Incorporating 3D Mechansims into 2D Dislocation Dynamics

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Background

- Micron-scale Plastic Behaviour:
  - Confined plasticity: e.g. fracture, contact
  - Inelastic deformation in small volumes
- 2D Dislocation Dynamics (“out-of-plane”)

  Lepinoux & Kubin; Gulluoglu et al.; Amodeo & Ghoniem; Lubarda et al.
- 3D Dislocation Dynamics: *(mostly periodic BC)* Devincre & Kubin; Canova et al.; Schwarz; Ghoniem et al.; Zbib et al.; Weygand et al.
- 2D Framework by van der Giessen & Needleman

  Solve BVP with plastic flow $\equiv$ glide of $\perp$’s

  composites; bending; stationary cracks; stress in thin films; fatigue

What?

Include 3D physics in 2D framework

- In discrete dislocation plasticity the long-range interactions are directly taken into account. Short-tange interactions are supplied through constitutive rules.
- Rules are needed in 2D as well as in 3D simulations but more rules are generally needed in 2D.
- More rules to incorporate more physics
  - *line tension*
  - *junction formation*
  - *dynamic sources*
  - *dynamic obstacles*

Why?

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  Real sources are dislocation segments

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- As a consequence, hardening is quite limited
- It is also important to identify the parameters affecting energy storage and dissipation
- 3D Dislocation Dynamics
  performance limited by computing power

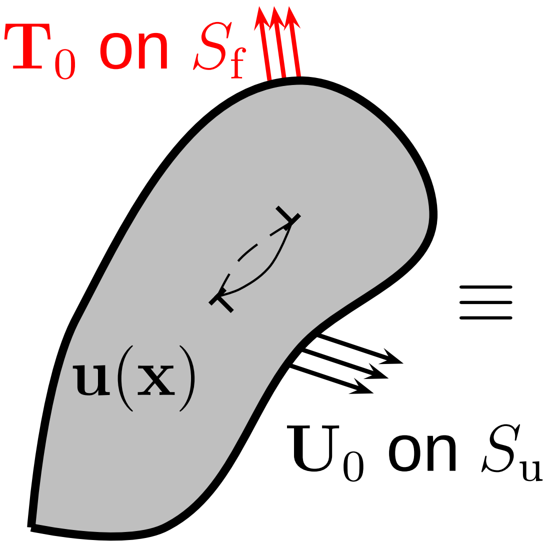
Outline

1. Discrete Dislocation Plasticity
2. 3D Rules in 2D Framework
3. Work-Hardening

   Benzerga, Bréchet, Needleman & Van der Giessen (MSMSE) 2004

4. Relation to geometric hardening and GNDs
5. The Stored Energy of Cold Work

Discrete Dislocation Plasticity



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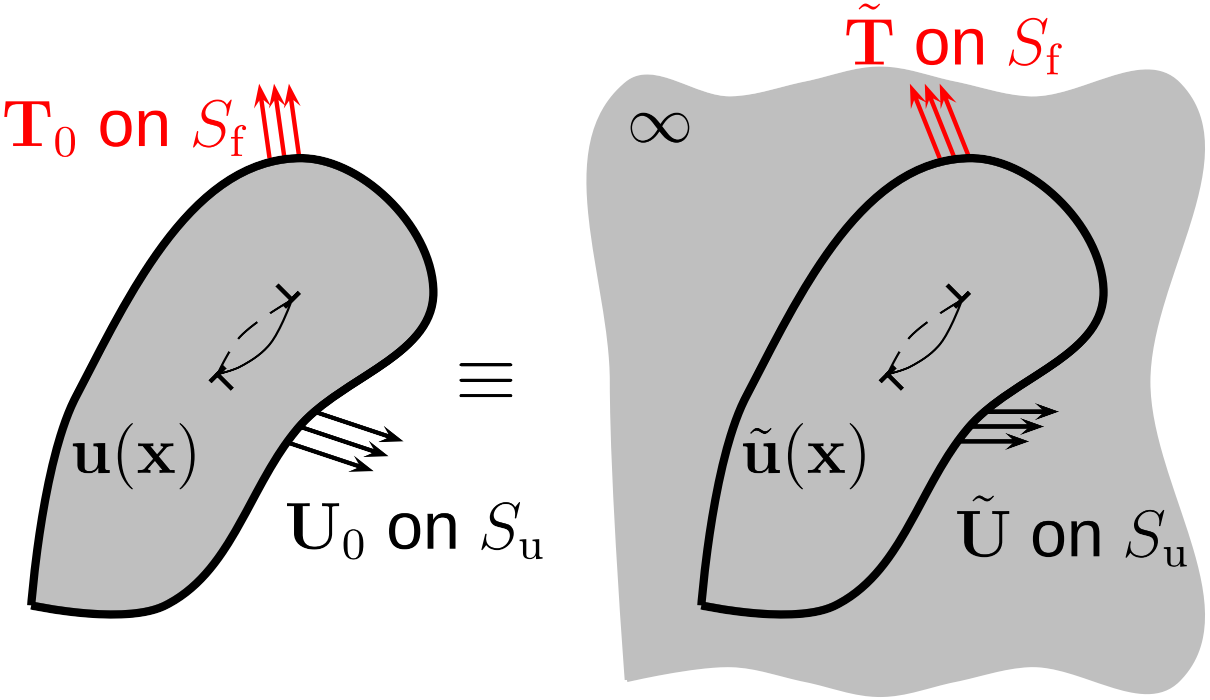

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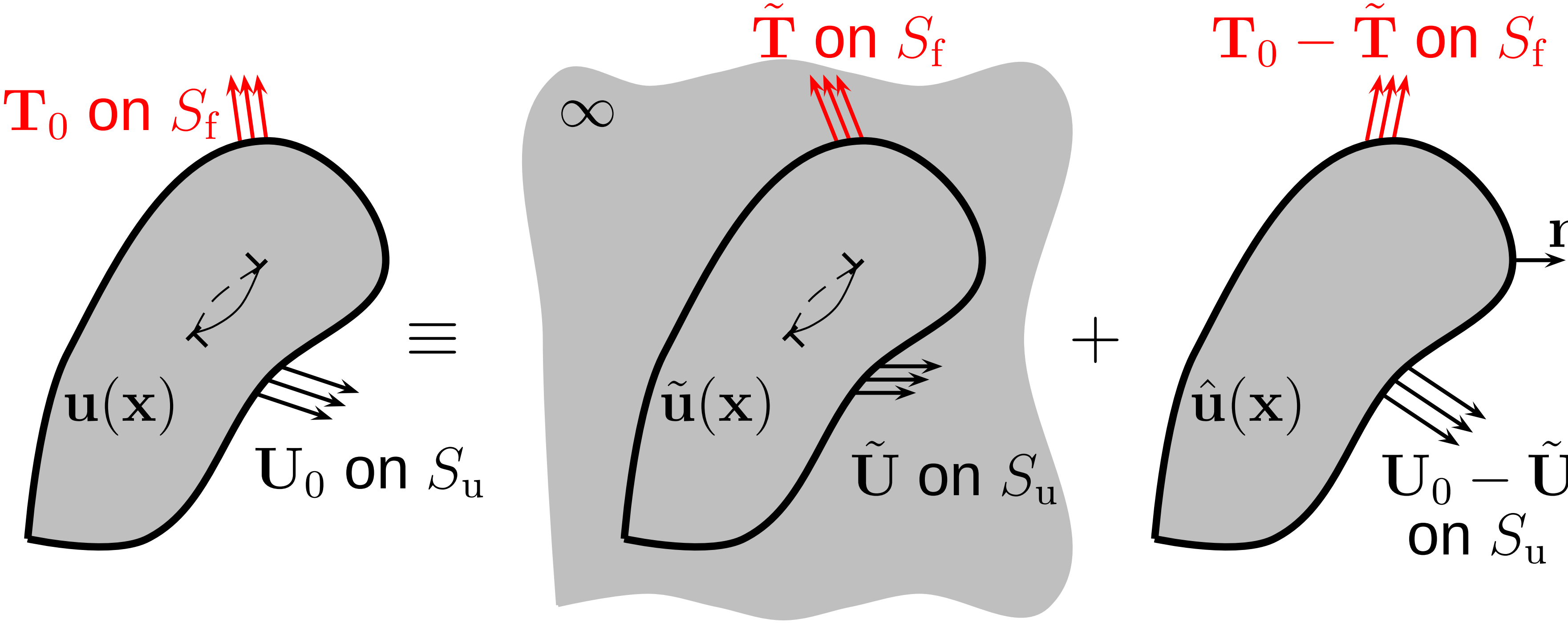

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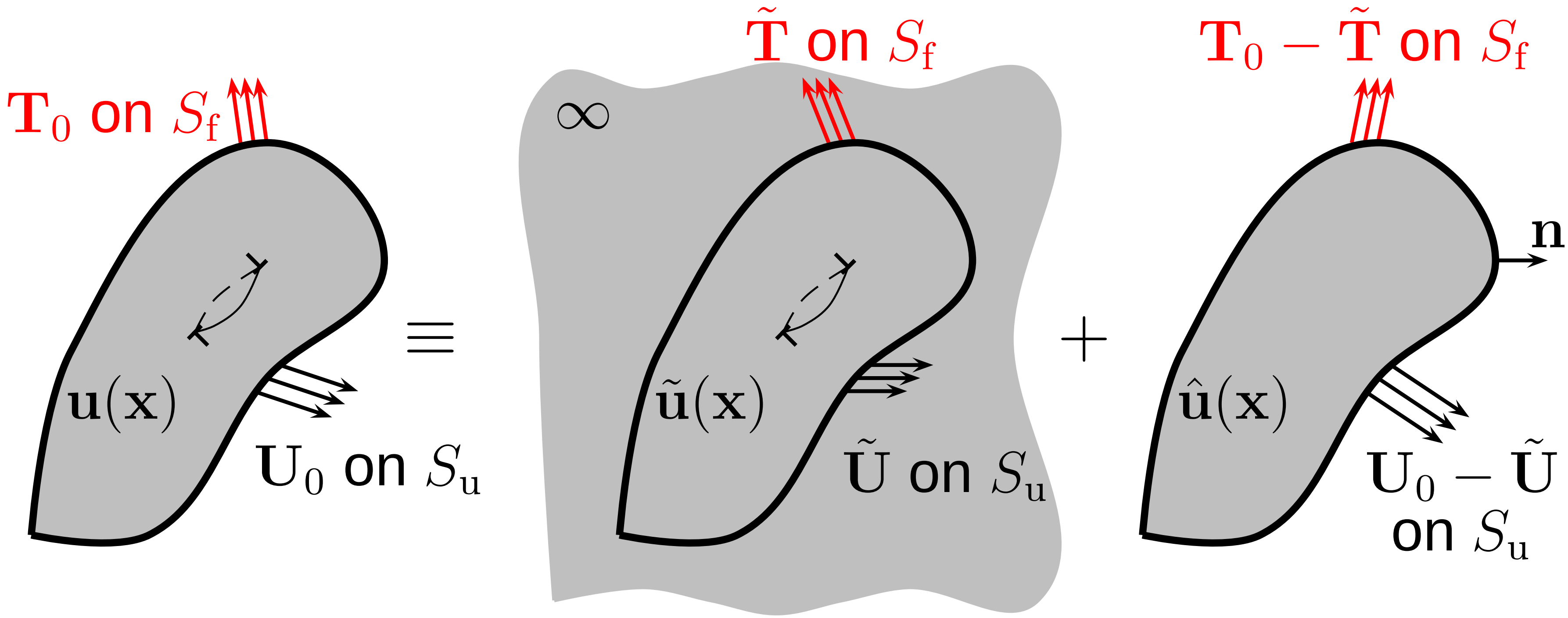

$$\nabla \cdot \hat{\boldsymbol{\sigma}} = \mathbf{0} \quad ; \quad \hat{\boldsymbol{\epsilon}} = \nabla \otimes \hat{\mathbf{u}} \quad ; \quad \hat{\boldsymbol{\sigma}} = \boldsymbol{\mathcal{L}} : \hat{\boldsymbol{\epsilon}} \qquad \text{for } \mathbf{x} \in V$$

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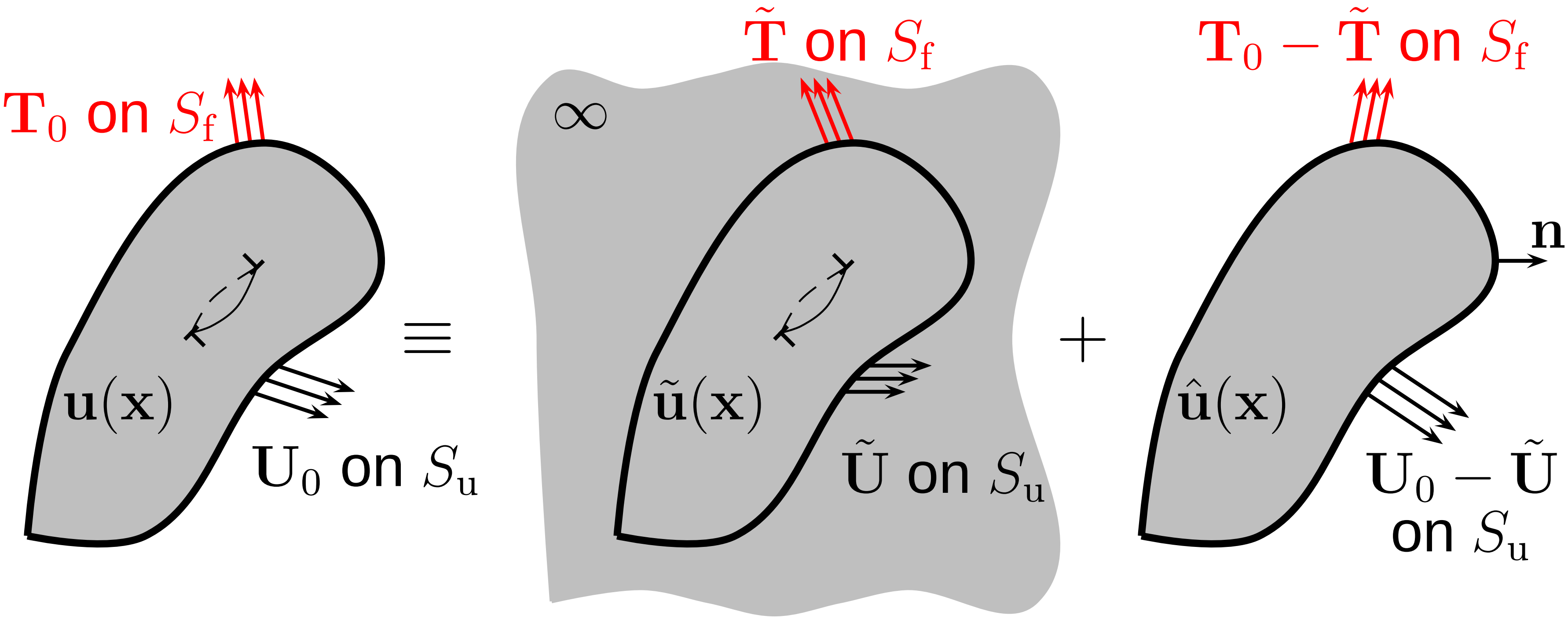

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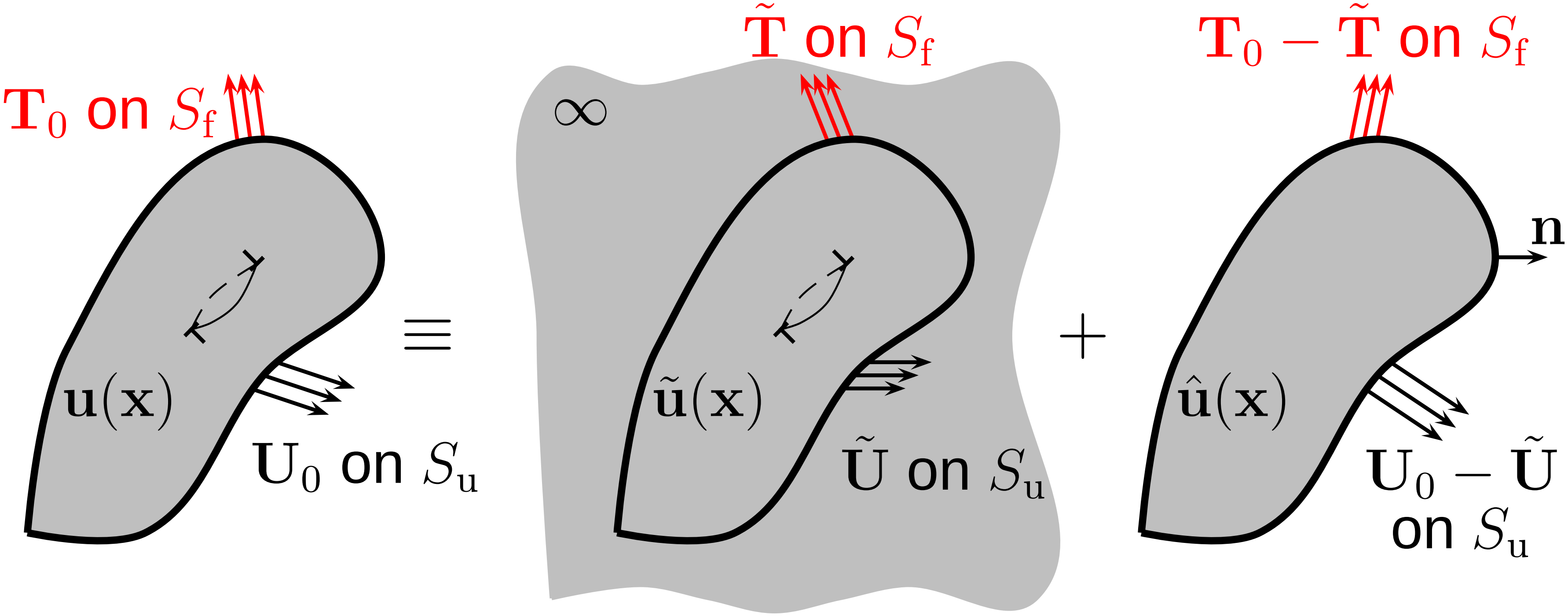
$$\mathbf{n} \cdot \hat{\boldsymbol{\sigma}} = \mathbf{T}_0 - \mathbf{n} \cdot \tilde{\boldsymbol{\sigma}} \quad \text{for } \mathbf{x} \in S_\mathrm{f} \quad ; \quad \hat{\mathbf{u}} = \mathbf{U}_0 - \tilde{\mathbf{U}} \quad \text{for } \mathbf{x} \in S_\mathrm{u}$$

Discrete Dislocation Plasticity



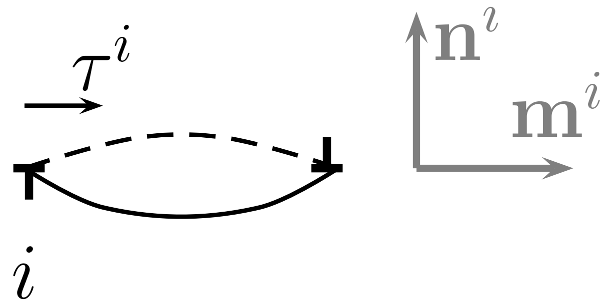
$$\mathbf{u}(\mathbf{x}) = \tilde{\mathbf{u}}(\mathbf{x}) + \hat{\mathbf{u}}(\mathbf{x}) \quad ; \quad \boldsymbol{\epsilon} = \tilde{\boldsymbol{\epsilon}} + \hat{\boldsymbol{\epsilon}} \quad ; \quad \boldsymbol{\sigma} = \tilde{\boldsymbol{\sigma}} + \hat{\boldsymbol{\sigma}}$$

2D Dislocation Dynamics

- **Nucleation:** Static initial sources of constant strength and nucleation time.

- **The Peach–Koehler force**:

$$f^i = \mathbf{n}^i \cdot \left(\hat{\boldsymbol{\sigma}} + \sum_{j \neq i} \boldsymbol{\sigma}^j \right) \cdot \mathbf{b}^i$$



$$b^i \equiv (\mathbf{b}^i \times \mathbf{t}^i) \cdot \mathbf{n}^i$$

- **Viscous drag**:

$$B v^i = f^i \approx \tau^i \, b^i$$

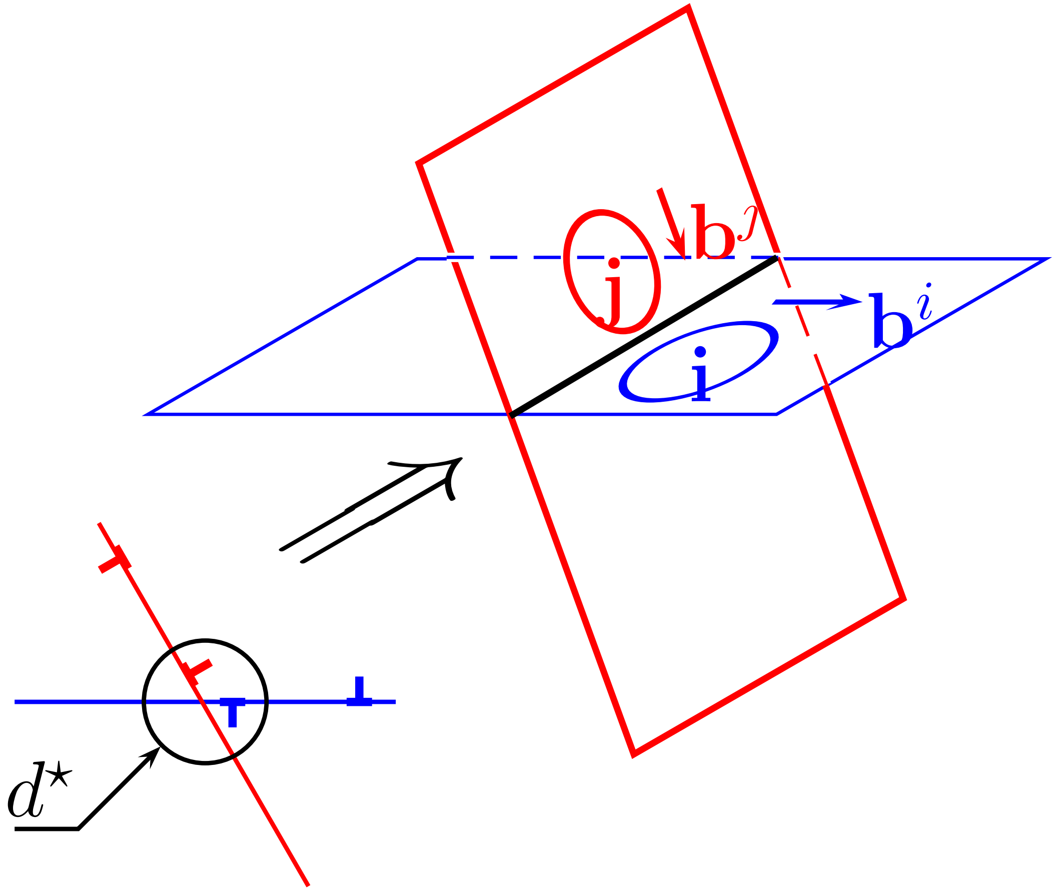
B: phonon drag coefficient

Incorporating 3D Mechanisms into 2D Dislocation Dynamics

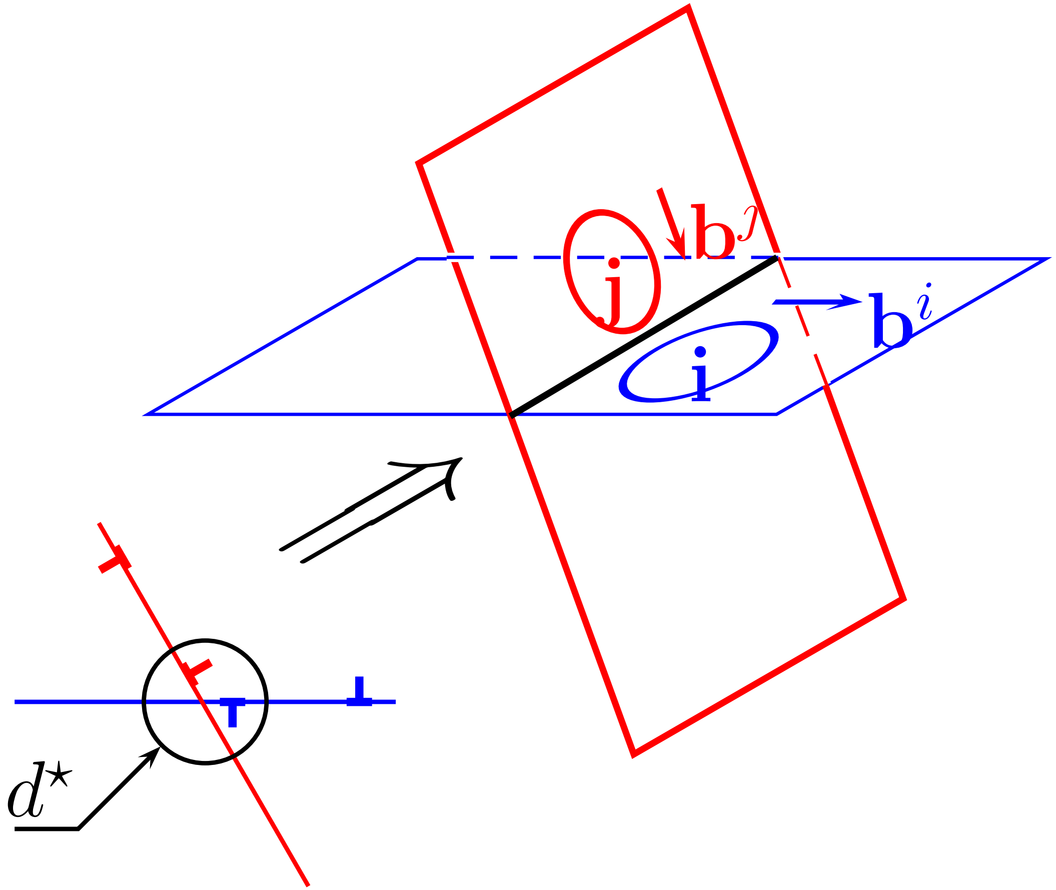
Constitutive rules are needed for:

