Discrete Dislocation Modeling of Contact and Friction

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based on work with

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Deshpande, V.S. et al. *Acta Mat.*, 2004, **52**, 3135.

Deshpande, V.S. et al. *Mat. Sci. Engin.*, 2005, **400-401**, 186.

Nicola, L. et al., work in progress.

Introduction

- Following Bowden and Tabor (2001), write

$$F_{\mathrm{fr}} = \tau_{\mathrm{fr}} A_c.$$

  where A_c is the contact area and τ_{fr} is the friction stress.
- Two contributions to τ_{fr}: adhesion at the interface and inelastic deformation of asperities.
- Confine attention to the initiation of sliding.
- Contact sizes between ≈ 0.05 μm to ≈ 100 μm.
- Issues considered:
  - The effect of contact size and spacing on τ_{fr}.
  - The energy dissipated in initiating sliding across a single contact.
  - The interaction between contacts (indentation only).

Background

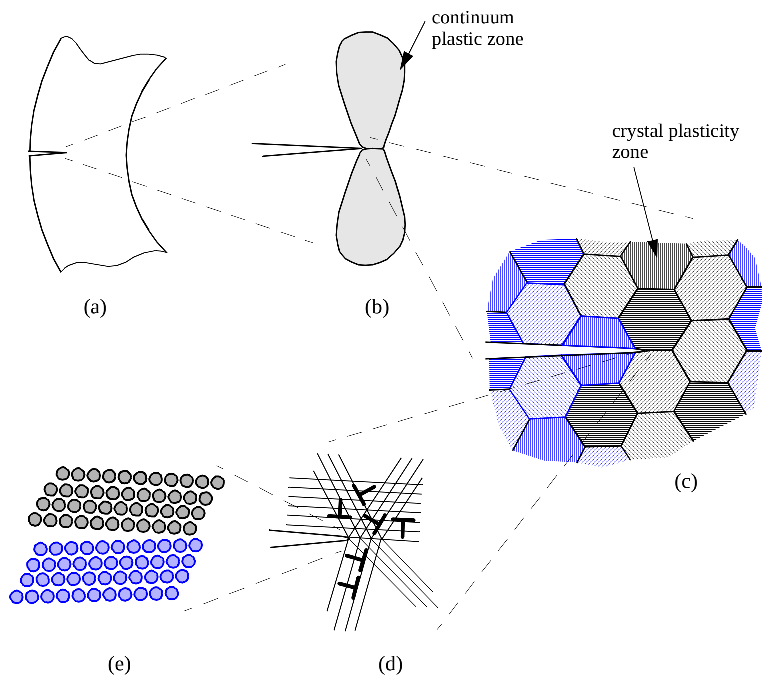
- Micron scale plasticity in crystalline solids is size dependent, e.g. the indentation size effect.
- Measurements of τ_{fr}: AFM, $A_c \approx 30 - 60$ nm^2, $\tau_{\text{fr}}/\mu \approx 1/40$ (Carpick et al., 1996); SFA, $A_c \approx 5 \times 10^9 - 2 \times 10^{11}$ nm^2, $\tau_{\text{fr}}/\mu \approx 1/1300$ (Homola et al., 1990).
- Previous discrete dislocation analyses.
  - Polonsky and Keer (1996) – size dependence of the hardness.
  - Hurtado and Kim (1999) – interface dislocations only: (i) small contacts – τ_{fr} is the theoretical shear strength; (ii) large contacts – τ_{fr} is the Peierls stress; (iii) transition – $\tau_{\text{fr}} \propto a^{-1/2}$ (nucleation controlled, Rice-Thompson model).

