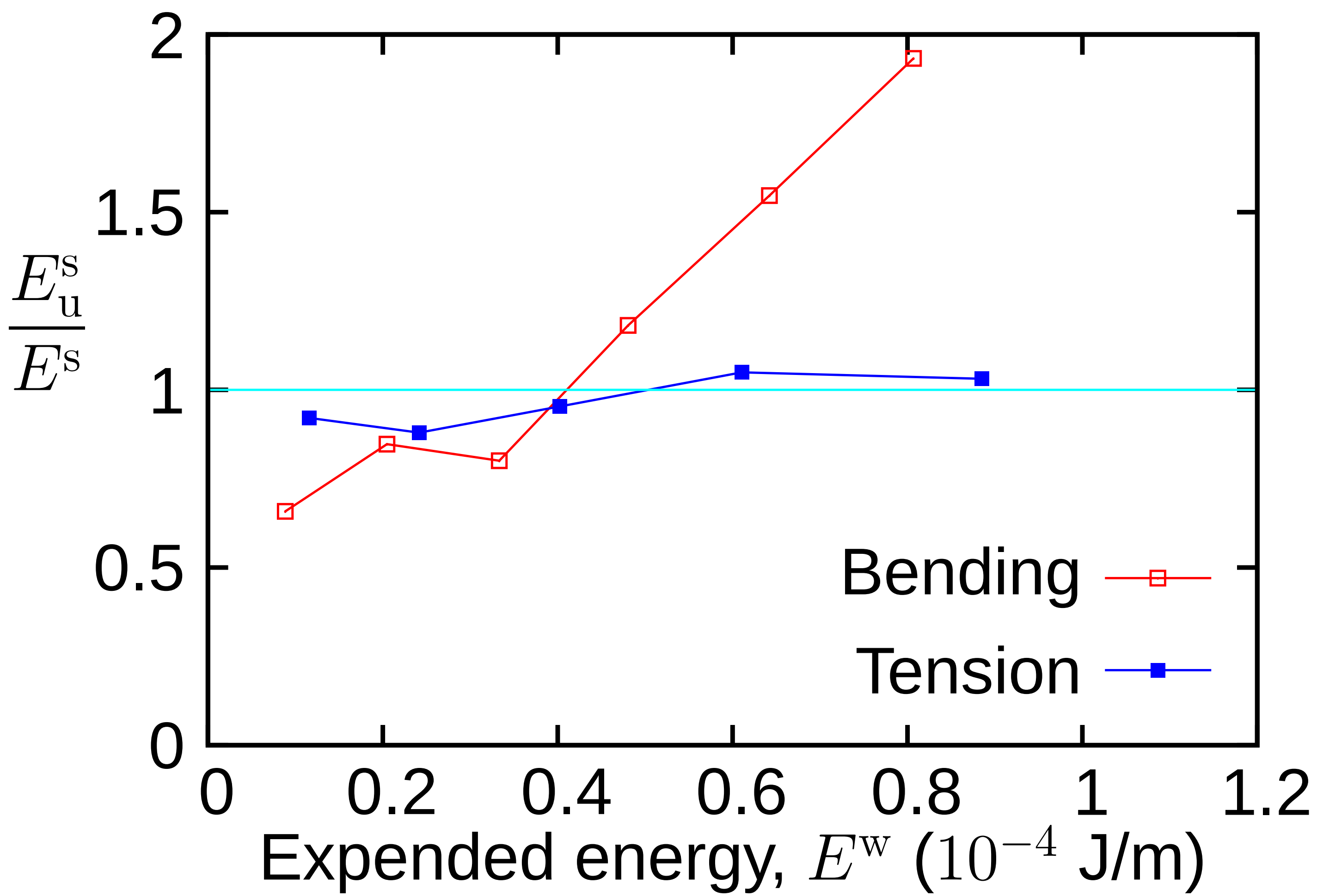
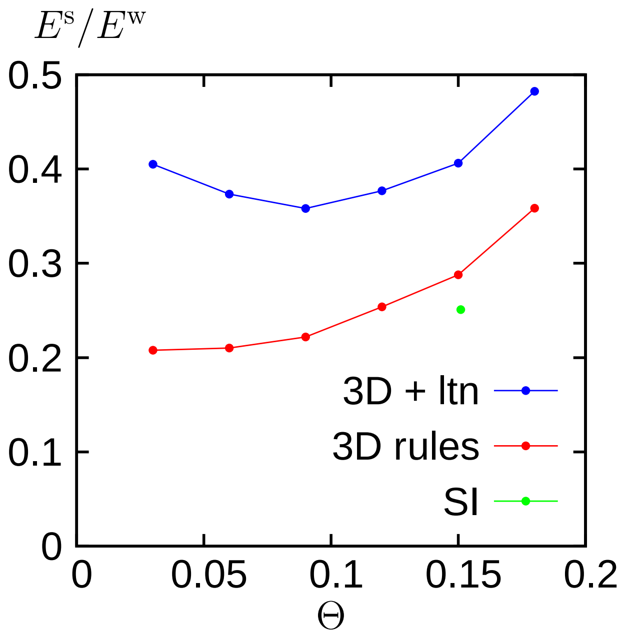