- Junction Formation
- Dynamic Sources
- Dynamic Obstacles
- Higher-order Interactions
- Line Tension

Junction Formation

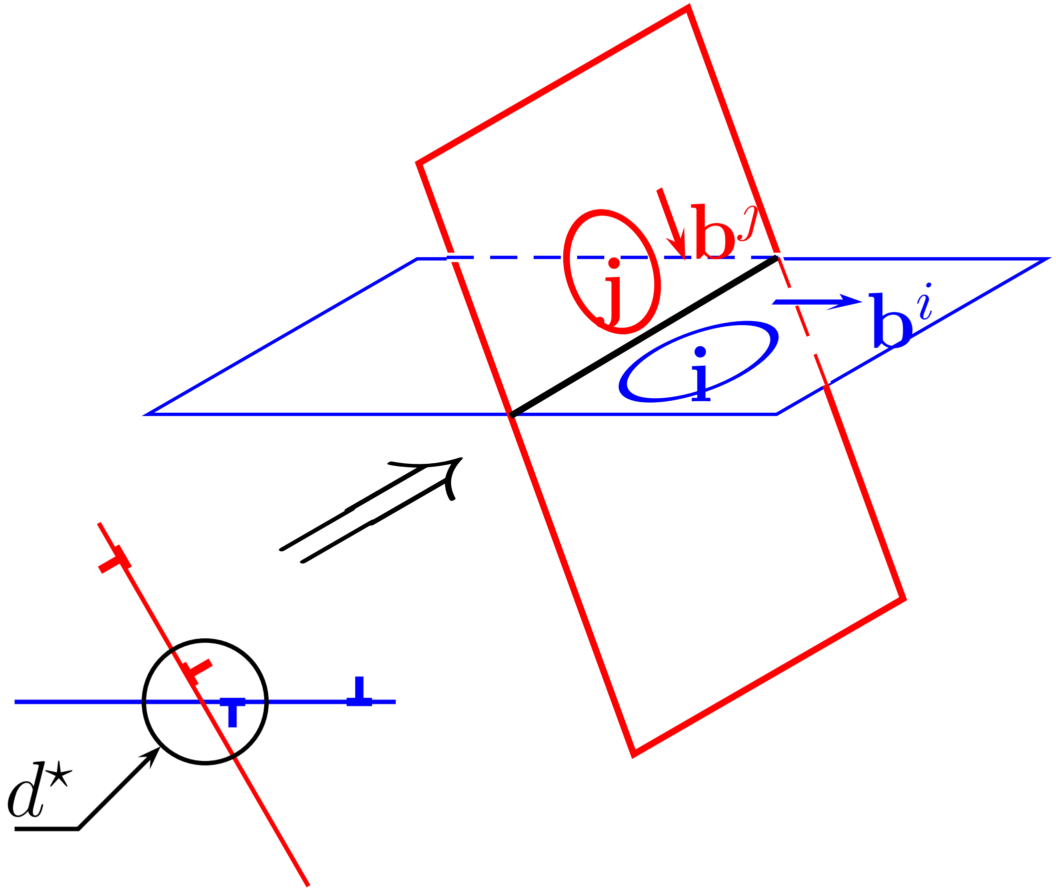


Junction Formation



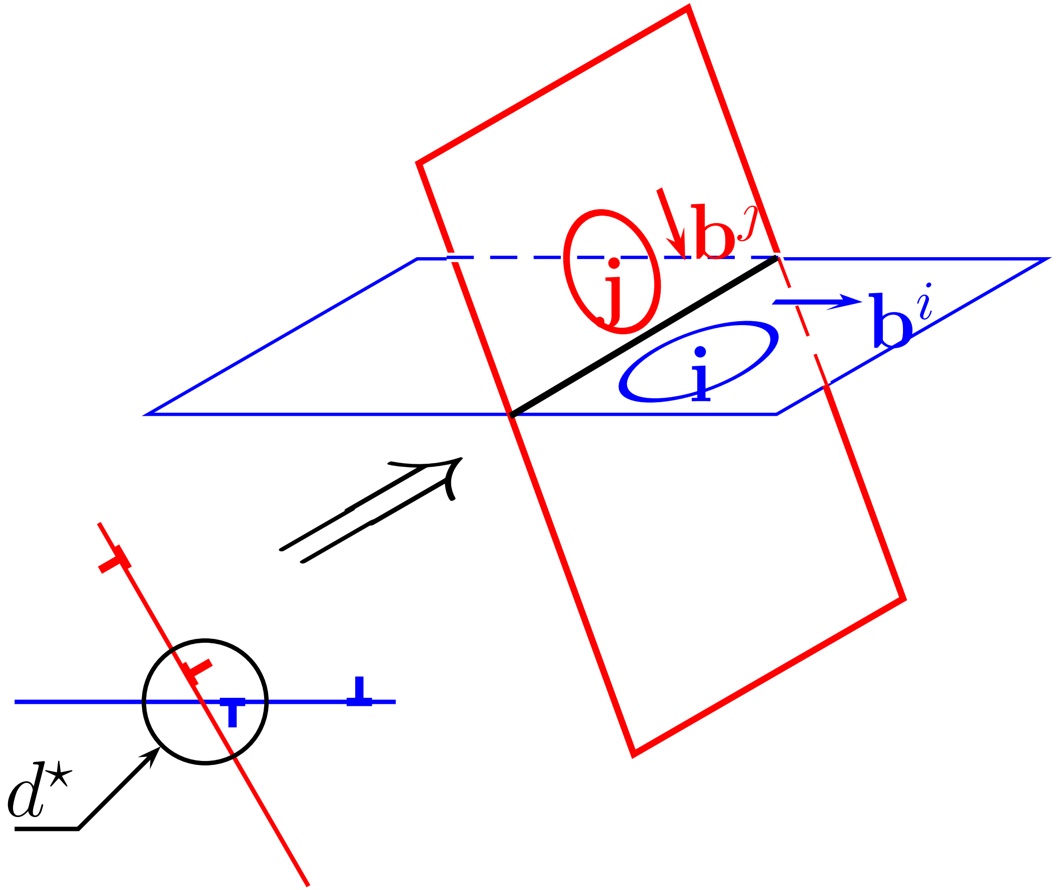
A stable junction is an *anchoring point*...

Junction Formation



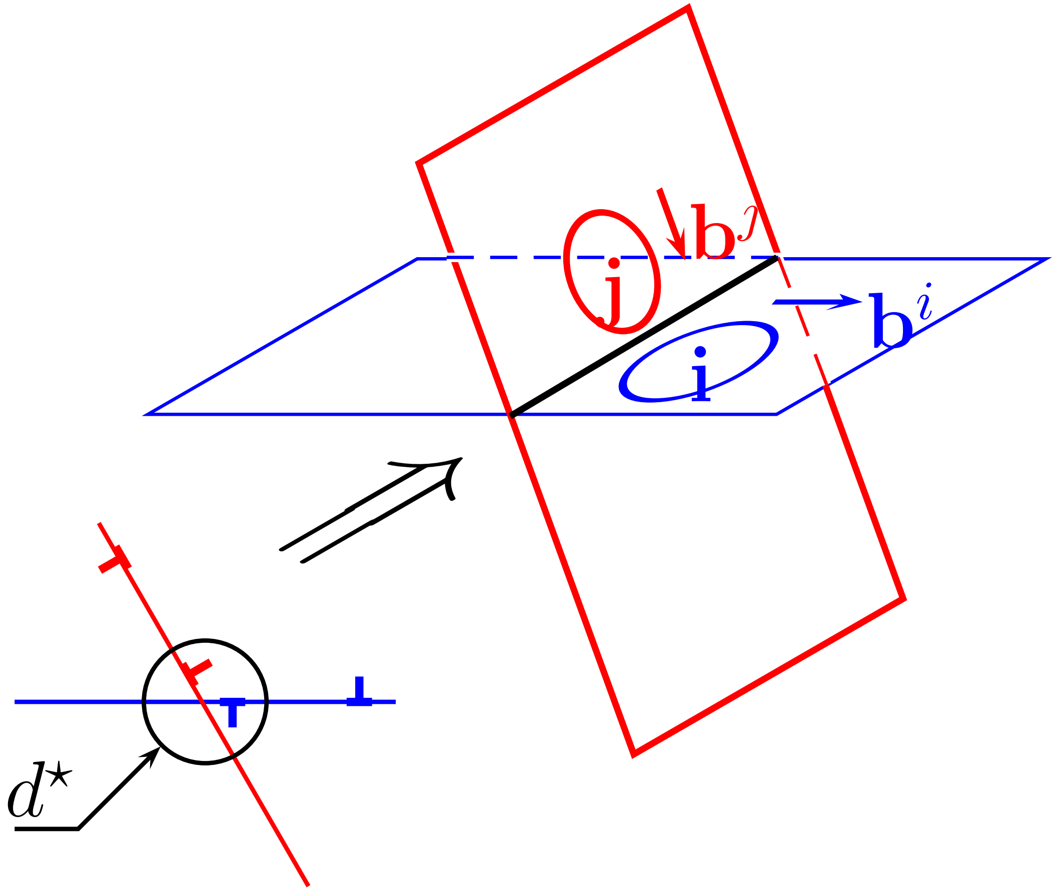
A breakable junction is an *obstacle*...

Junction Formation



Presumably, cross-slip favors anchoring points...

Junction Formation



in 2D, anchoring points have formation probability p.

Dynamic Sources

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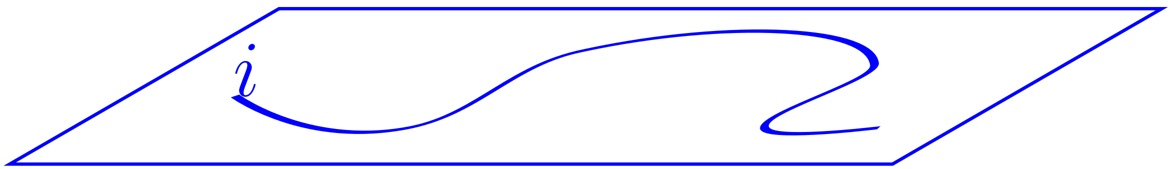

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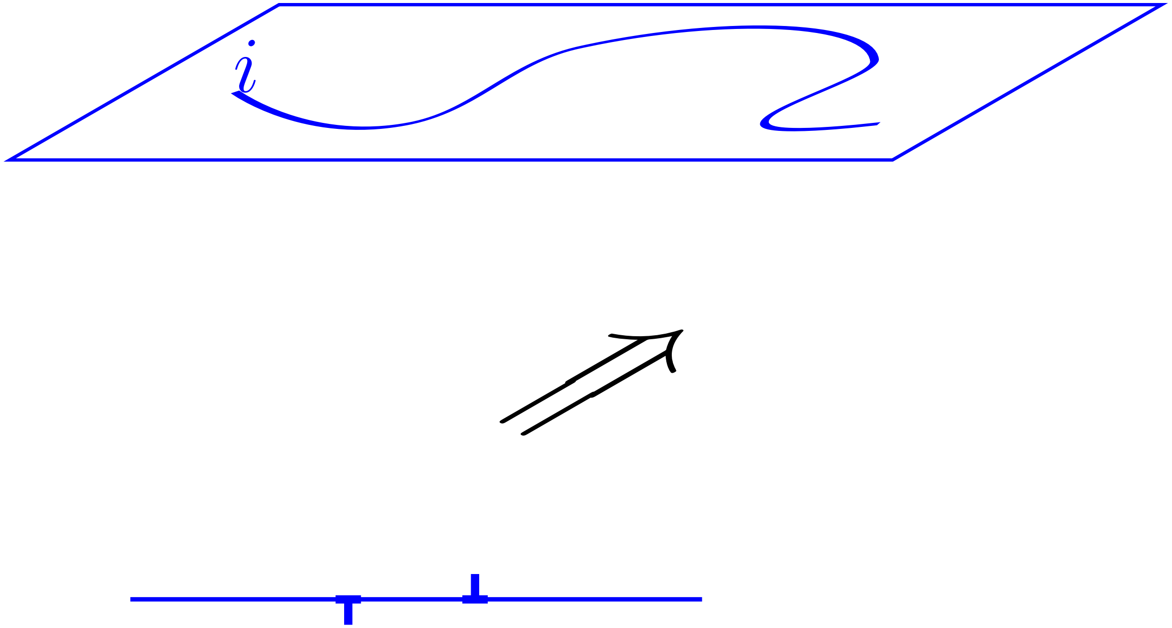

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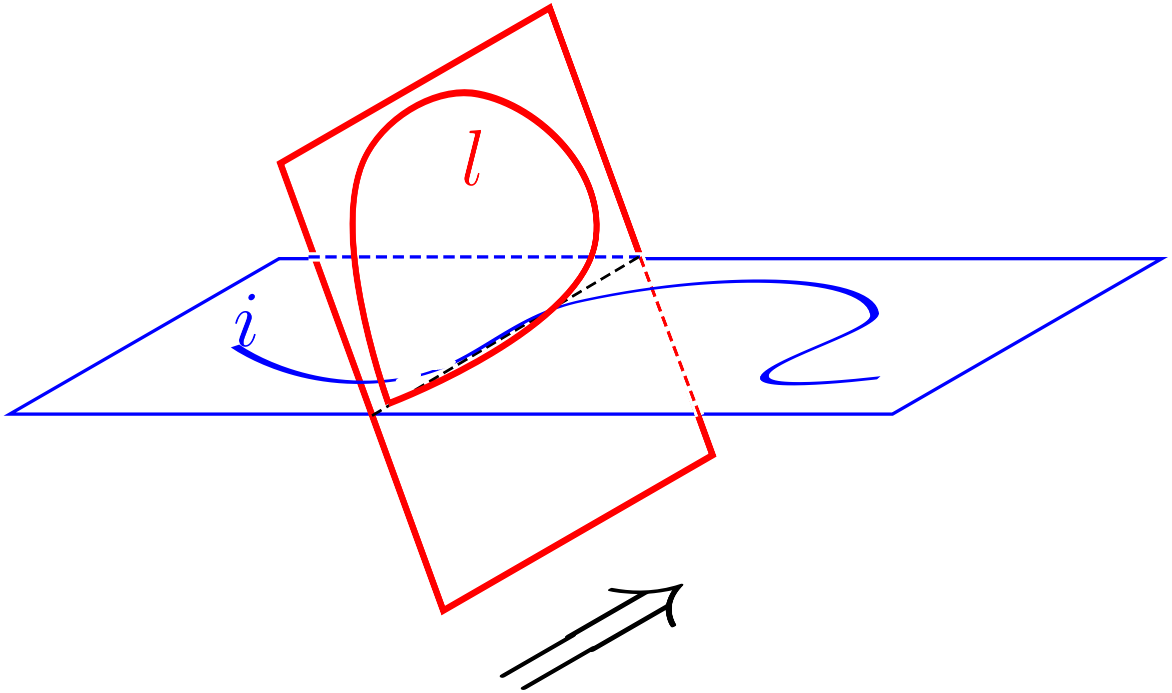

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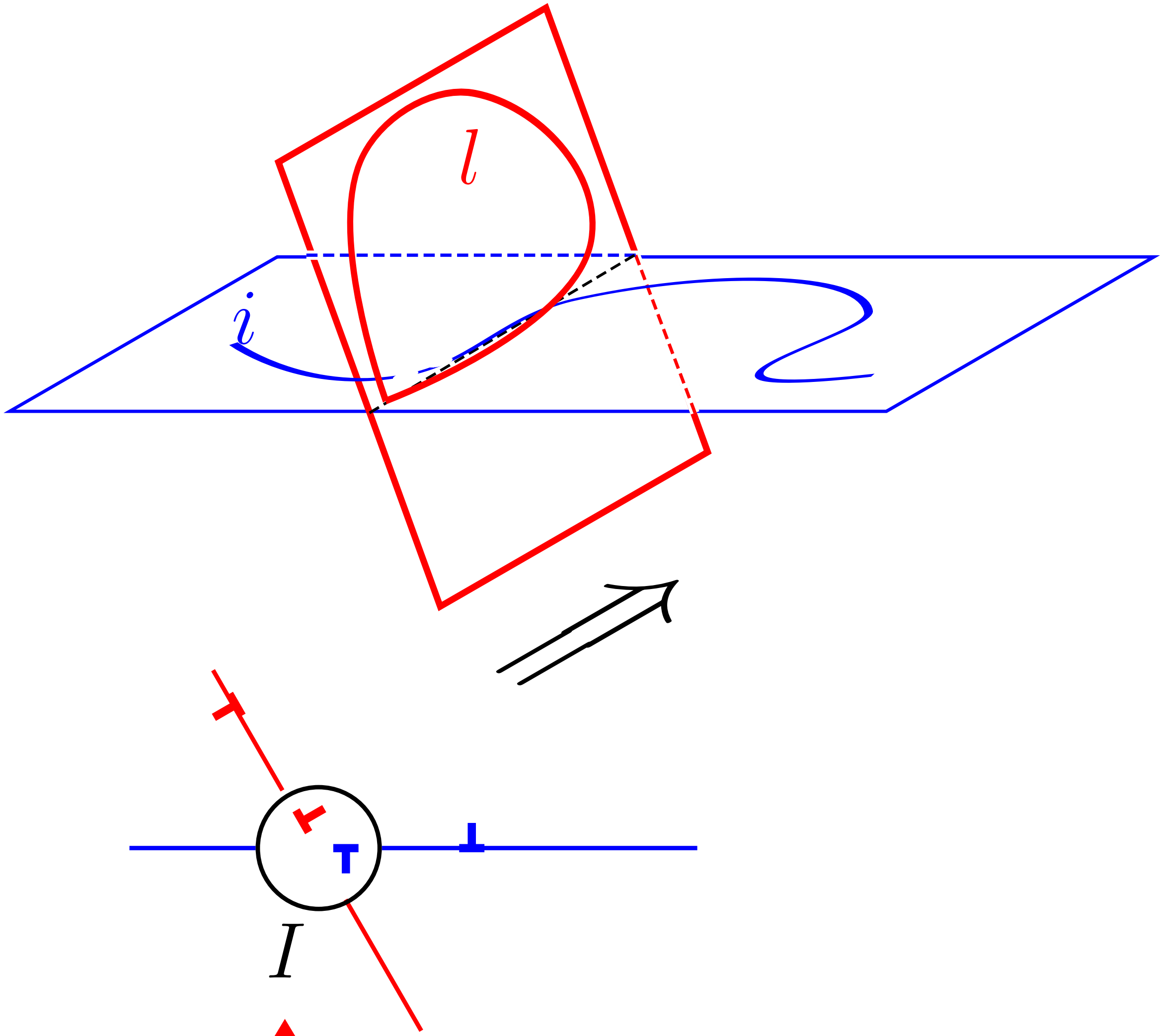

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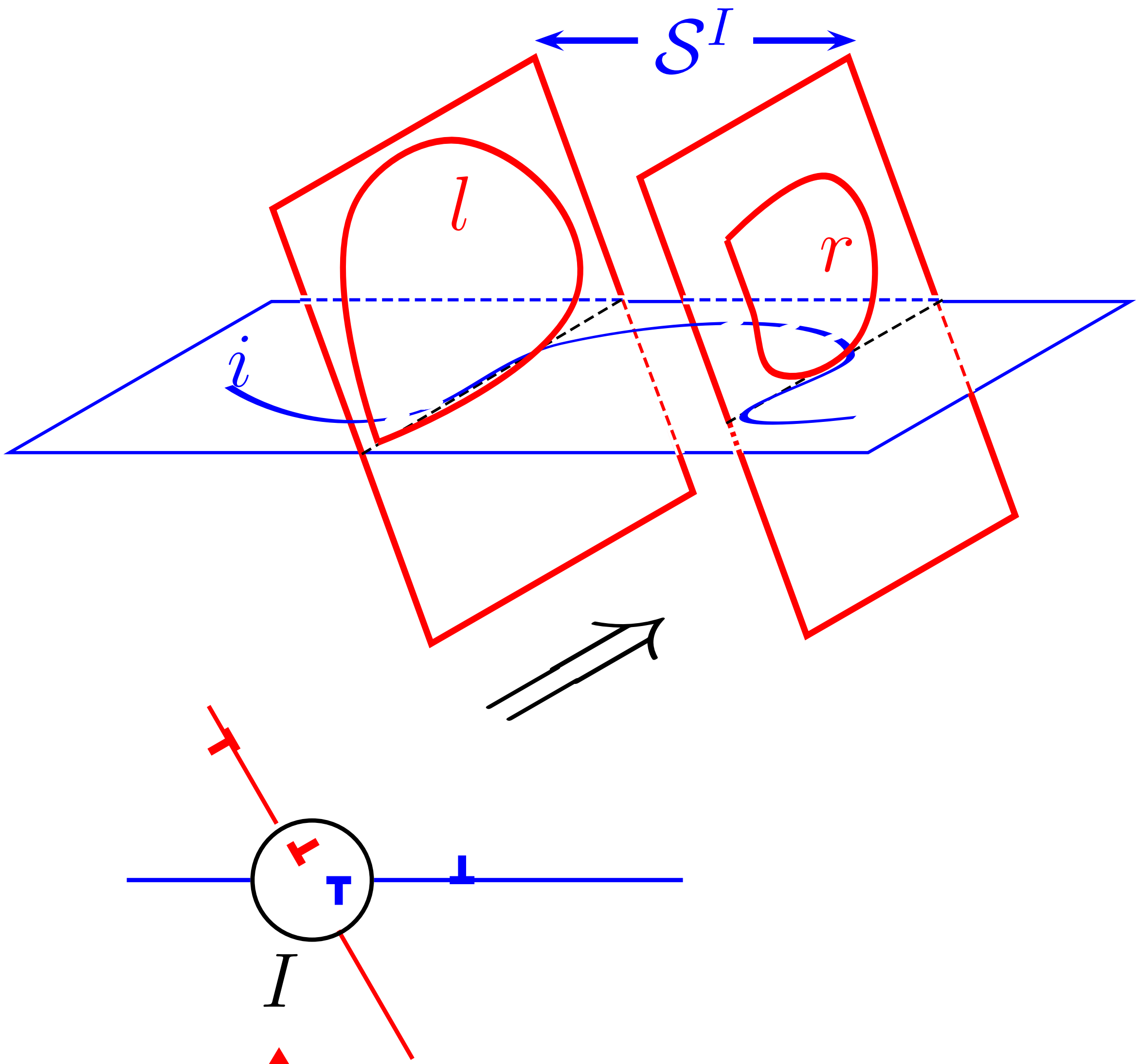