Modeling Framework

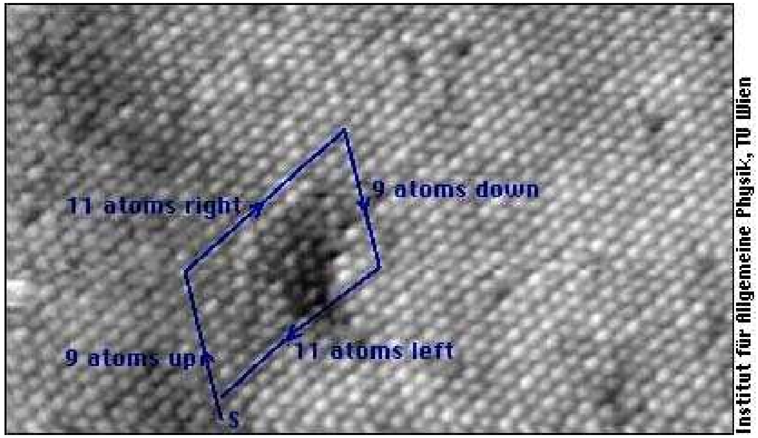
- Single crystals.
- Attention is confined to crystals where the only inelastic deformation mechanism is dislocation glide.
- Two-dimensional, plane strain analyses.
- Small deformation formulation – geometry change effects neglected.
- Quasi-static analyses.
- Discrete dislocation plasticity.
  - Comparison with continuum slip plasticity for the multi-contact (indentation) analysis.

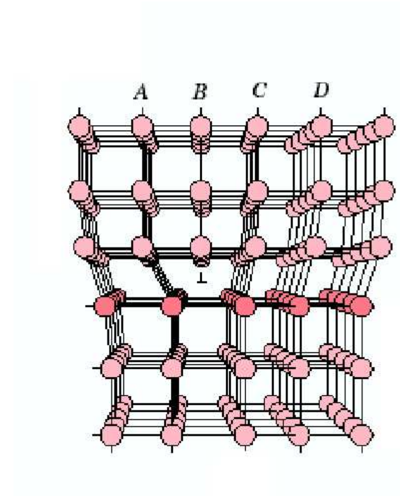
Discrete Dislocation Plasticity

- Dislocations are treated as discrete entities and modeled as line singularities in an elastic solid.
- Long range interactions between dislocations come directly from elasticity theory.
- Formulate and solve general boundary value problems where plastic flow is represented by the collective motion of discrete dislocations.



Dislocations





- Burgers vector magnitude b.
- Elasticity – accurately represents dislocation fields beyond $5b - 8b$ from the core.
- The stress field is long range.

$$\sigma_{ij} \propto b \frac{f_{ij}}{r}$$

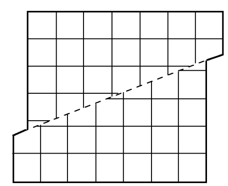
- A dislocation density of 10^{13} m^{-2} corresponds to 10 μm^{-2}.

Boundary Value Problems

Issue:

- Singular dislocation fields are not well-represented numerically.

$$\sigma_{ij}^{(k)} \propto \frac{f_{ij}^{(k)}}{r} \qquad \oint_\Gamma \frac{\partial u_i}{\partial x_j} dx_j \neq 0$$



Resolution:

- Represent the singular fields explicitly.
- Use superposition.
- Exploit fact that the singular fields satisfy

$$\frac{\partial \sigma_{ij}^{(k)}}{\partial x_j} = 0$$

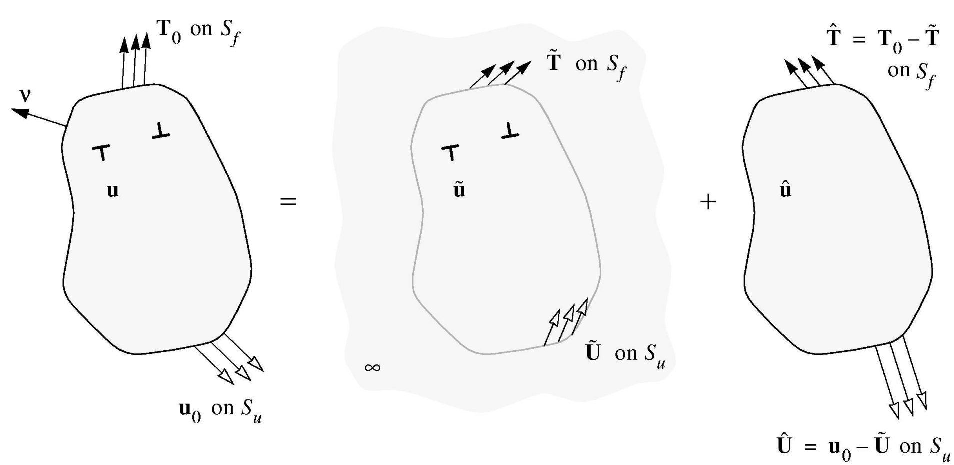
Boundary Value Problems – Small Strain Theory

$$u_i = \tilde{u}_i + \hat{u}_i \, , \qquad \epsilon_{ij} = \tilde{\epsilon}_{ij} + \hat{\epsilon}_{ij} \, , \qquad \sigma_{ij} = \tilde{\sigma}_{ij} + \hat{\sigma}_{ij} \, .$$