Size effects (bending)



$1\mu\mathrm{m}\times 3\mu\mathrm{m}$

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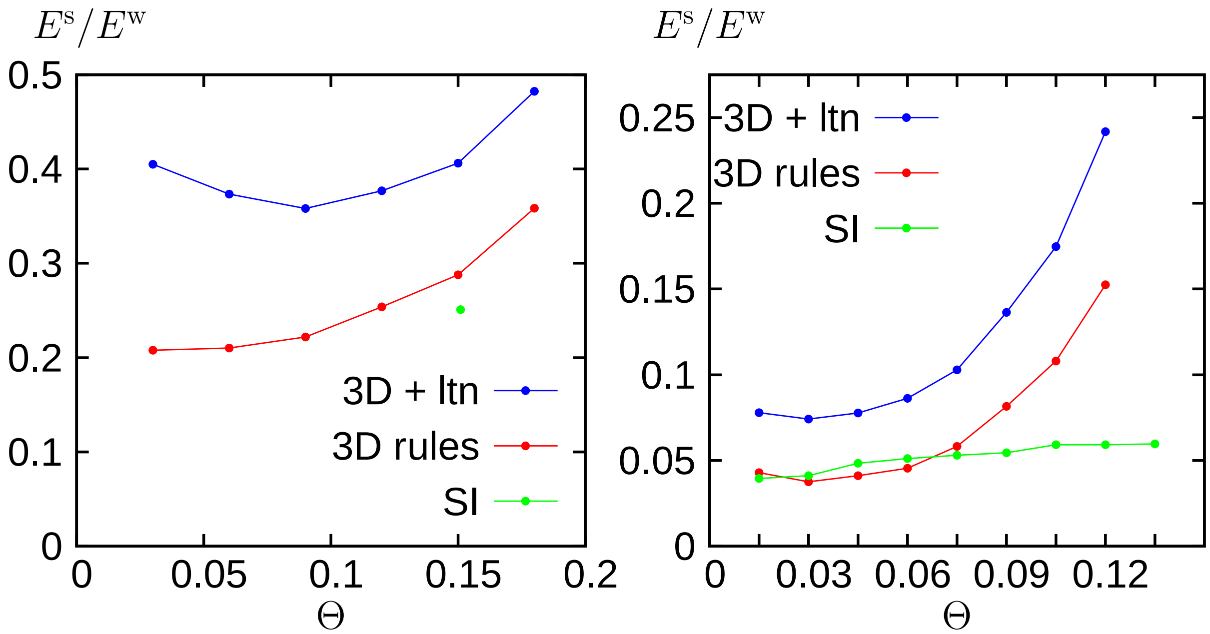

$1\mu m \times 3\mu m$ $2\mu m \times 6\mu m$

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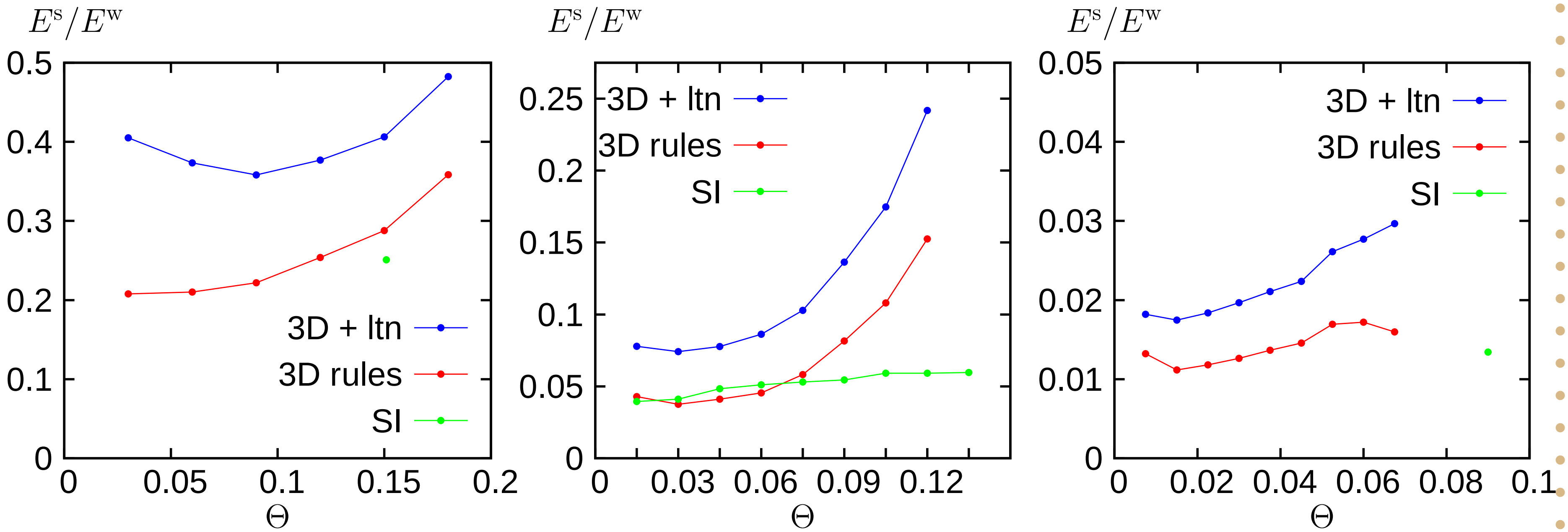