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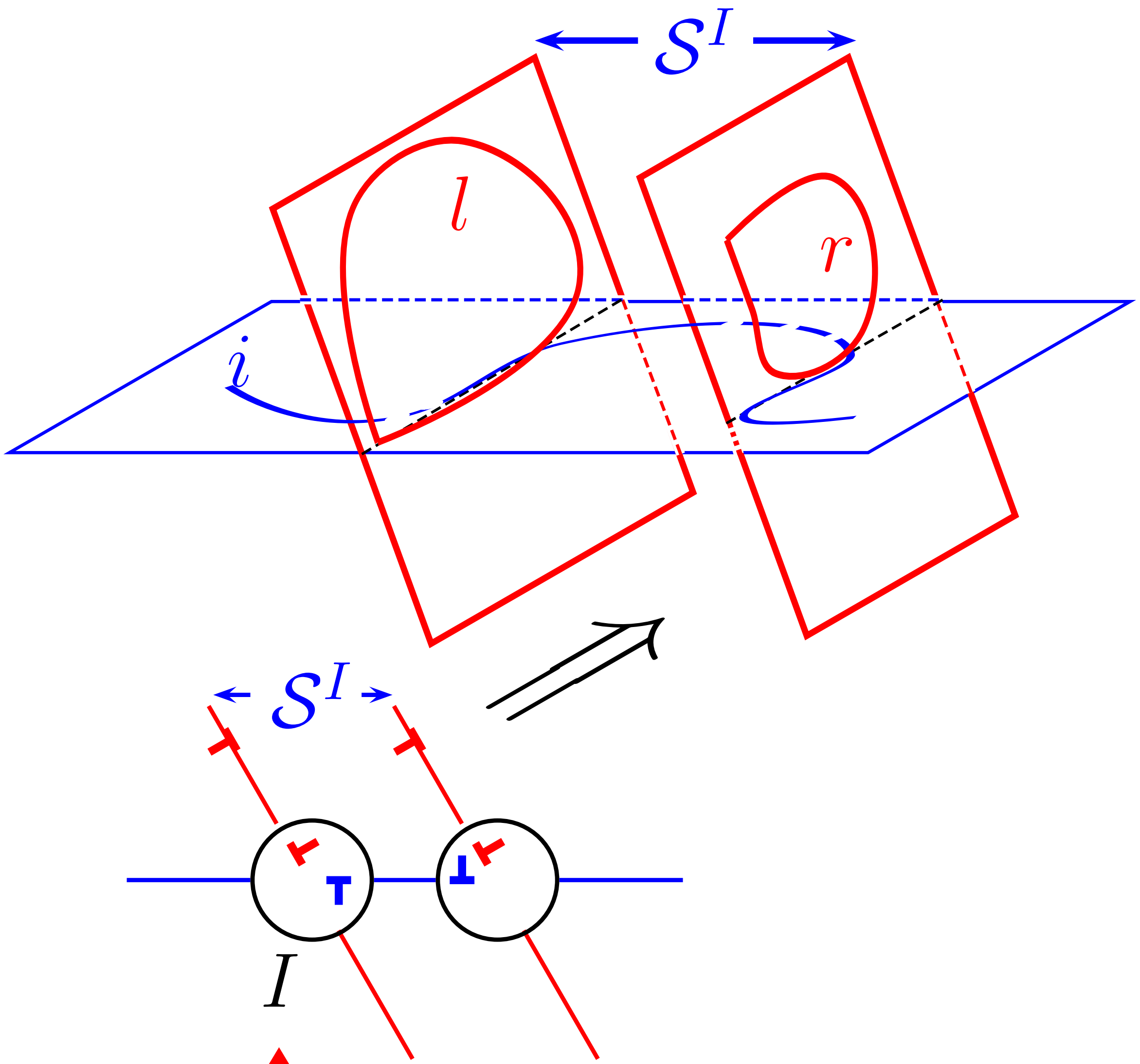

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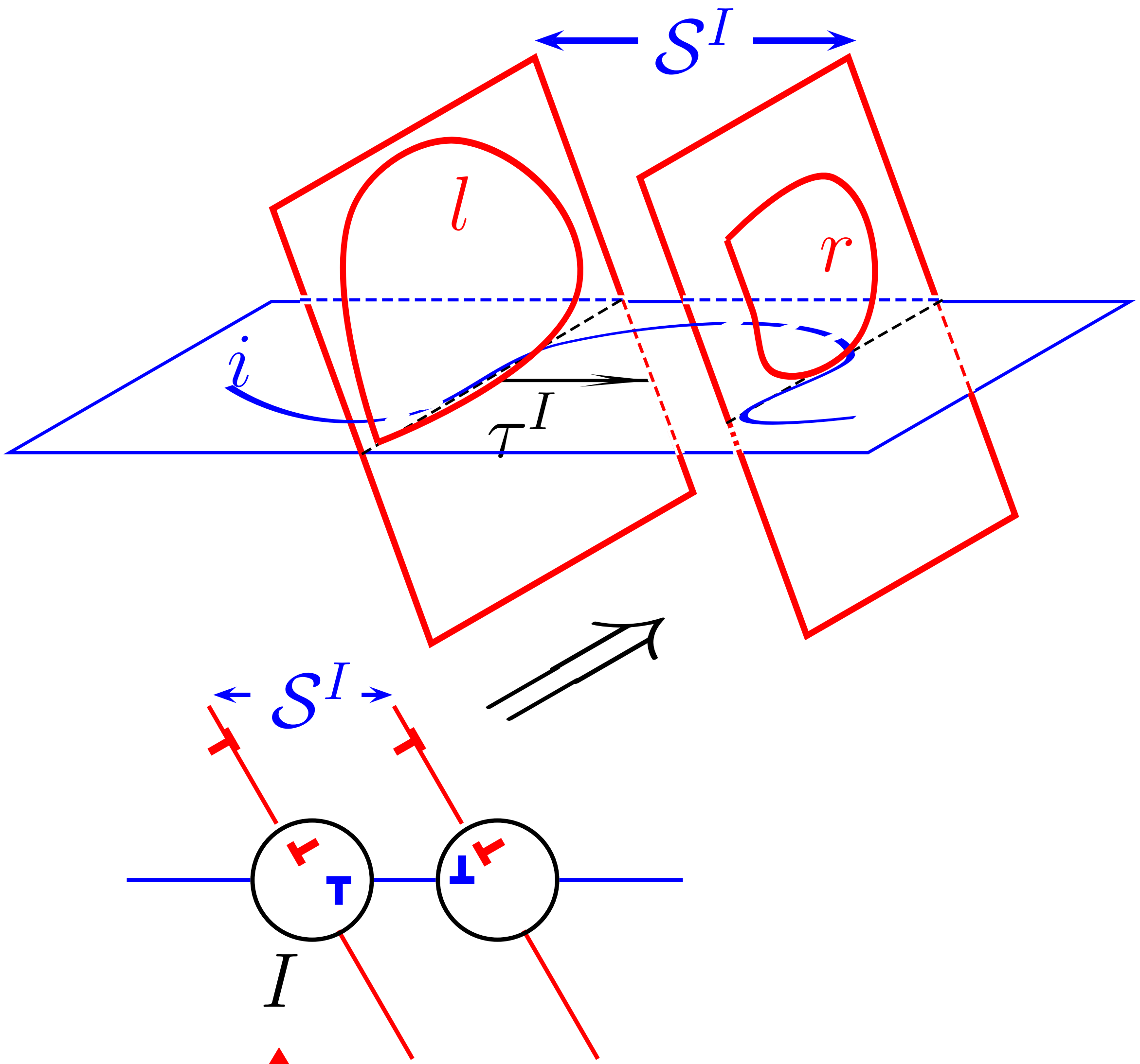

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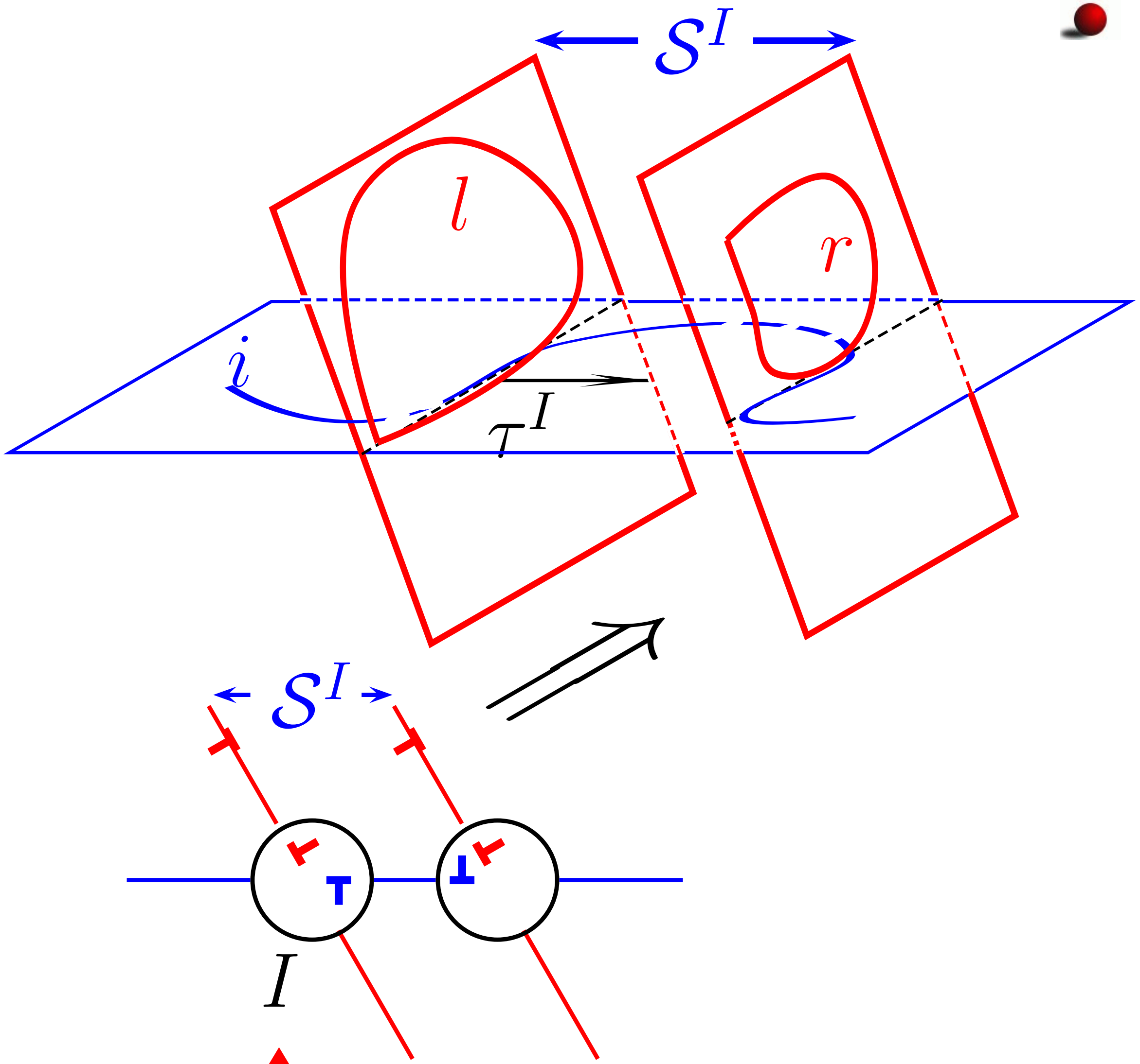

- **Critical Stress**

$$\tau^I_{\text{nuc}} = \beta \frac{\mu b^i}{\mathcal{S}^I}$$

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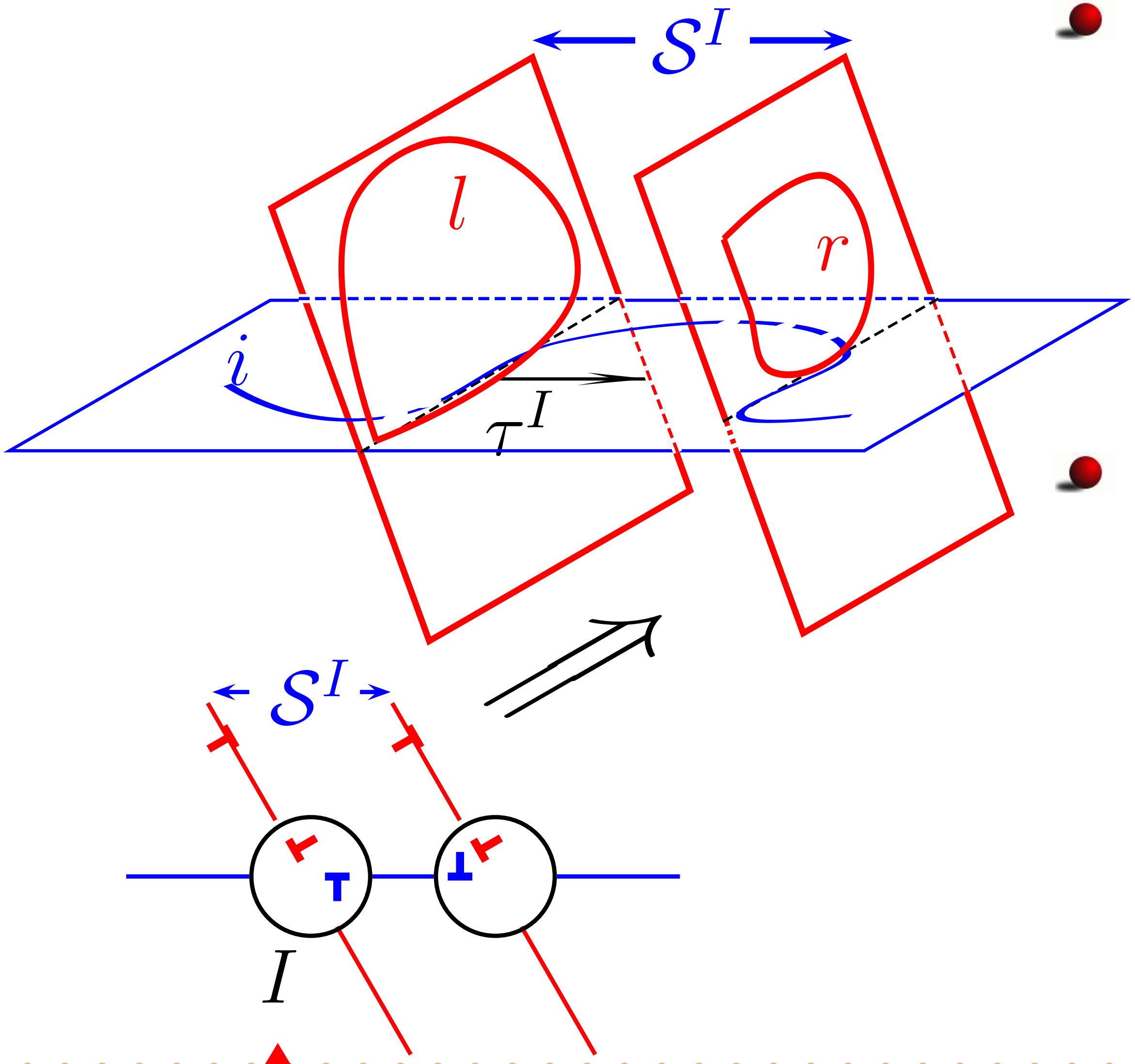

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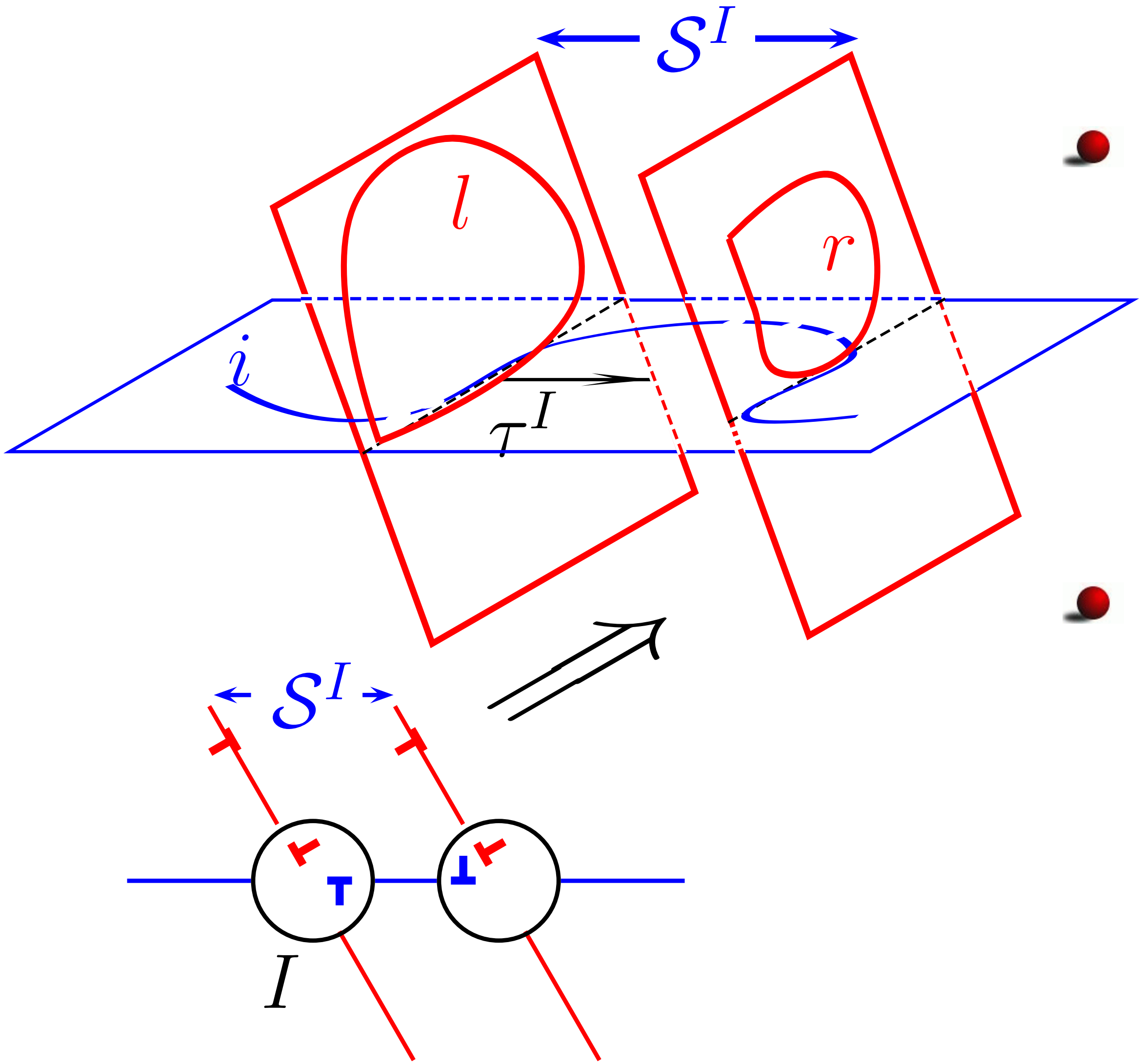

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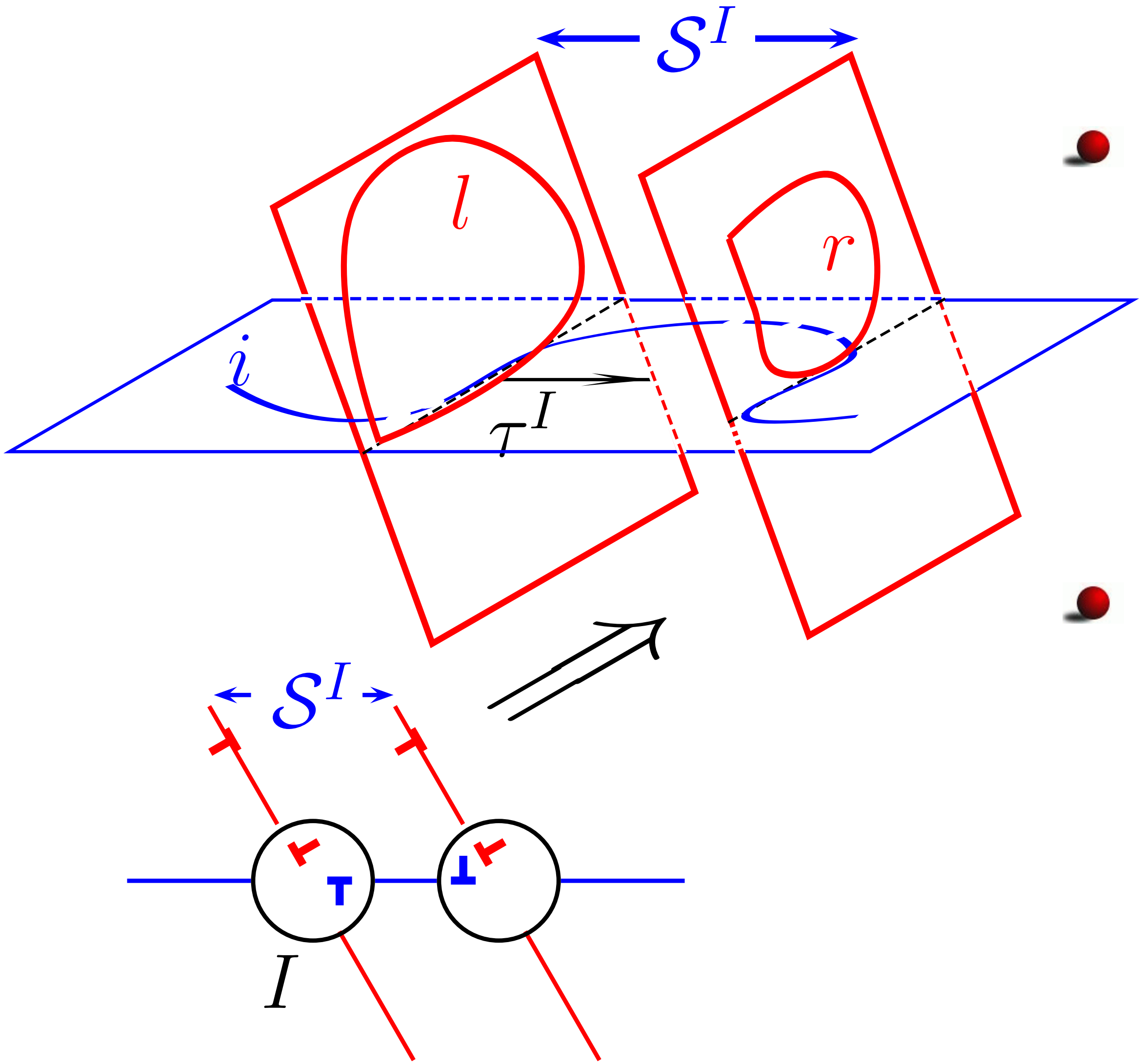