- $(\tilde{\ })$ fields – sum of the singular equilibrium fields of the individual dislocations, e.g. $\tilde{\sigma}_{ij} = \sum_k \sigma_{ij}^{(k)}$, $\sigma_{ij,j}^{(k)} = 0$.
- $(\hat{\ })$ fields – image fields that correct for the boundary conditions and are non-singular.

$$\hat{\sigma}_{ij,j} = 0 \qquad \hat{\sigma}_{ij} n_j = T_i^0 - \tilde{T}_i \text{ on } S_f \qquad \hat{u}_i = u_i^0 - \tilde{u}_i \text{ on } S_u$$

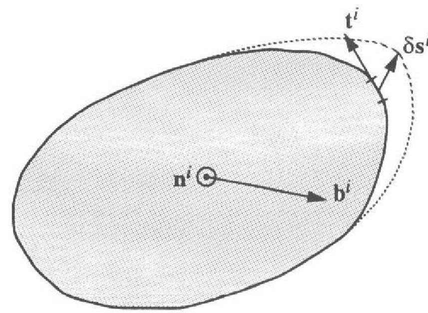
$$\int_V \hat{\sigma}_{ij} \delta \hat{u}_{i,j} dV = \int_{S_T} (T_i^0 - \tilde{T}_i) \delta \hat{u}_i dS$$



Peach-Koehler Force

- The change in potential energy Π associated with a change in dislocation position.

$$\delta\Pi = -\sum_i \int_{\mathcal{L}^i} \mathbf{f}^i \cdot \delta\mathbf{s}^i \, dl$$



- Glide component of the Peach-Koehler (configurational) force $\mathbf{f}^i$

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

Dislocation Constitutive Rules – 2D

- Plane strain, single crystals, isotropic elasticity; edge dislocations only.
- Glide component of the Peach-Koehler force.

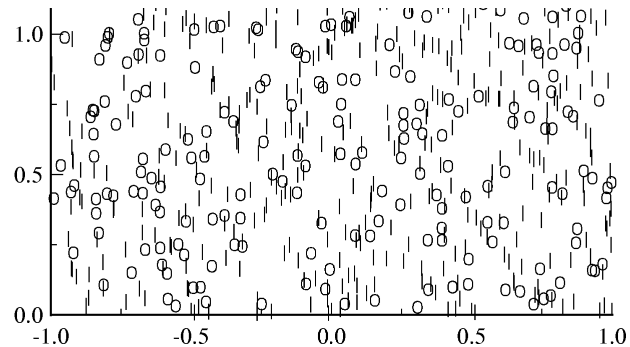
$$f^{(k)} = \mathbf{n}^{(k)} \cdot \left[\hat{\boldsymbol{\sigma}} + \sum_{j \neq k} \boldsymbol{\sigma}^{(j)} \right] \cdot \mathbf{b}^{(k)}$$

- Dislocation nucleation (Frank-Read sources) – nucleation occurs when $f^{(k)}$ at a source reaches $b\tau_{\mathrm{nuc}}$ during t_{nuc}.
- Dislocation motion – $v^{(k)} = f^{(k)}/B$.
- Dislocation annihilation – annihilation distance L_{e}.
- Obstacles – pin dislocations and release them once $f^{(k)}$ attains $b\tau_{\mathrm{obs}}$.

Computational Procedure

1. At time t the state of the body is known including $\sigma_{ij}(x_k, t)$ and the positions of all dislocations.
2. An increment of loading is prescribed.
3. The state of the body at $t + dt$ needs to be determined.
   - Calculate the dislocation interaction force.
     - Multi-body interaction calculation.
   - Calculate the change in dislocation structure caused by dislocation nucleation, dislocation annihilation, etc.
     - Evaluation of constitutive rules.
   - Calculate the image fields for the updated dislocation arrangement, i.e. the $(\hat{\ })$ fields.
     - Finite element calculation.