$1\mu m \times 3\mu m$ $2\mu m \times 6\mu m$ $4\mu m \times 12\mu m$

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- **Application to work-hardening**
  - **Two-stage hardening is natural outcome of the simulation. Work-hardening rates in agreement with experimental values**
  - **Dislocation storage parameters suggest scaling is correct**
  - **Organized dislocation structures form at multiple scales**

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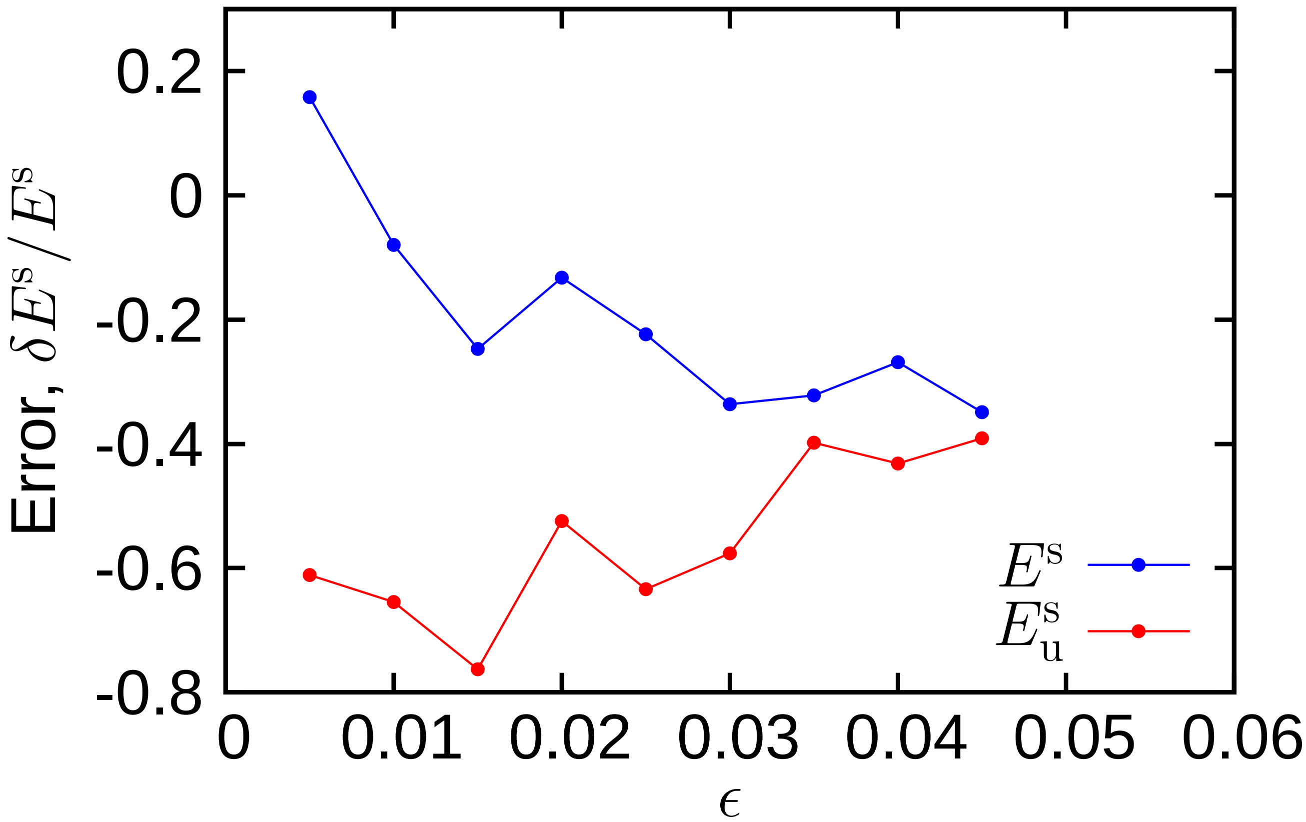
- At larger sample sizes and/or higher imposed curvature, there is an enhancement of strength due to statistical dislocations but GNDs essentially govern the moment-rotation response; A size effect results
- The ratio of stored energy to expended energy increases with decreasing sample size. There is no simple scaling with the dislocation density.
- Neglecting image contributions may lead to “uncontrolled” approximations

Effect of image stresses (tension)



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