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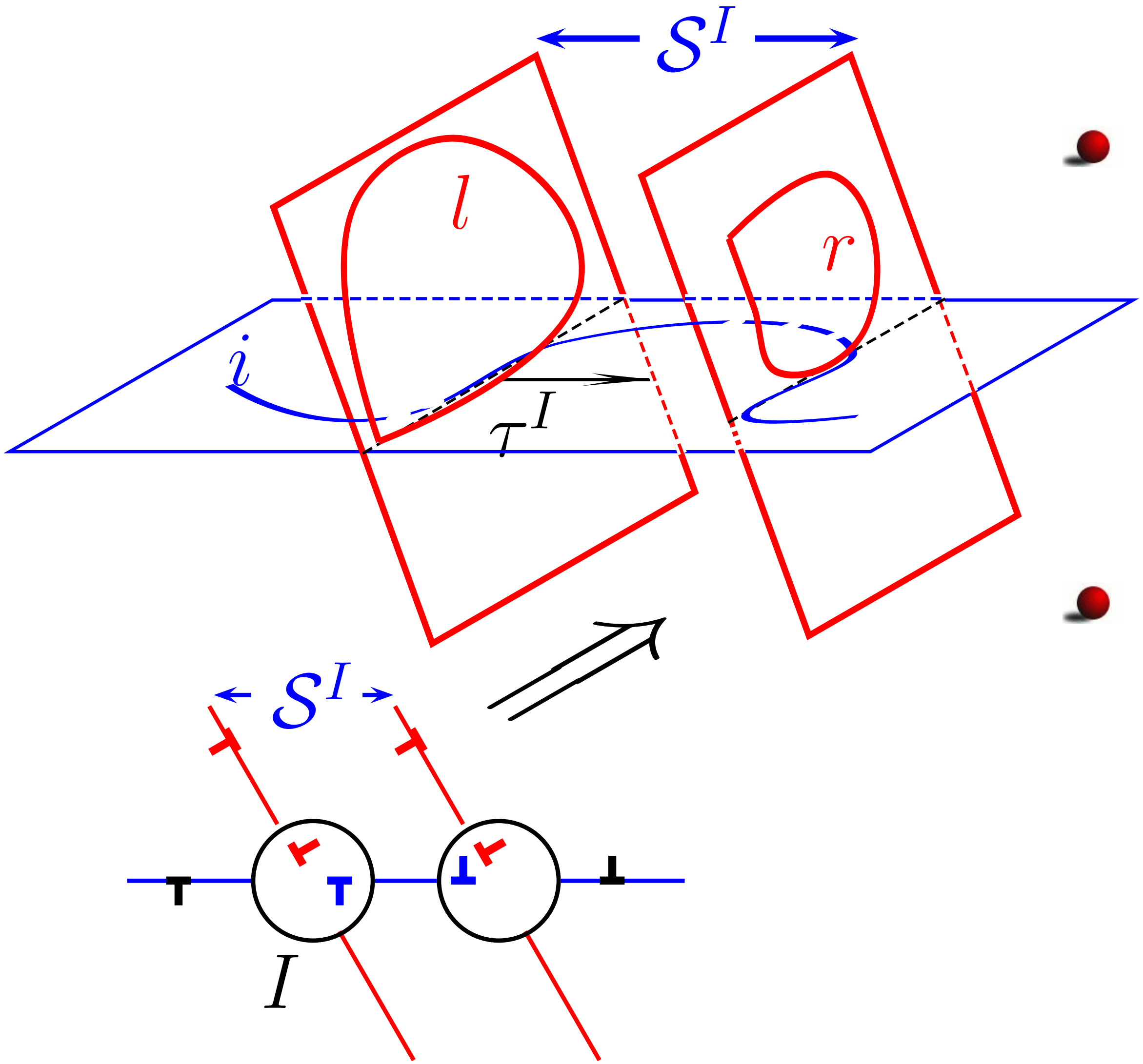

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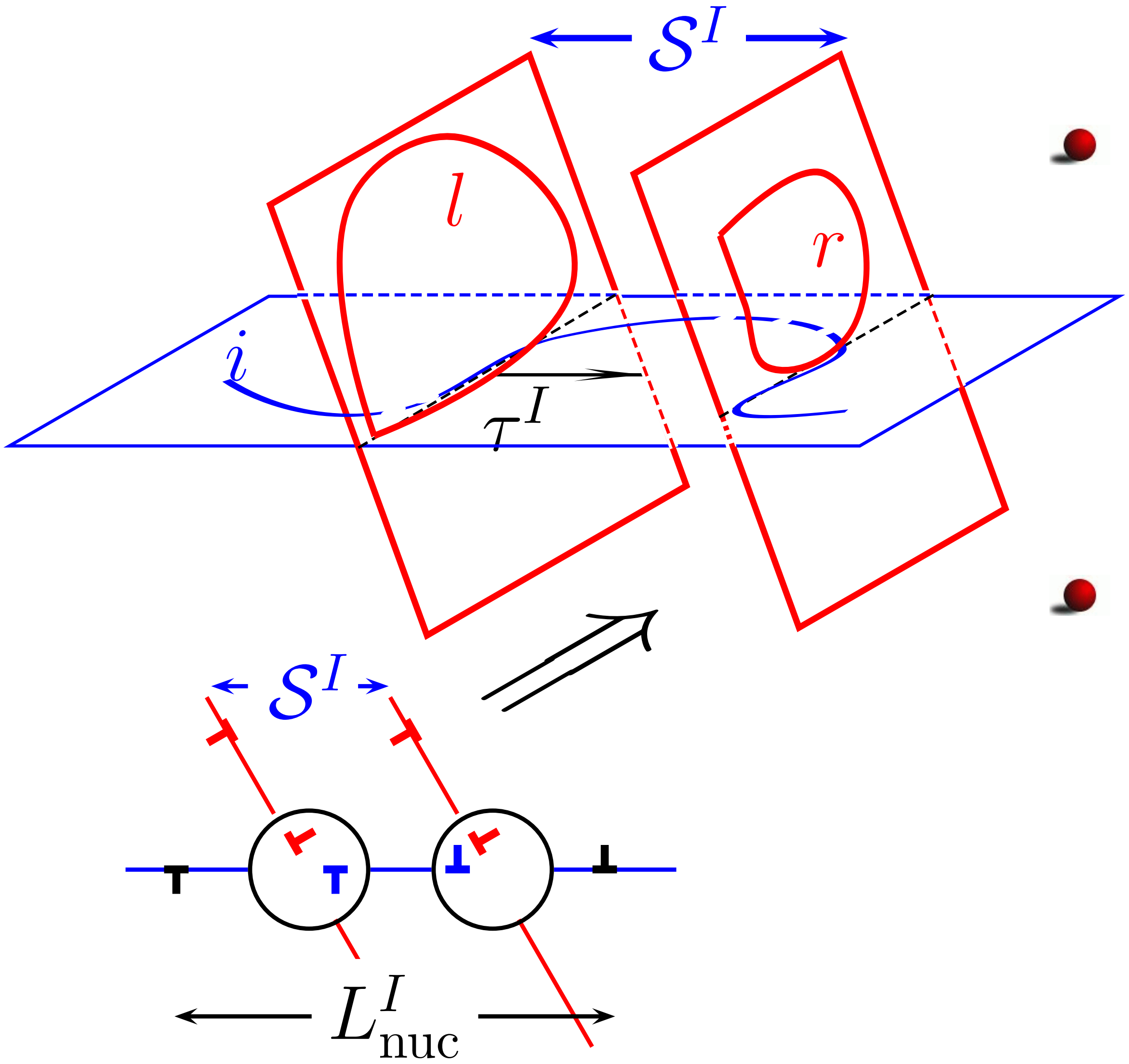

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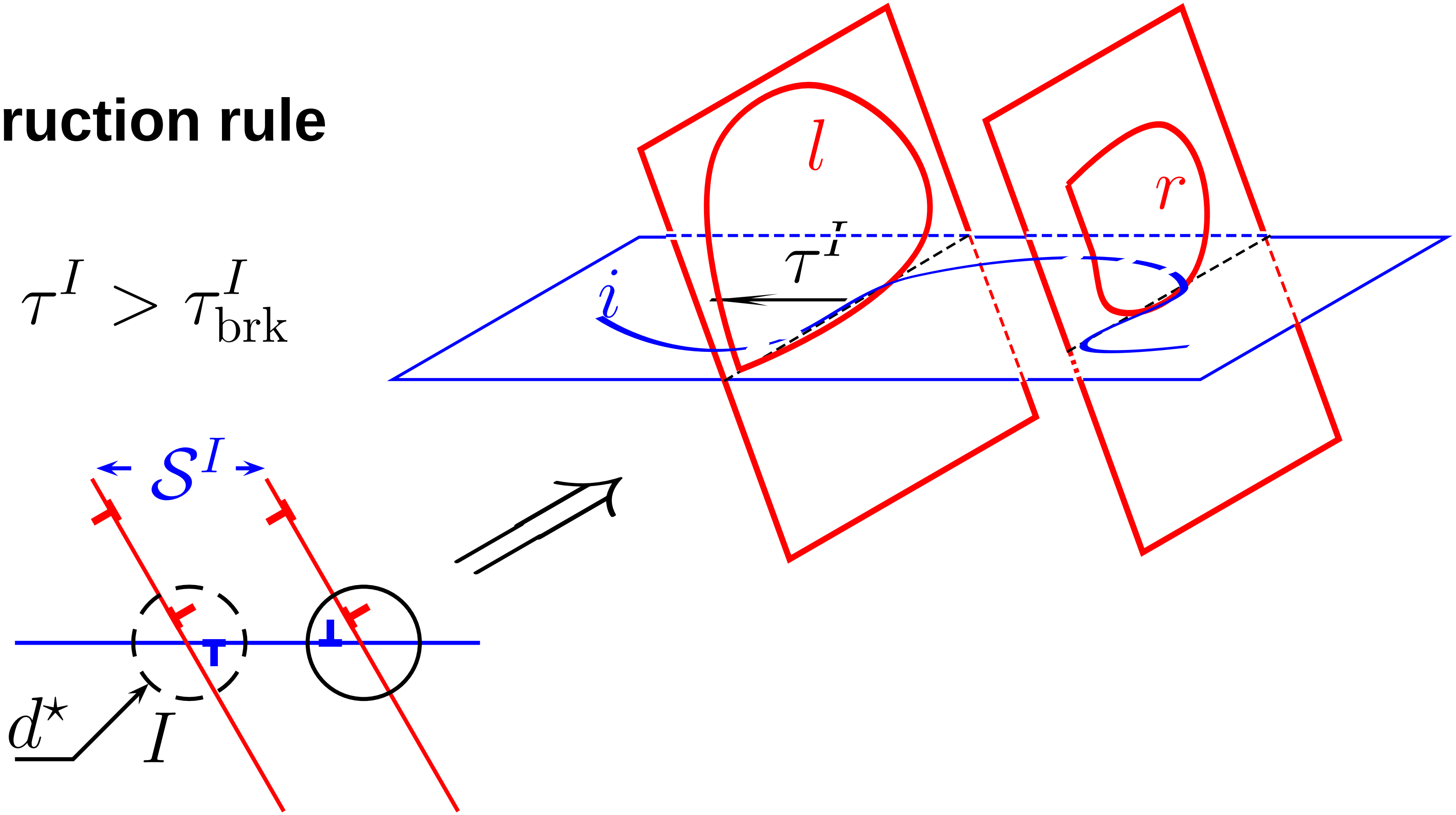
Dynamic Obstacles

- **Destruction rule**

$$\frac{f^I}{b^i} = \tau^I > \tau^I_{\text{brk}}$$

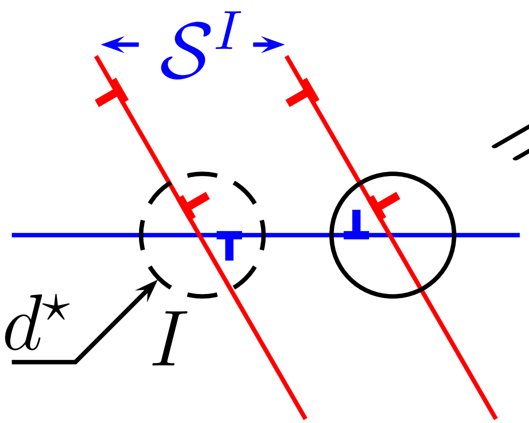


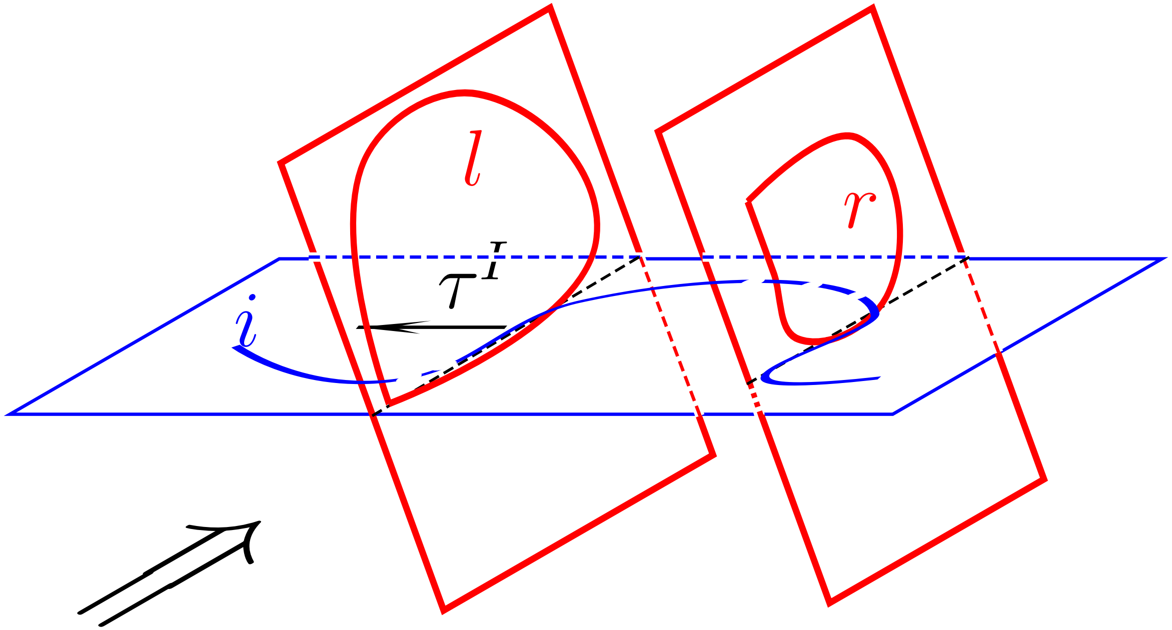
$\mathcal{S}^I \equiv$ nearest neighbor spacing (on either slip plane)

Dynamic Obstacles

- **Breaking Stress**

$$\tau^I_{\mathrm{brk}} \equiv \beta\mu\,\frac{b^i}{\mathcal{S}^I}$$





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Interaction junction/dislocation

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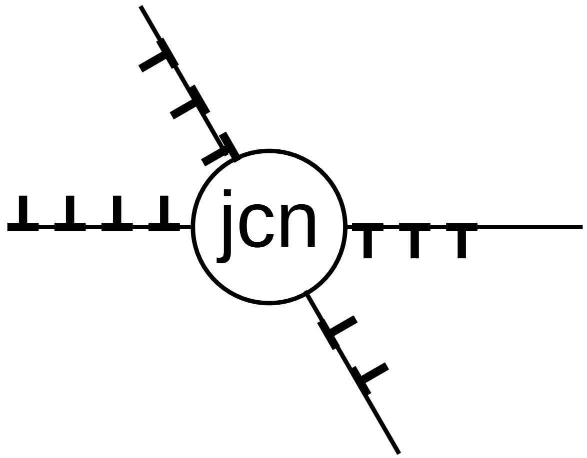

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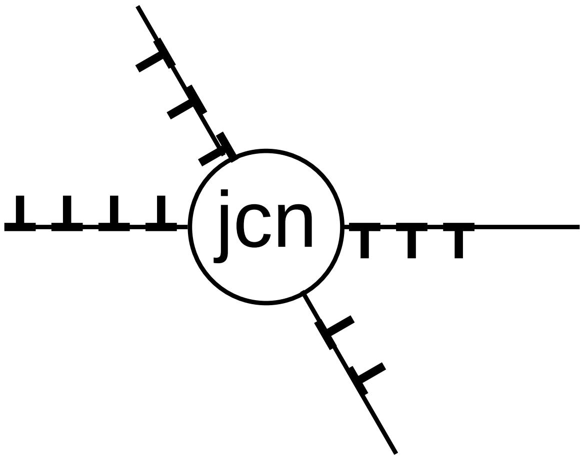
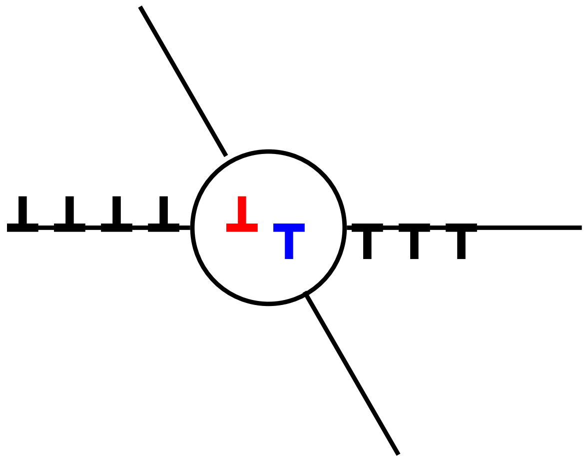


- **Special behavior of sources:**
  - Rule of destruction by annihilation

vs.



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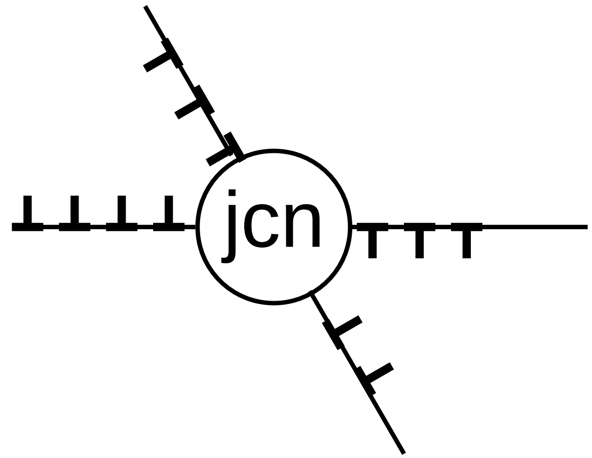

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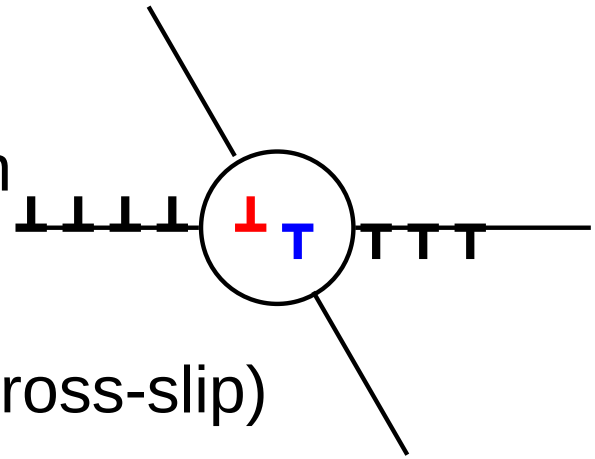

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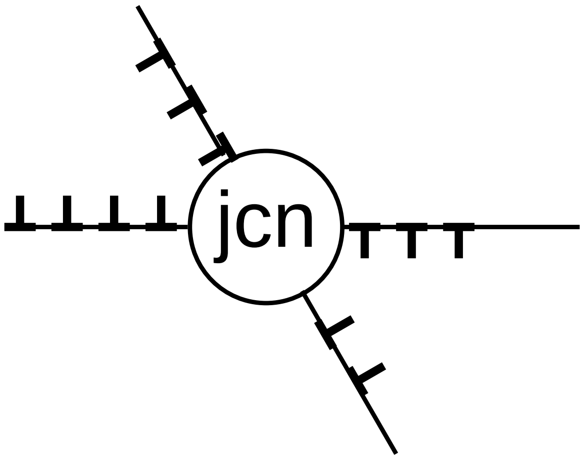

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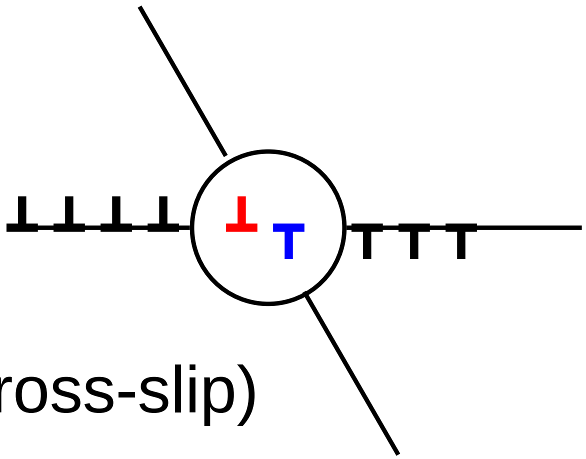

Annihilation & Line Tension

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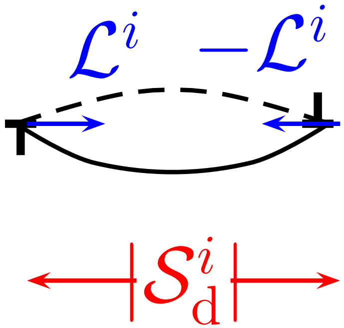

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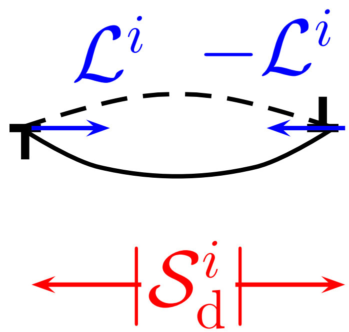

- **Change of partner:**

Annihilation & Line Tension

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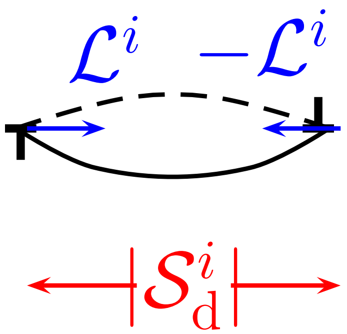
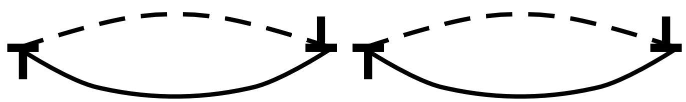