Discrete Dislocation Plasticity



Input:

- Elastic constants; slip systems; dislocation constitutive parameters; dislocation sources and obstacles.

Output:

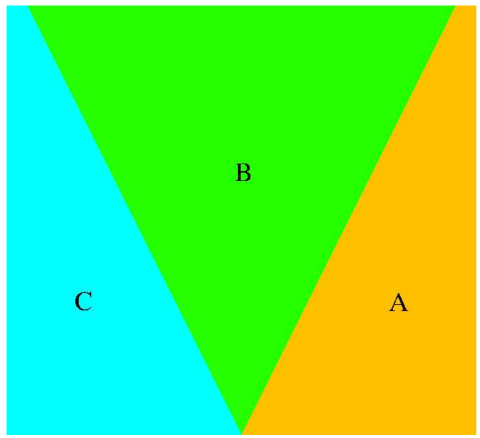
- The stress and deformation response.
- Evolution of the dislocation structure.

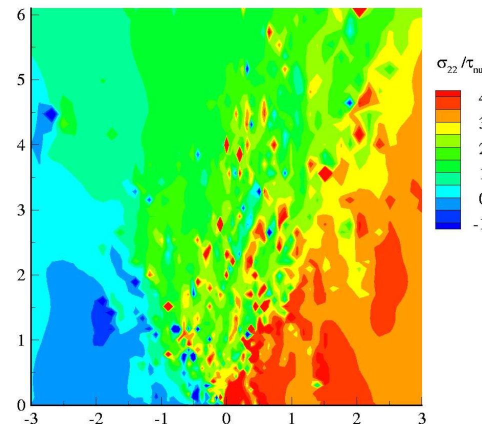
Comments:

- Dislocations form self-organized patterns.
- Dislocation dynamics is chaotic.

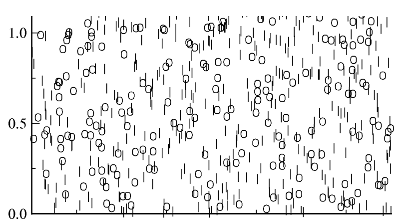
Mode I Crack, Single Crystal, Two Slip Systems

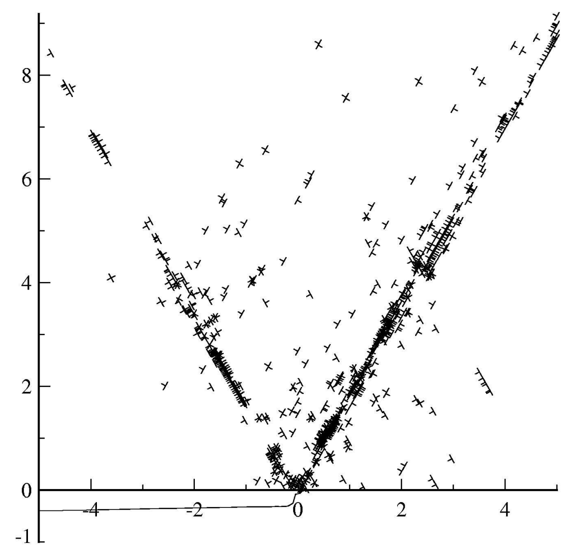
- Classical crystal plasticity – sectors of constant stress, Rice (1987).





- Dislocation structure.