- **Change of partner:**
  - *after annihilation*



Annihilation & Line Tension

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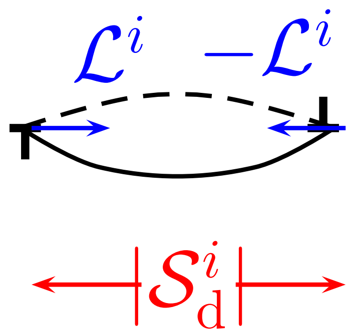
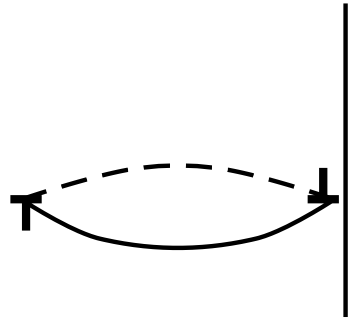


$$\mathcal{L}^i = -\alpha \frac{\mu |b^i|}{\mathcal{S}_{\mathrm{d}}^i}$$

- **Change of partner:**
  - *after annihilation*
  - *exiting at free surface*



Dislocation Glide

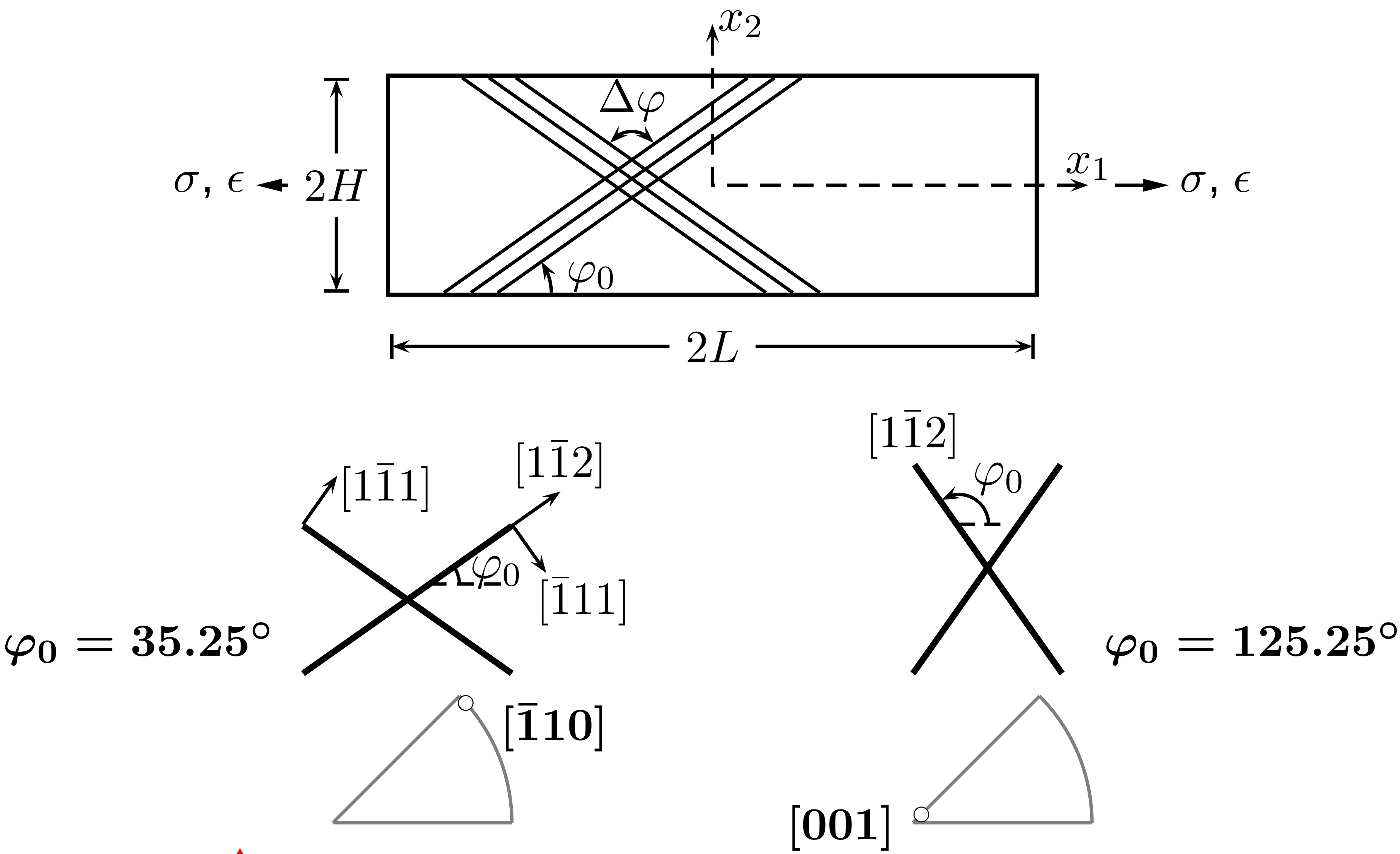
Viscous drag generalized into:

$$Bv^i = \left(\tau^i - \tau_\mathrm{P} + \mathcal{L}^i\right) b^i$$

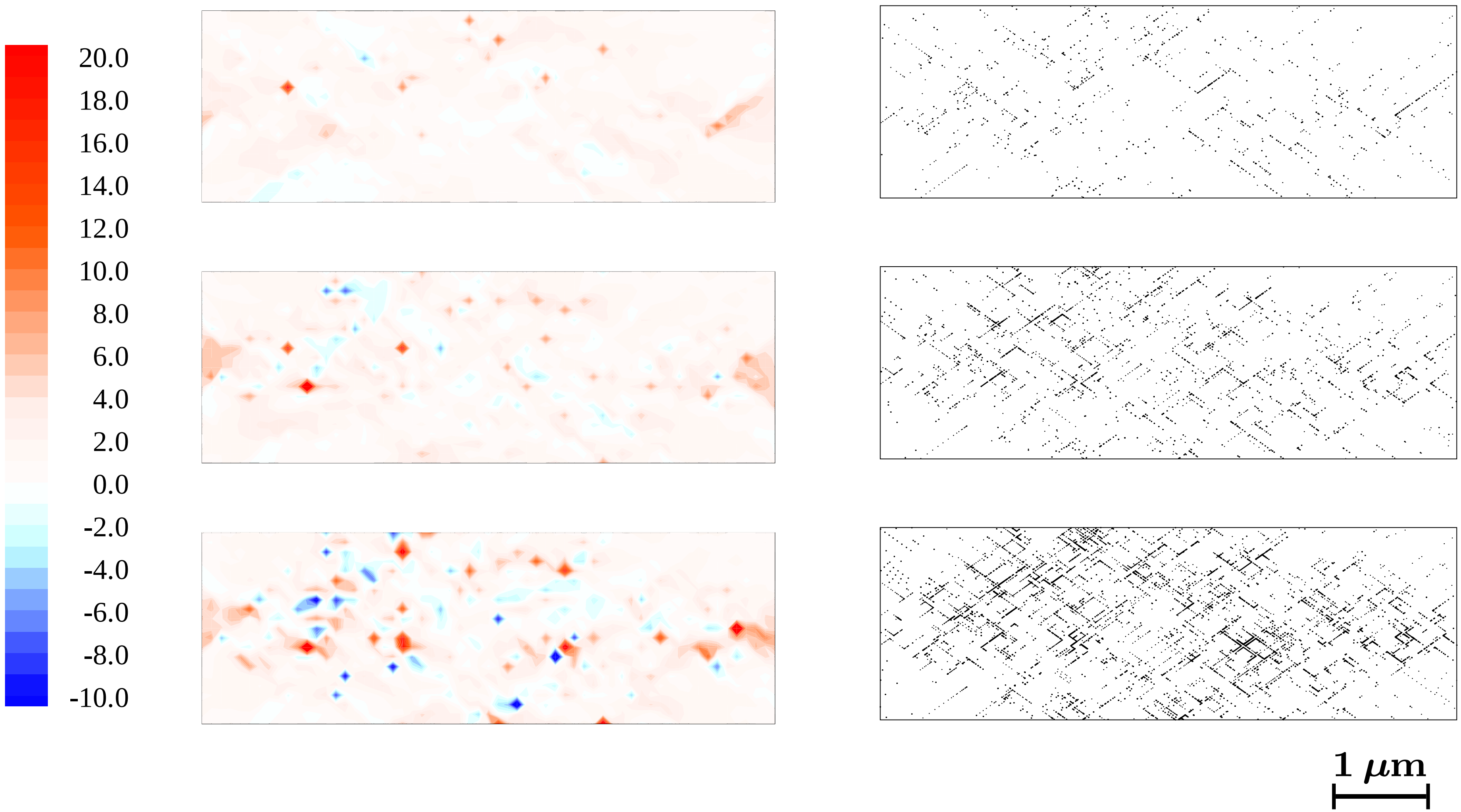
Outline

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

Work-Hardening



Phenomenology



stress σ_{11}/σ pattern

Two-Stage Hardening

- slip plane spacing $d = 50b$
- static sources with $\rho_0 = 4.9 \times 10^{13}\,\mathrm{m}^{-2}$
- **initially non-symmetric glide**
- **crystal size:** $6\,\mu\mathrm{m} \times 2\,\mu\mathrm{m}$

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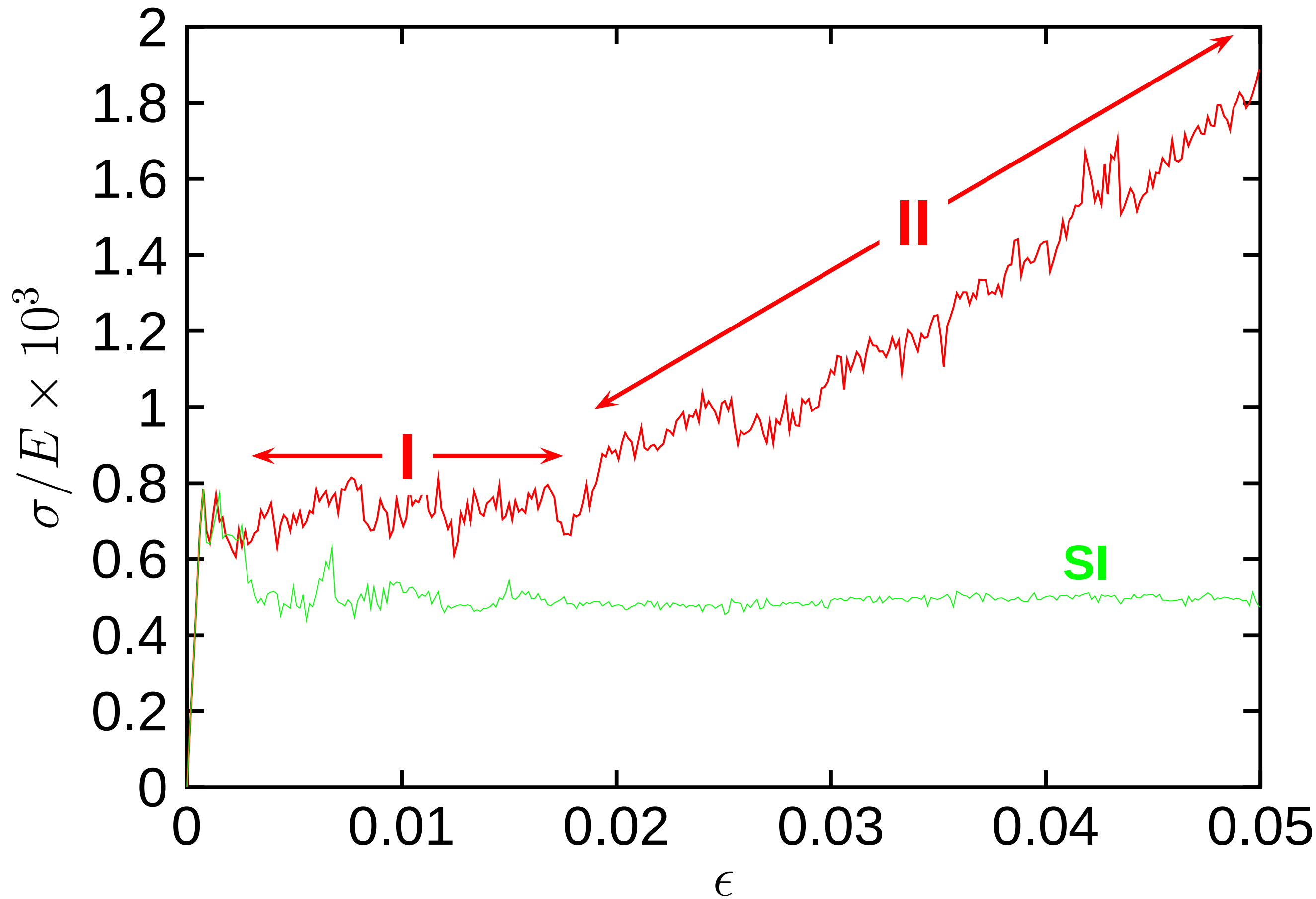
- **initially non-symmetric glide**
- **crystal size:** $6\,\mu\mathrm{m} \times 2\,\mu\mathrm{m}$
- **parameters for 3D rules:**
  - *critical junction distance* $d^{\star} = 6b$
  - *formation probability of anchoring points* $p = 0.05$
  - *breaking stress parameter* $\beta = 1$
  - *nucleation time parameter* $\gamma = 0.1$
  - *line tension coefficient* $\alpha = 0$

Two-Stage Hardening



Comparison with experiments

- slip plane spacing $d = 25b$
- static sources with $\rho_0 = 9.7 \times 10^{13}\,\mathrm{m}^{-2}$
- **parameters for 3D rules:**
  - *formation probability of anchoring points* $p = 0.02$
  - *breaking stress parameter* $\beta = 5$

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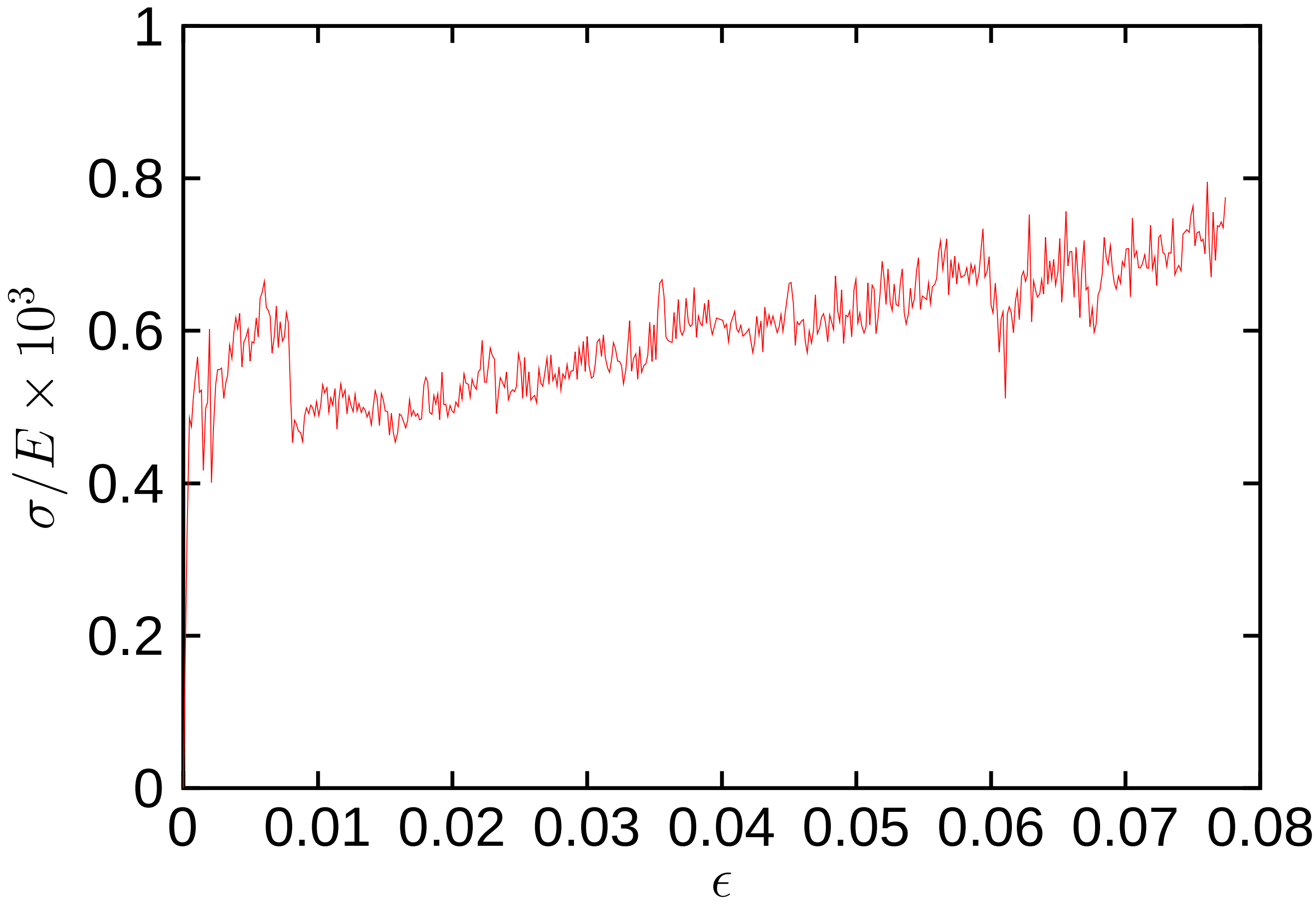
- **parameters for 3D rules:**
  - *formation probability of anchoring points* $p = 0.02$
  - *breaking stress parameter* $\beta = 5$
- Sources can be destroyed by annihilation

Comparison with experiments



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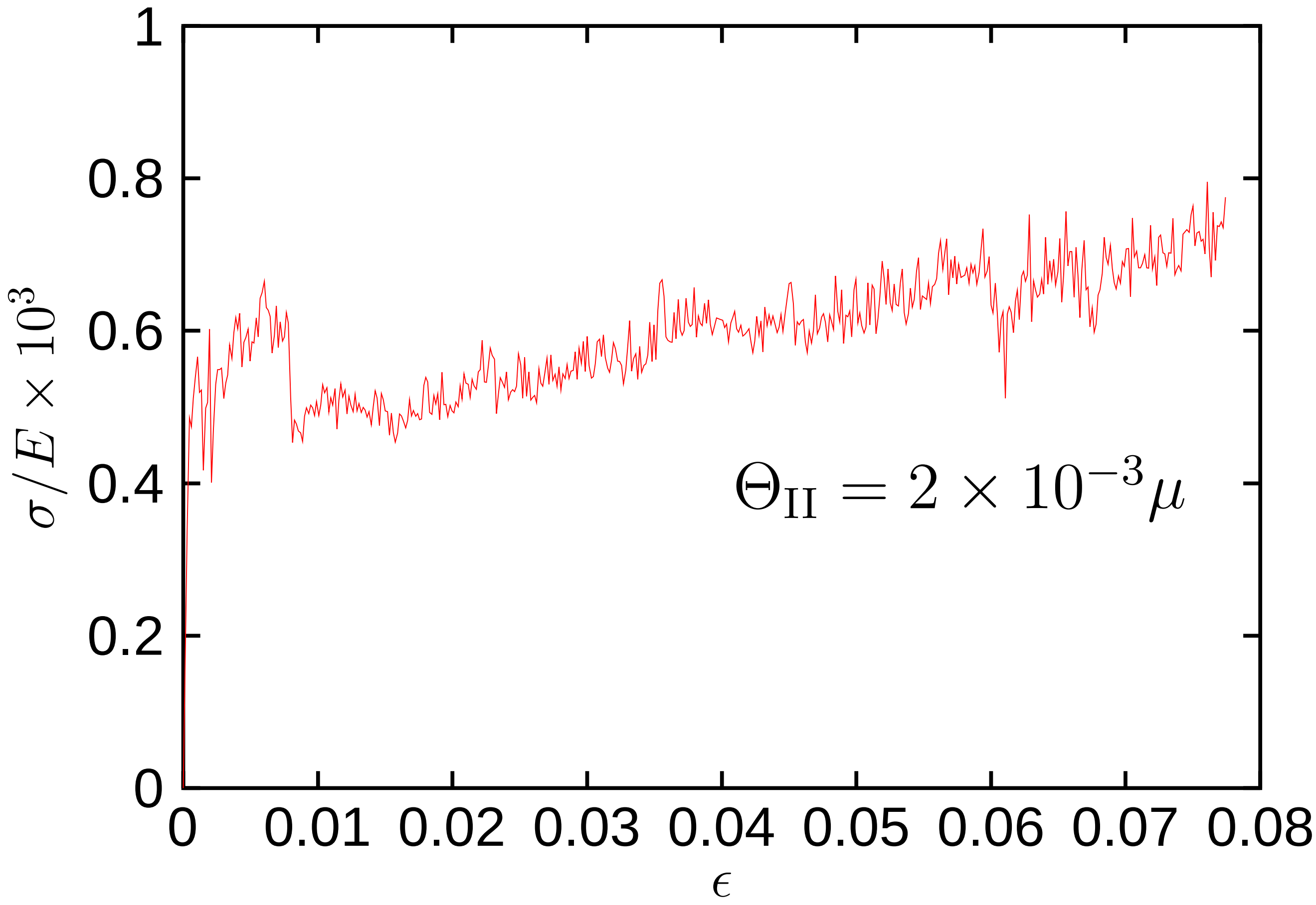
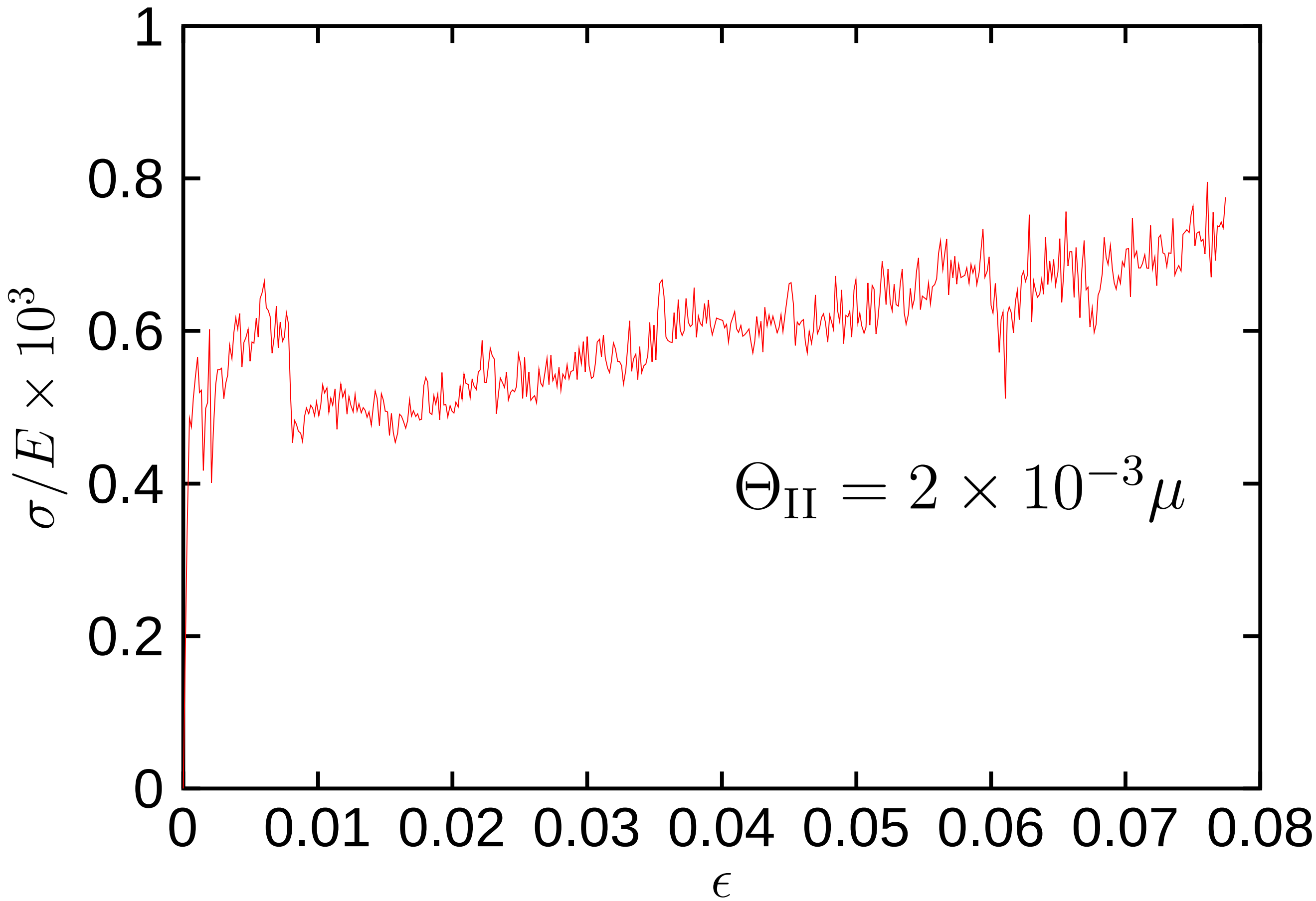
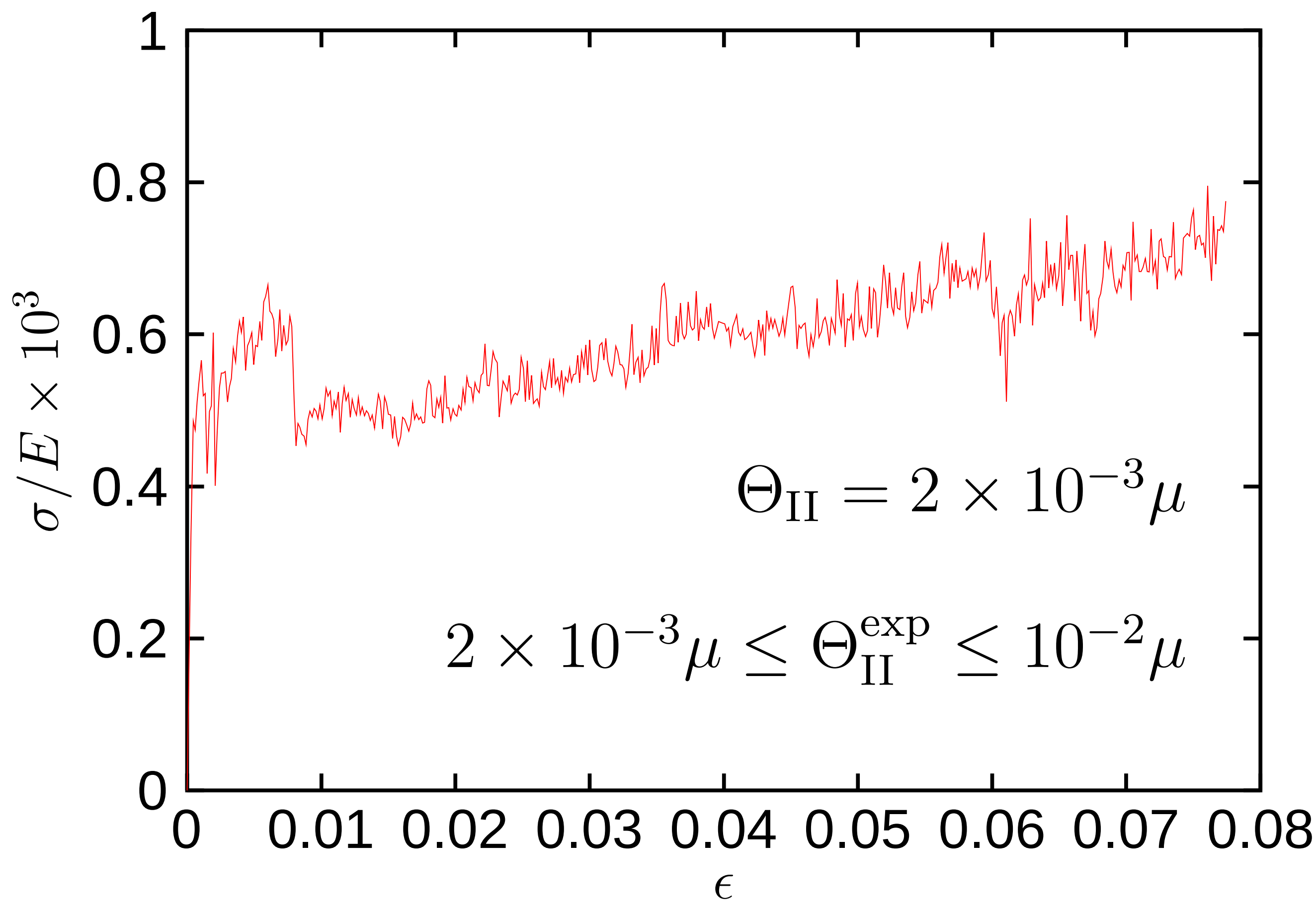


Comparison with experiments



Sources can be destroyed by annihilation

Comparison with experiments



Sources can be destroyed by annihilation

Flow Stress

With $\mathcal{T} = \sigma f_s = \sigma\,(1/2\sin(2\varphi_0))$

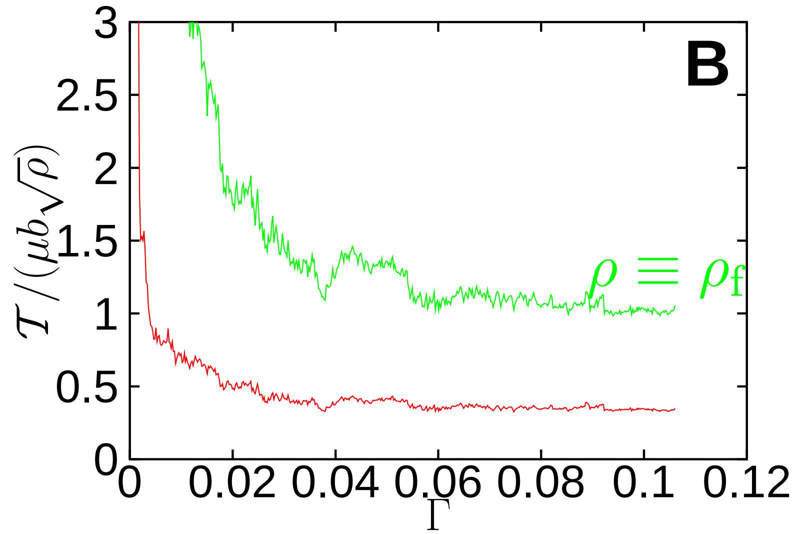
For stage II

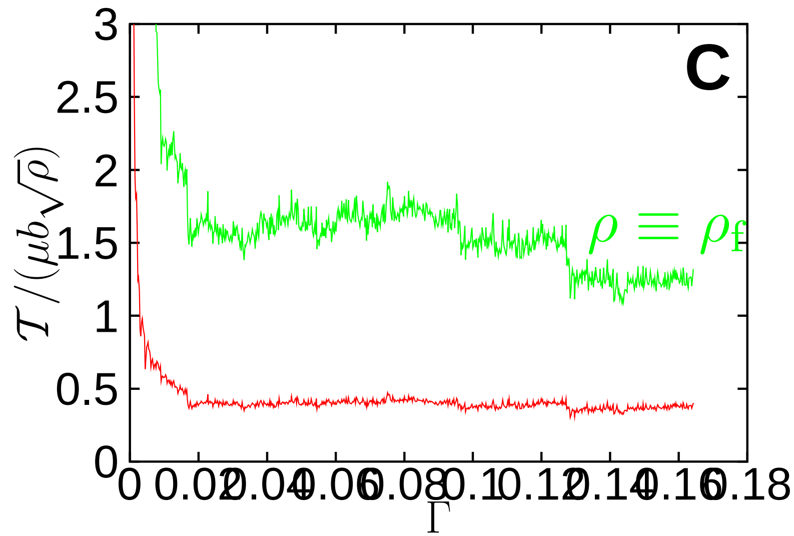
$$\mathcal{T}/\mu = A \times b \times \sqrt{\rho}$$

$$\mathcal{T}/\mu = A^{\mathrm{f}} \times b \times \sqrt{\rho_{\mathrm{f}}}$$

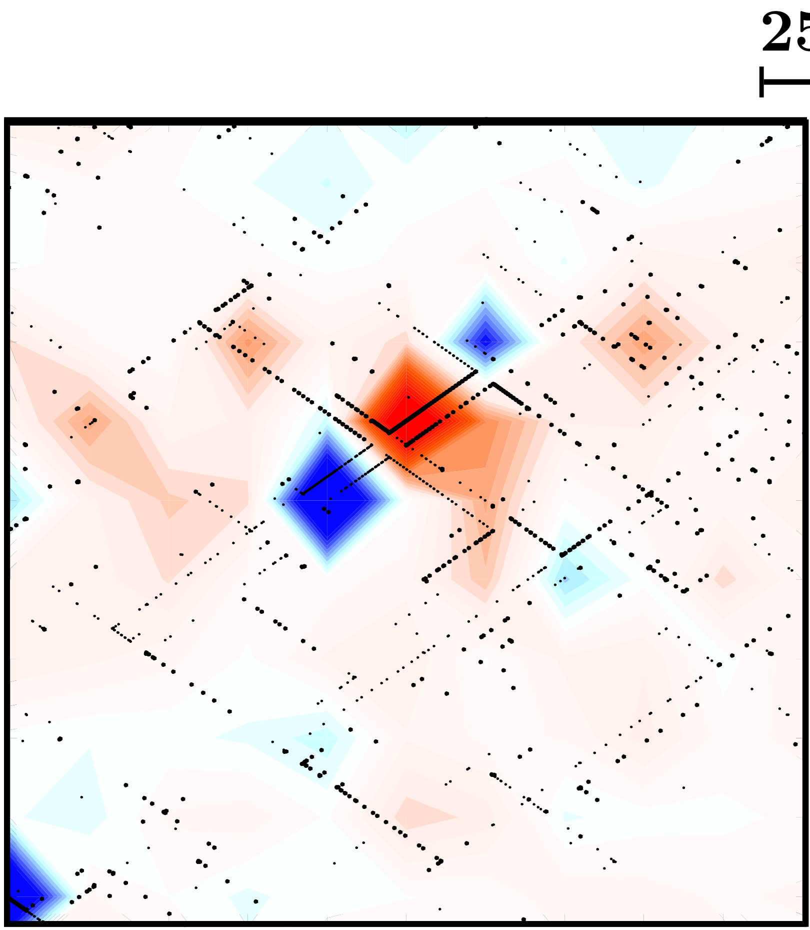
Averaging over several runs:

- $\mathbf{0.4 \leq A \leq 0.5}$
- $\mathbf{1.0 \leq A^{f} \leq 1.8}$

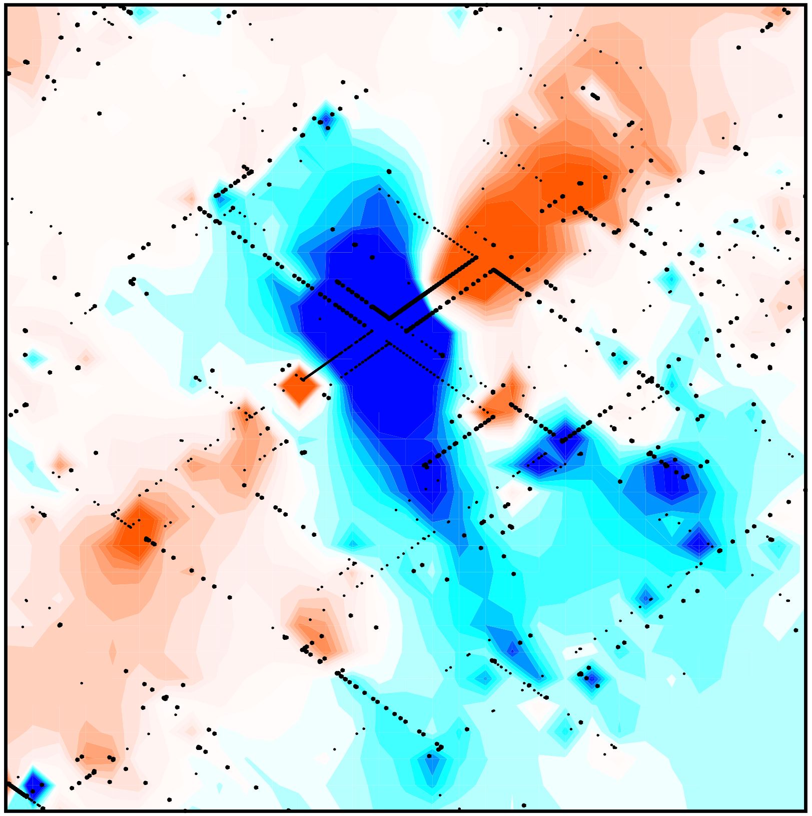




Cell Formation

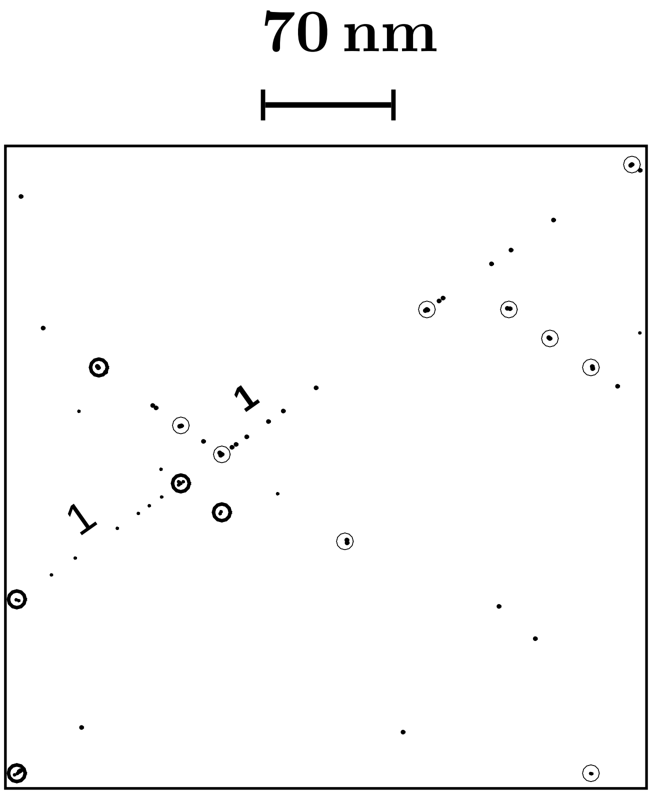


Superposed σ_{11}/σ-field



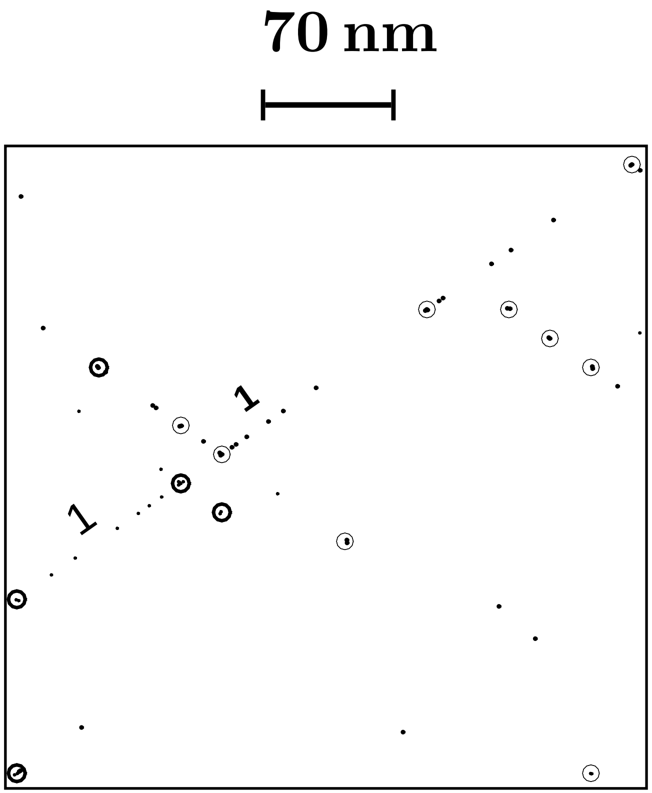
Superposed θ-field

Structure of Incipient Cell

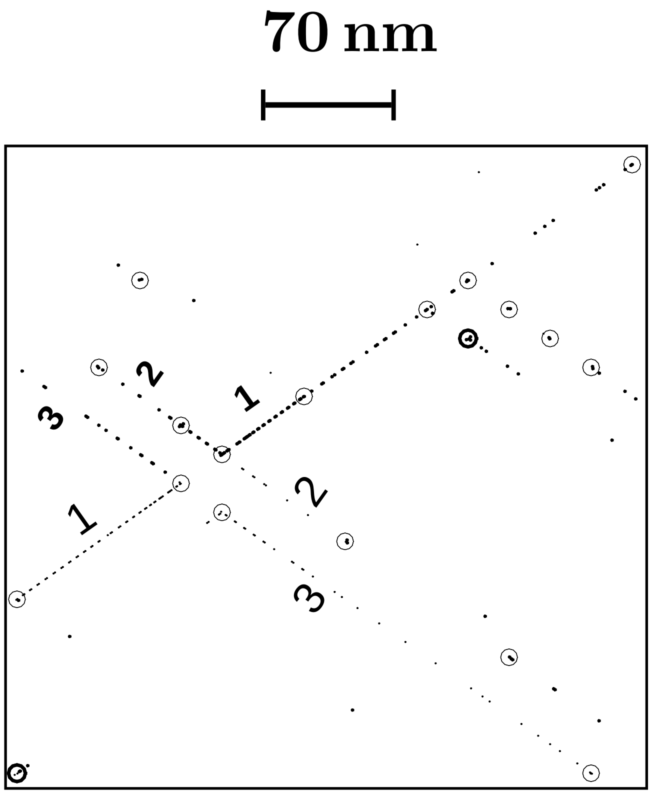


$\epsilon = 0.020$

Structure of Incipient Cell

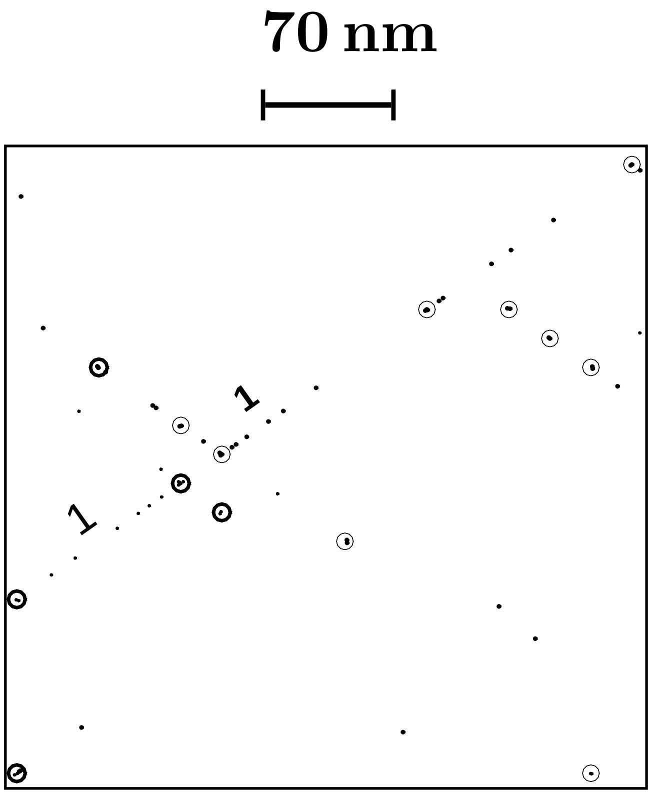


$\epsilon = 0.020$

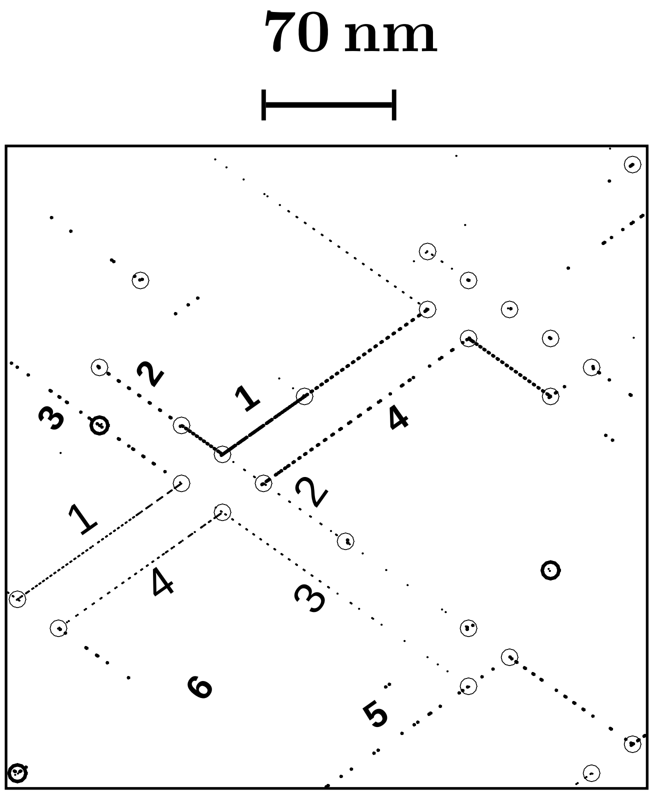


$\epsilon = 0.025$

Structure of Incipient Cell

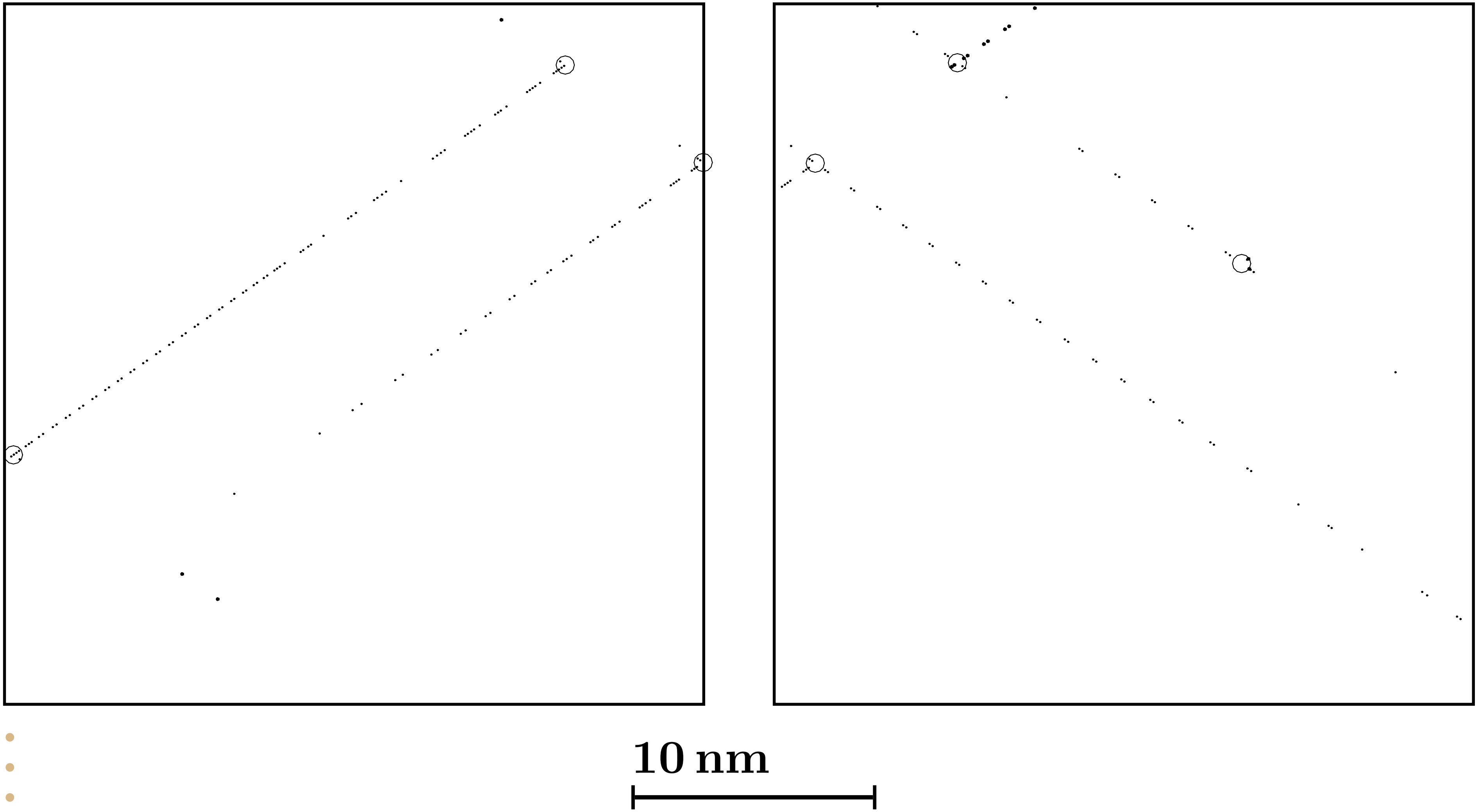


$\epsilon = 0.020$



$\epsilon = 0.035$

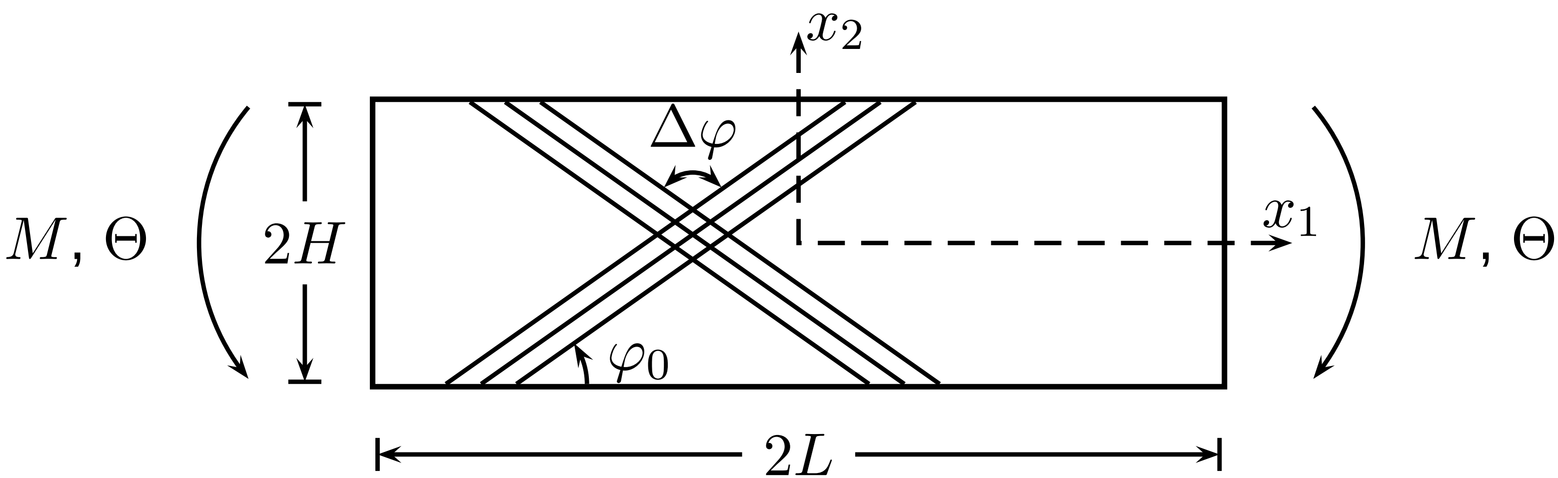
Fine Wall Structure



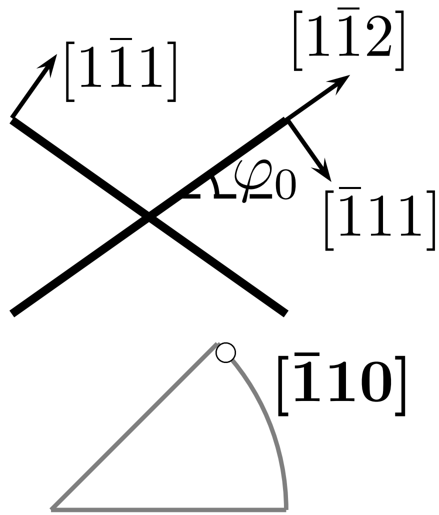
Outline

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

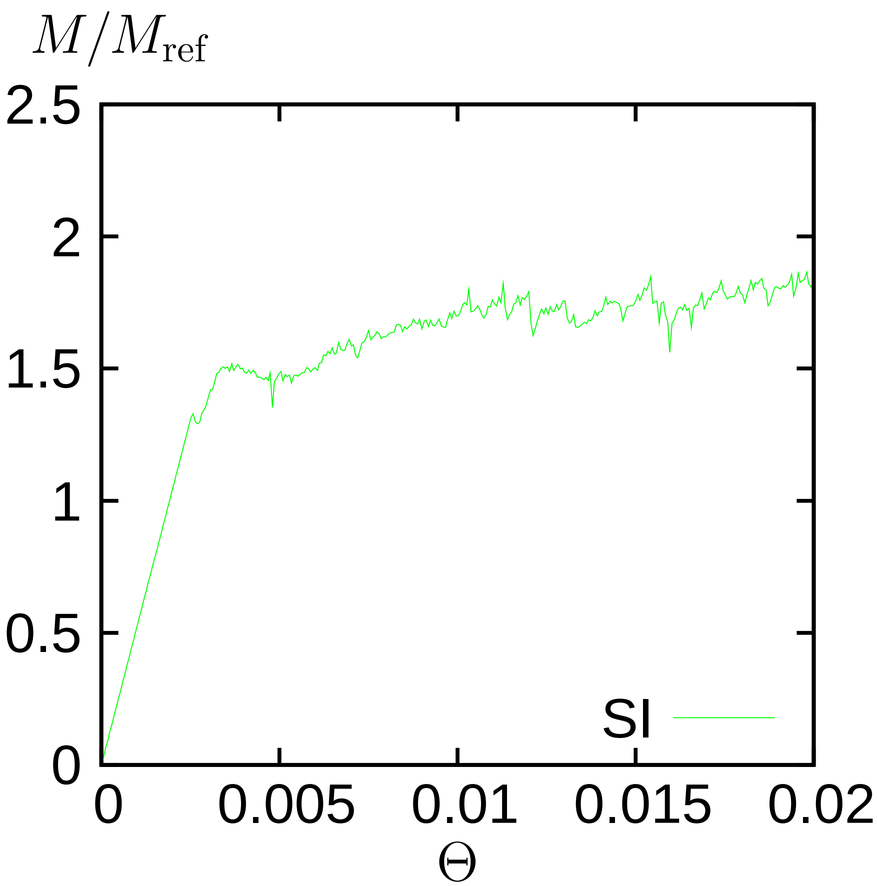
Bending

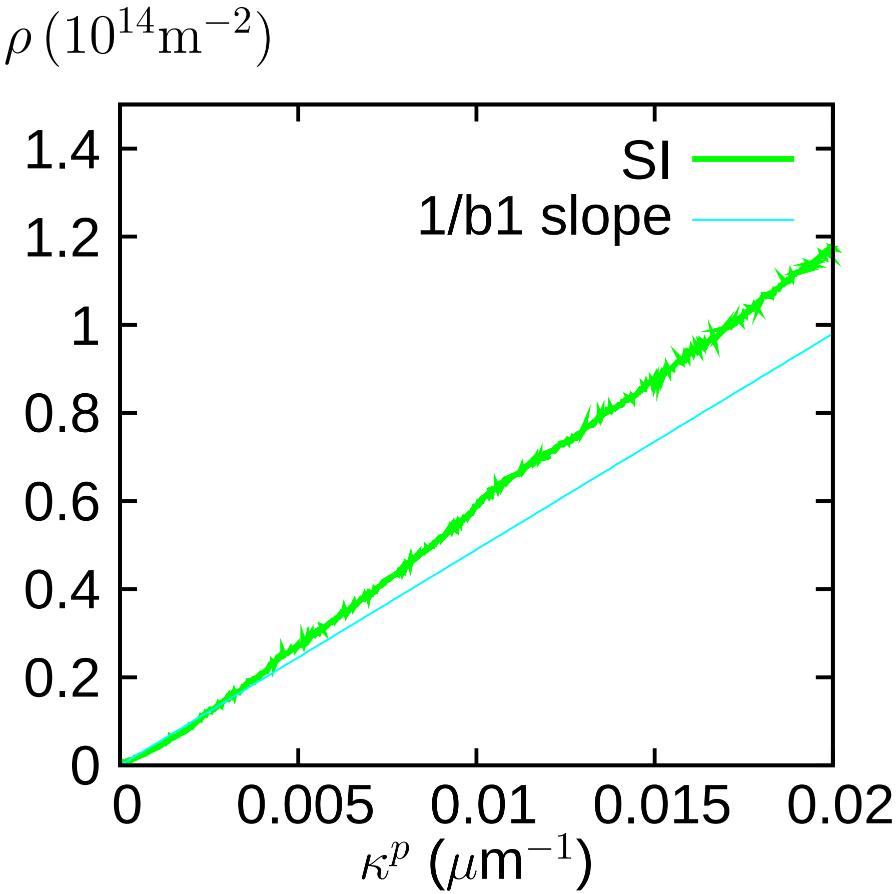


$$\boldsymbol{\varphi_0 = 35.25^\circ}$$



Bending (2D rules)

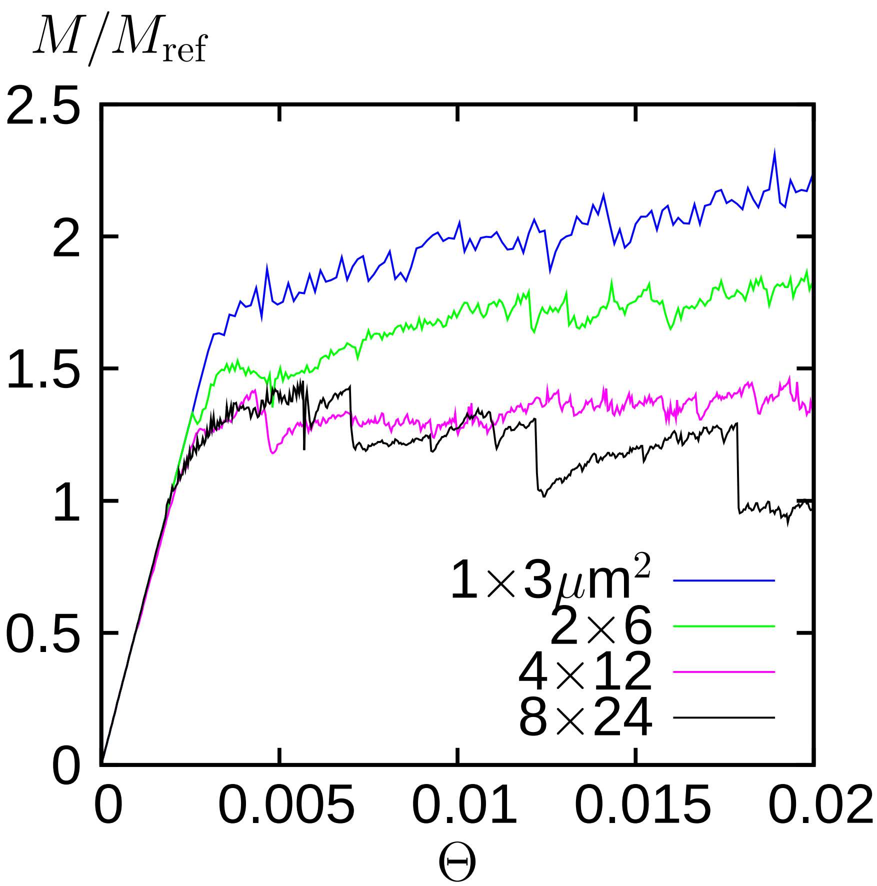


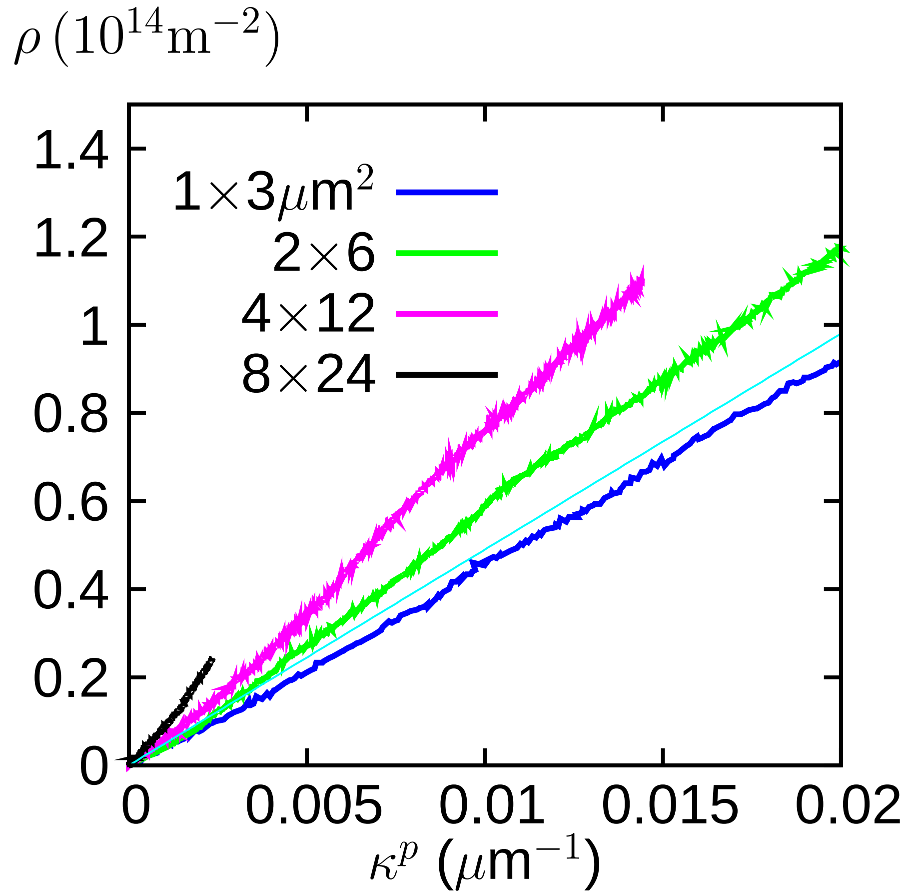


$$M = \int_R \sigma_{11} x_2 dx_2$$

$$\kappa^p = \frac{\Theta}{L} - \frac{M}{D}$$

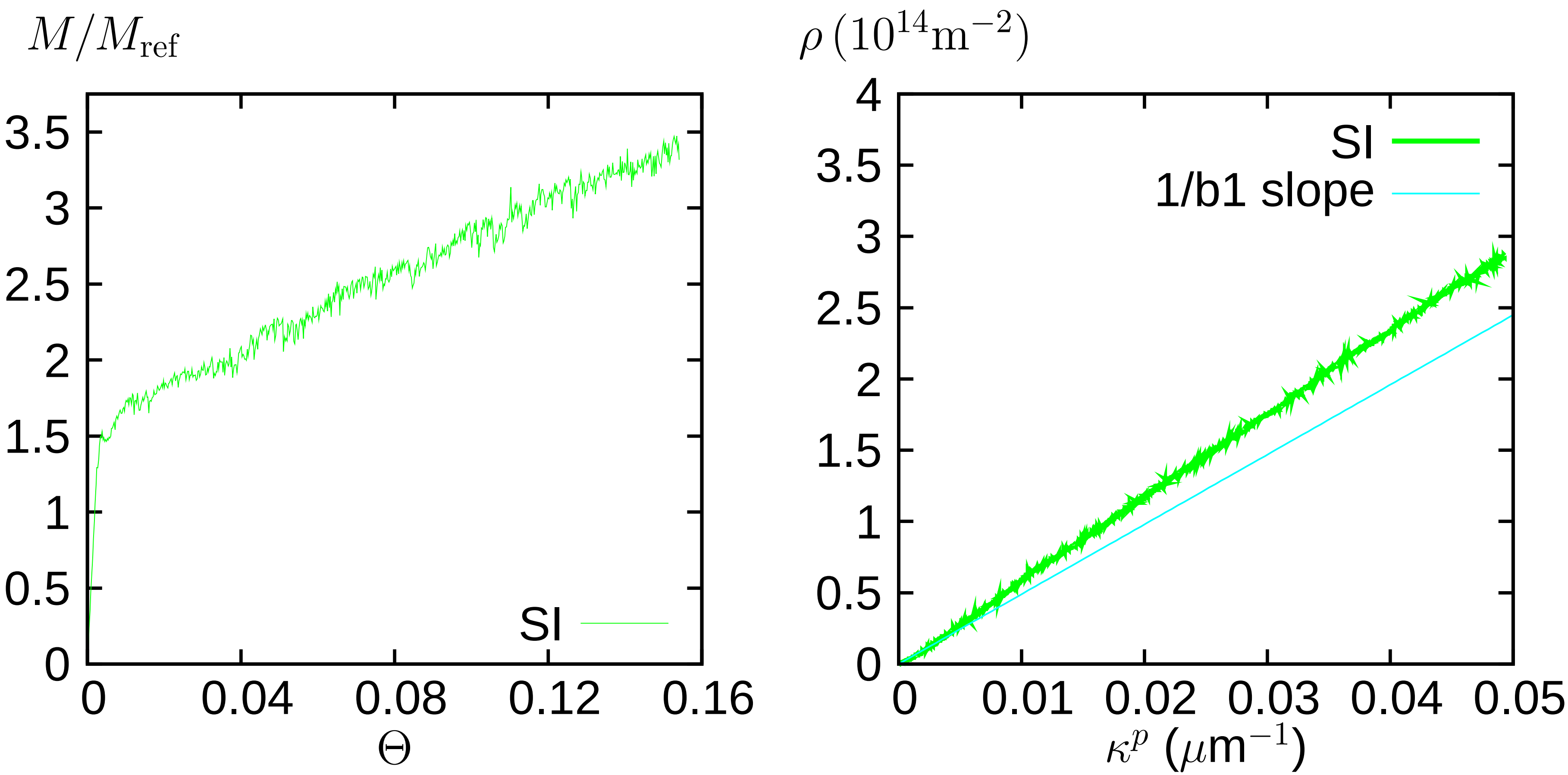
Bending (2D rules)



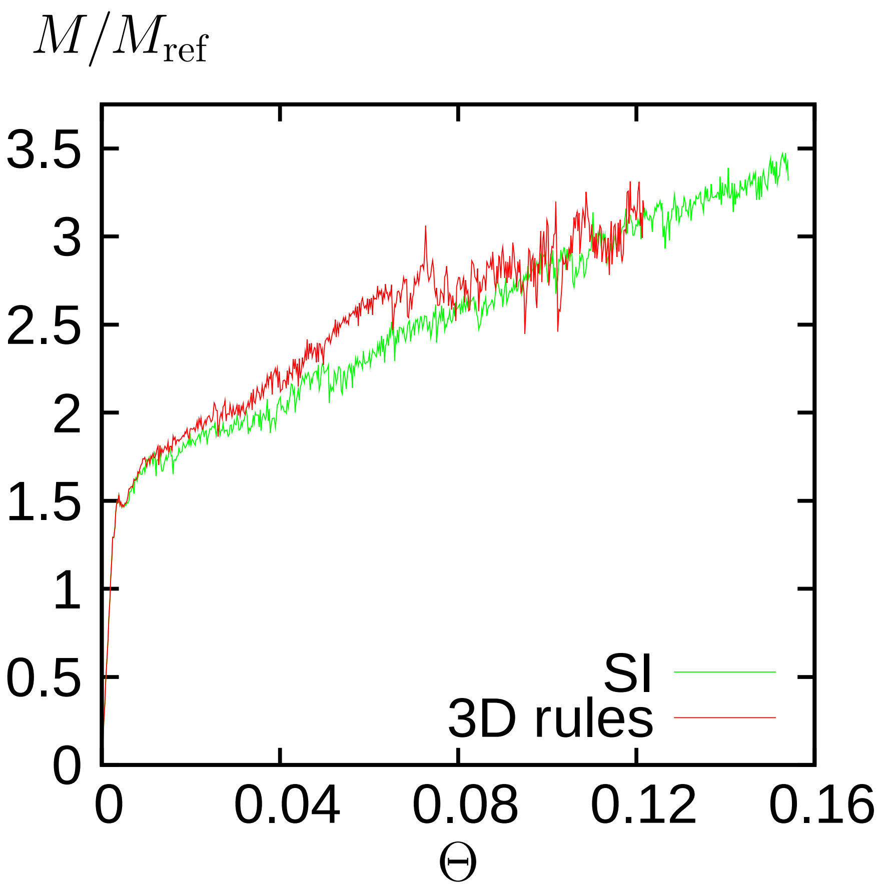


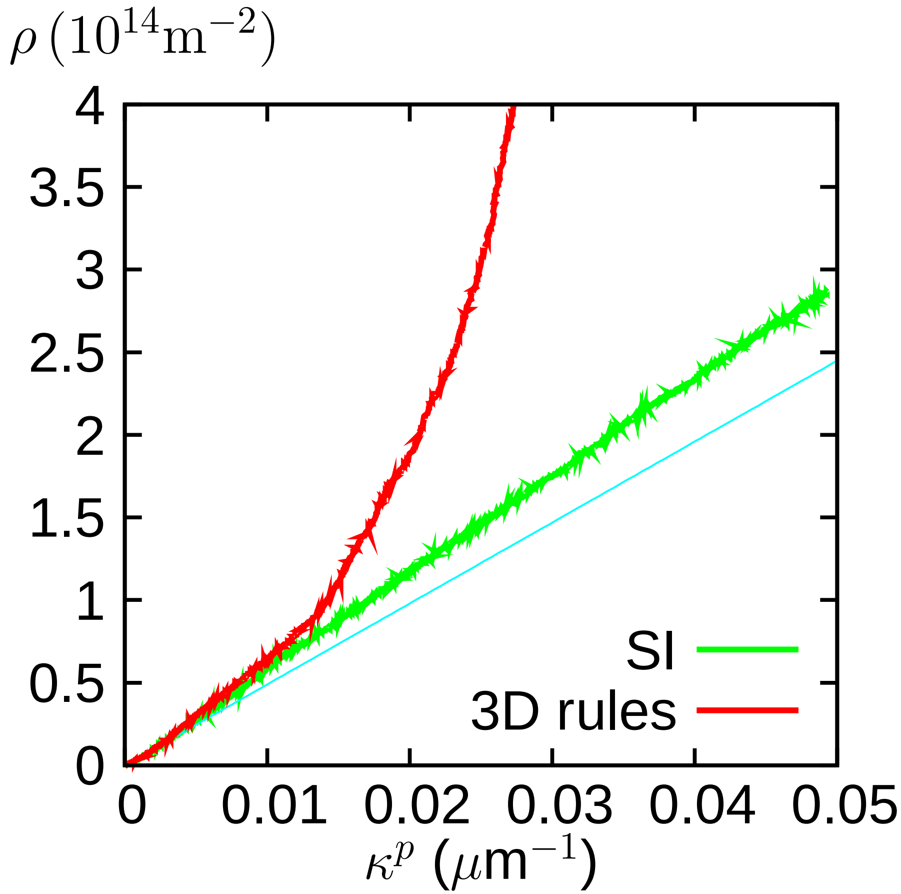
$$\rho_{\rm G} = \frac{\kappa^p}{b_1} = \frac{\kappa^p}{b\cos(\varphi_0)}$$

Bending (new results)



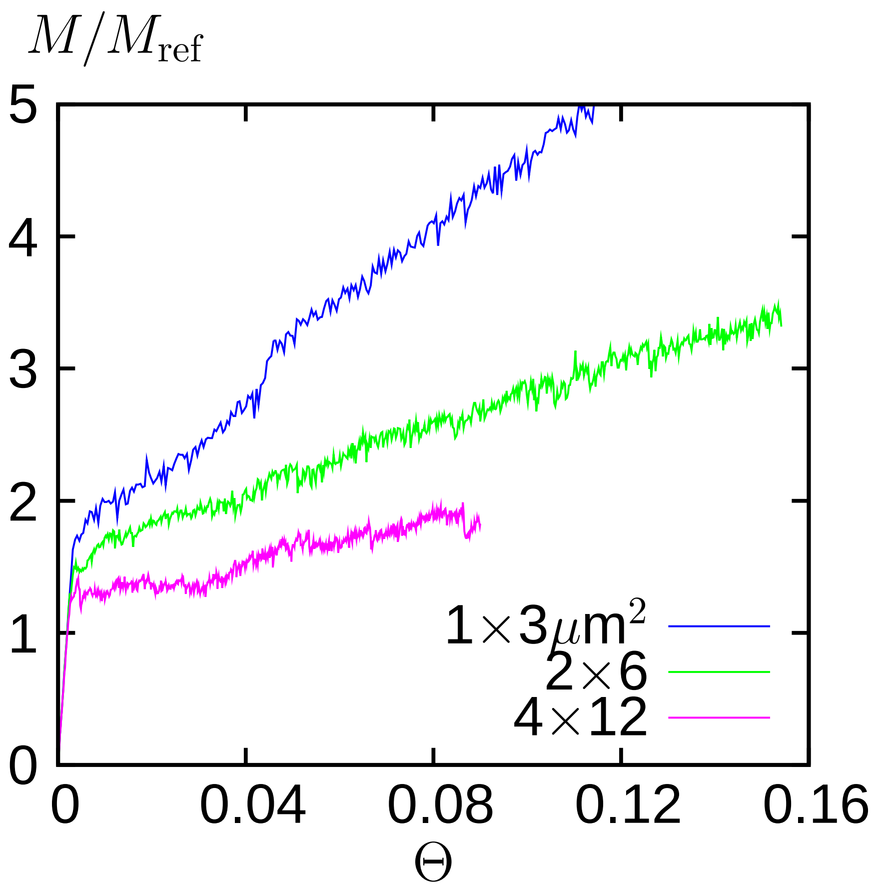
Bending (new results)

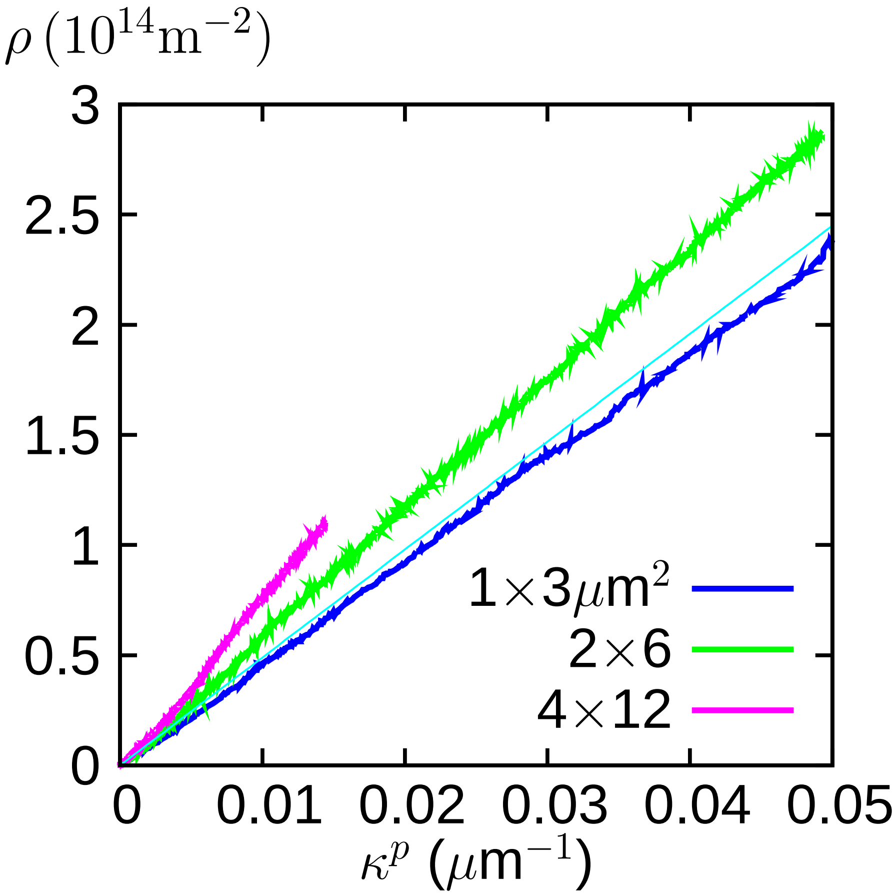




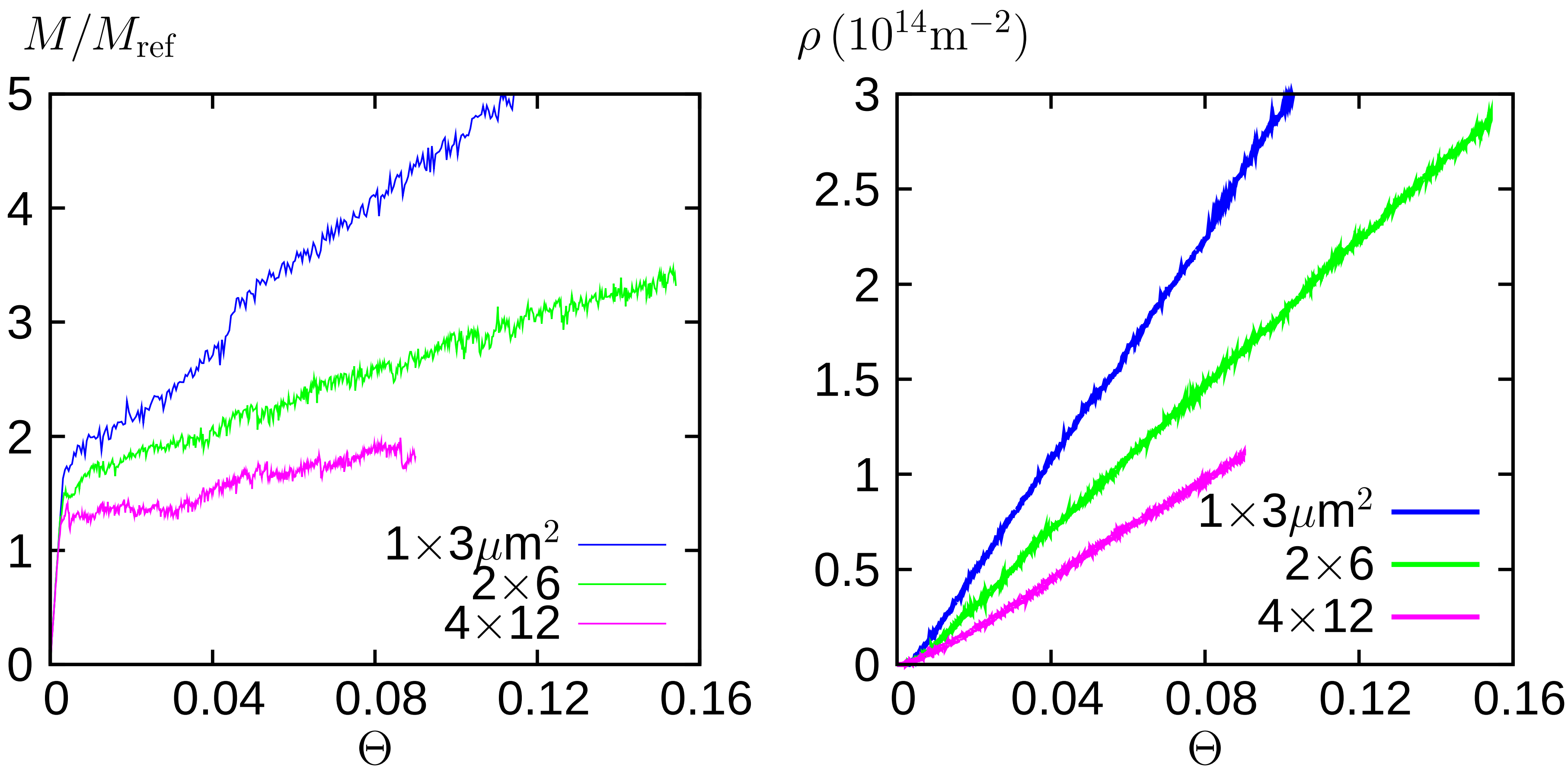
dislocation density is not the only structural parameter governing strength

Bending (new results)



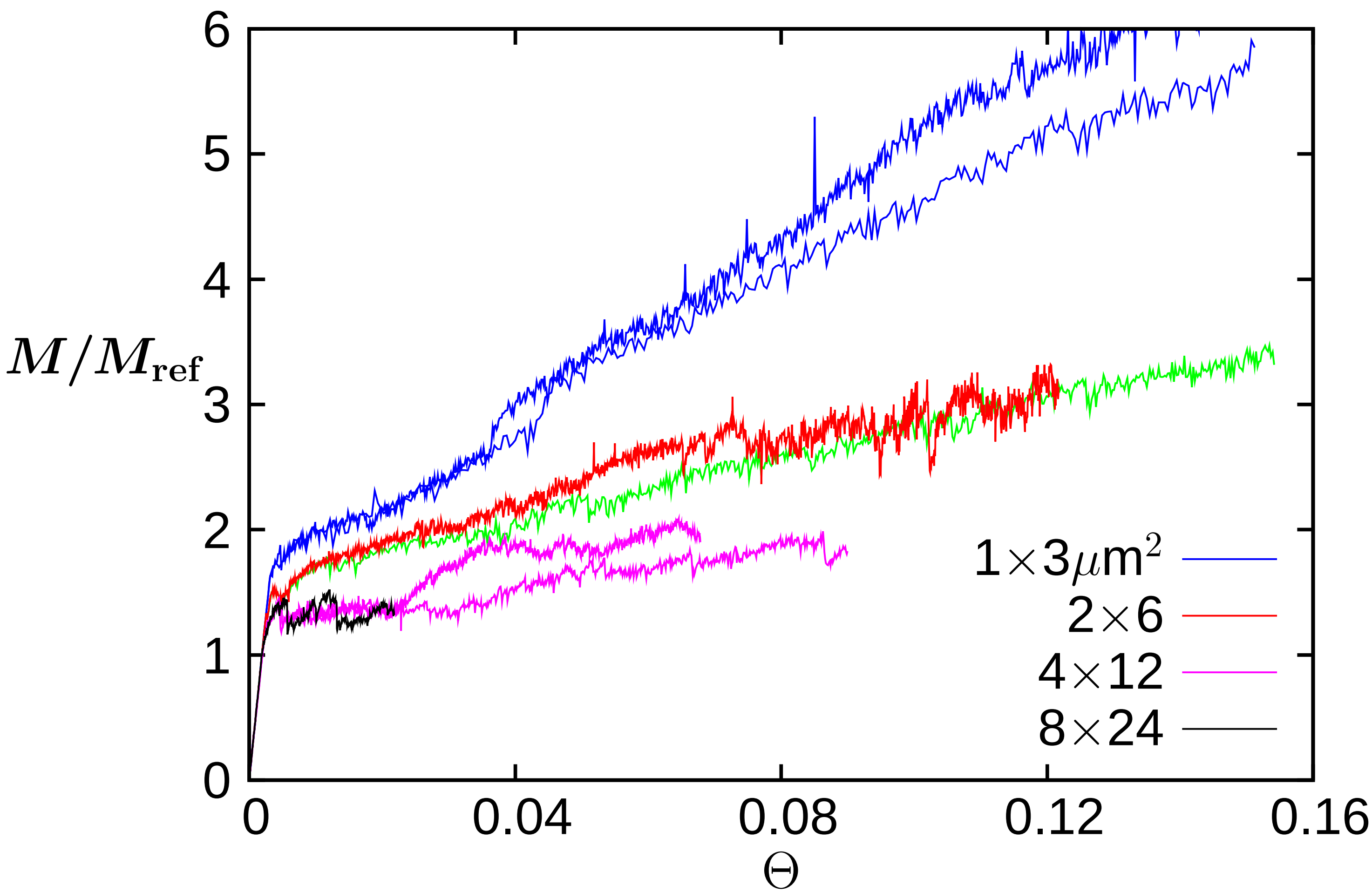


Bending (new results)

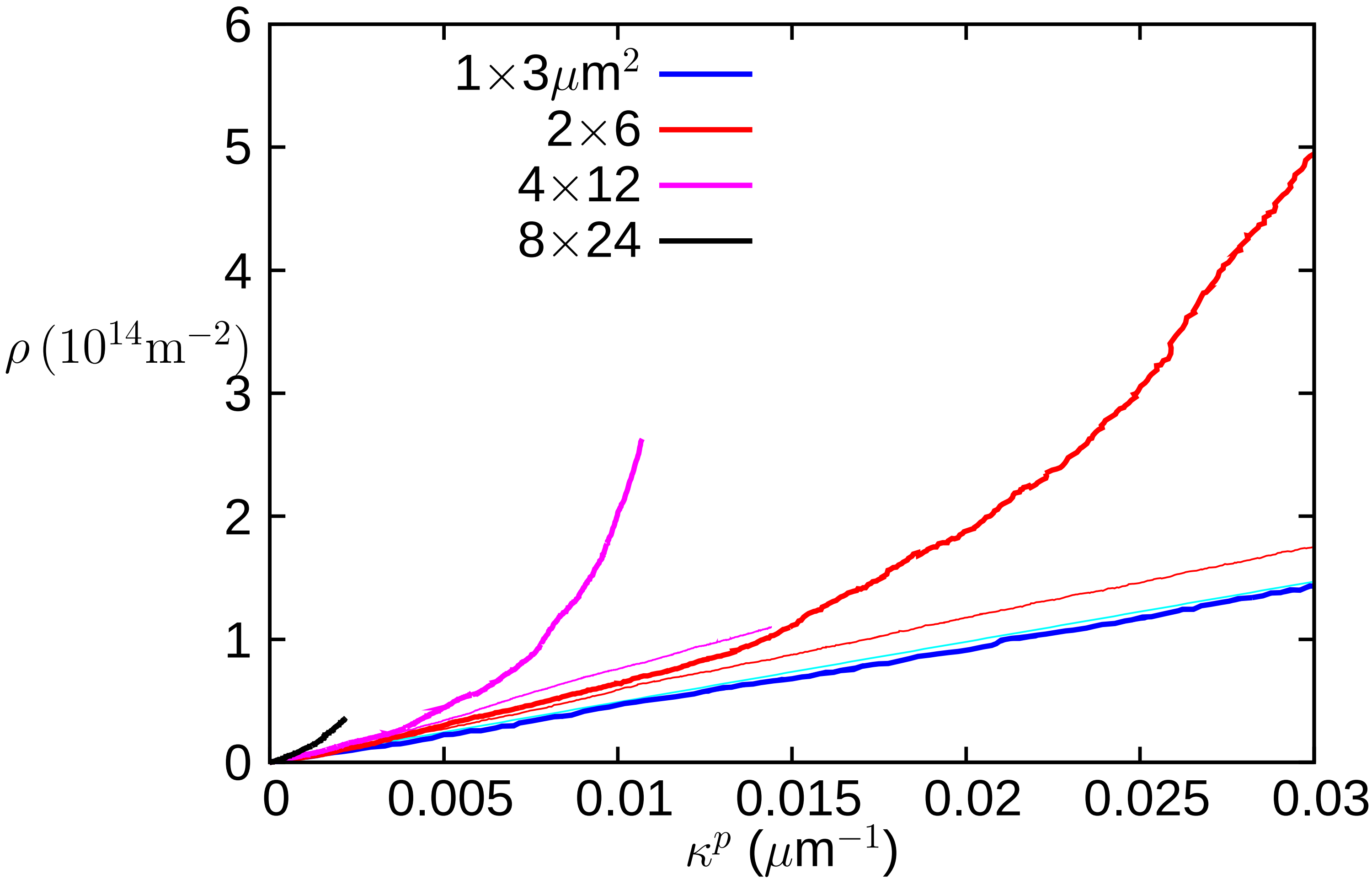


The size effect is seen in M_{yield} and the "hardening"

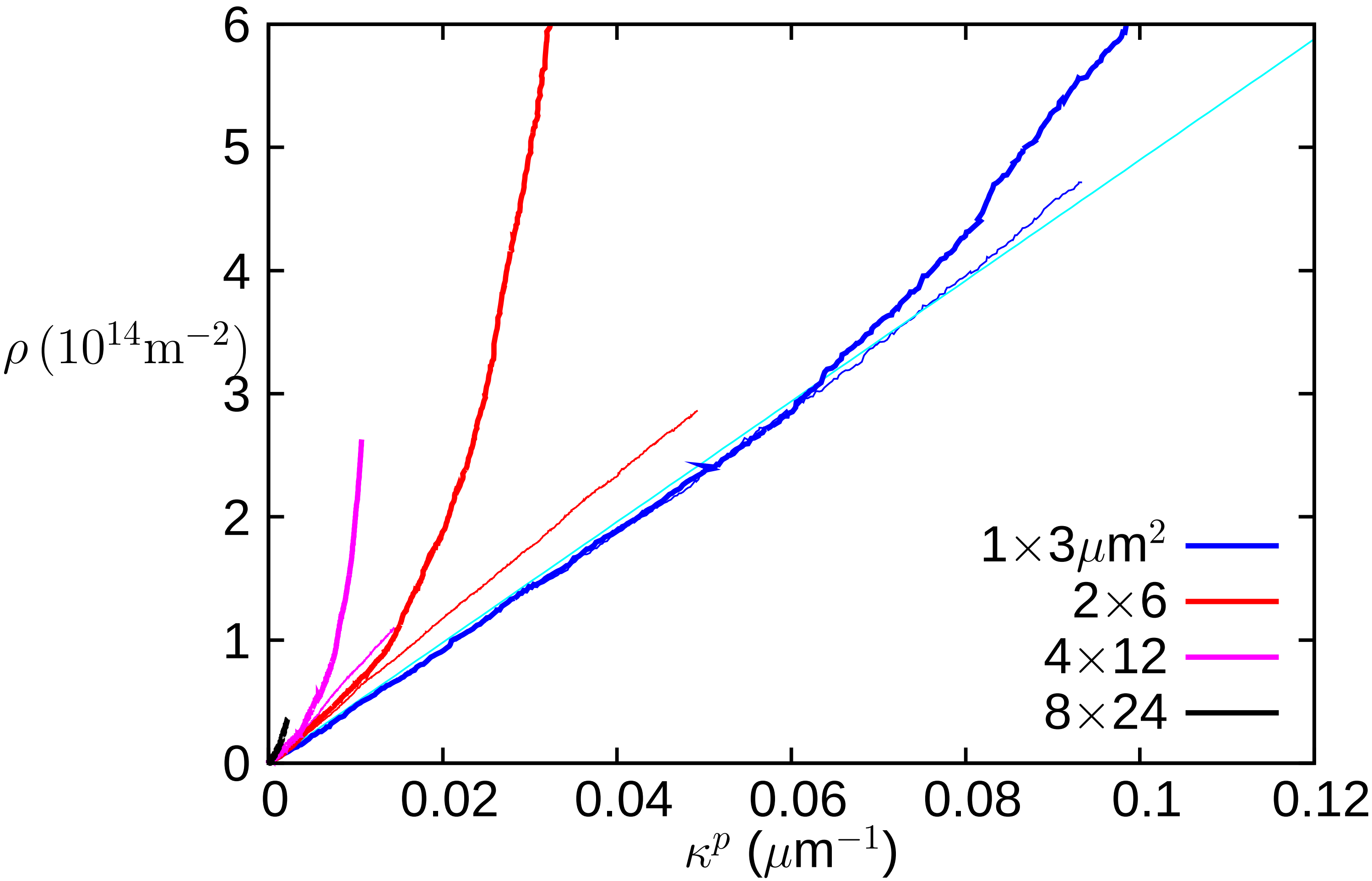
Bending (effect of 3D Rules)



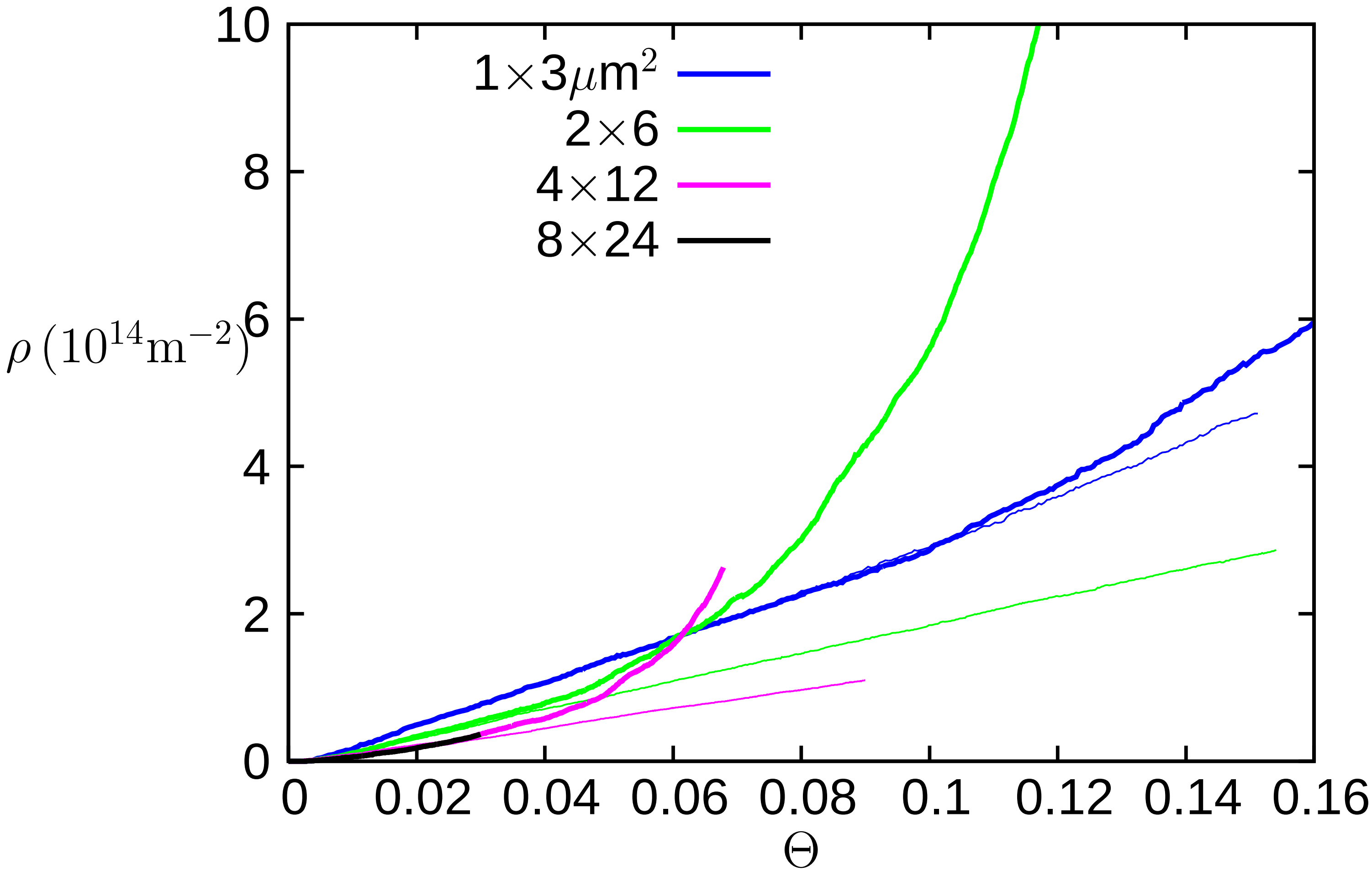
Bending (effect of 3D Rules)



Bending (effect of 3D Rules)



Bending (effect of 3D Rules)



Bending (effect of 3D Rules)