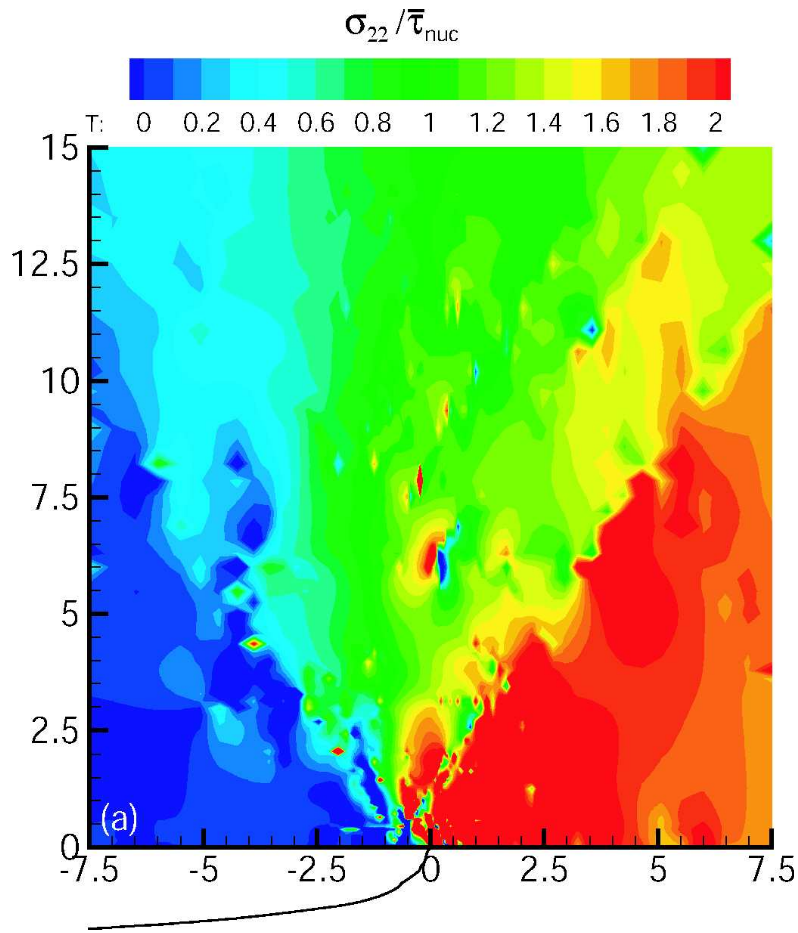




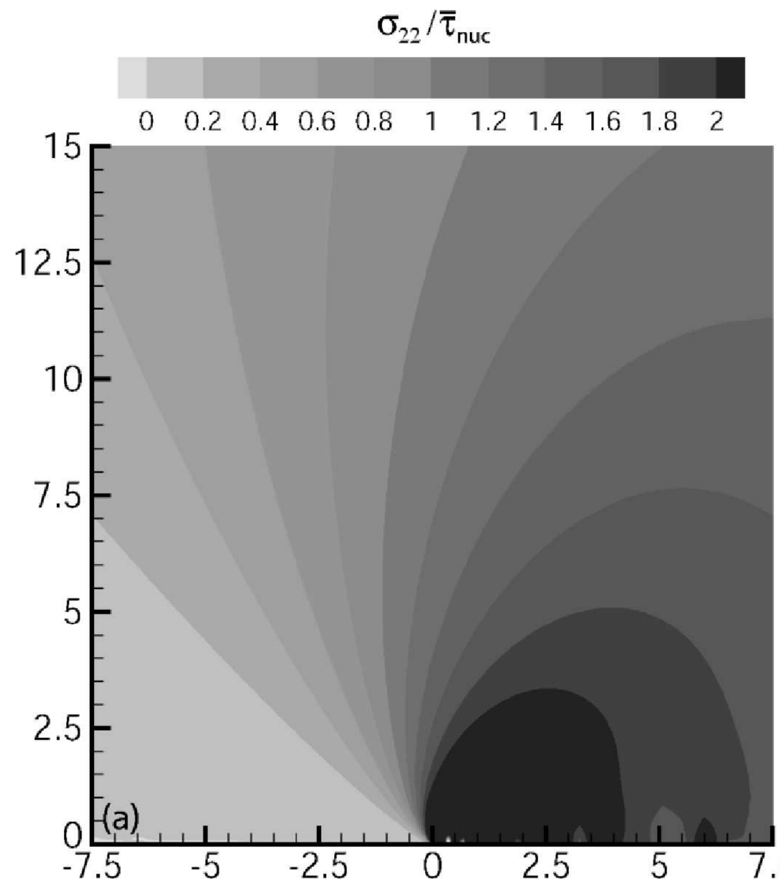
Many internal sources – no special dislocation nucleation from the crack tip.

Total and (ˆ) Field Stress Distributions

- Three slip systems.

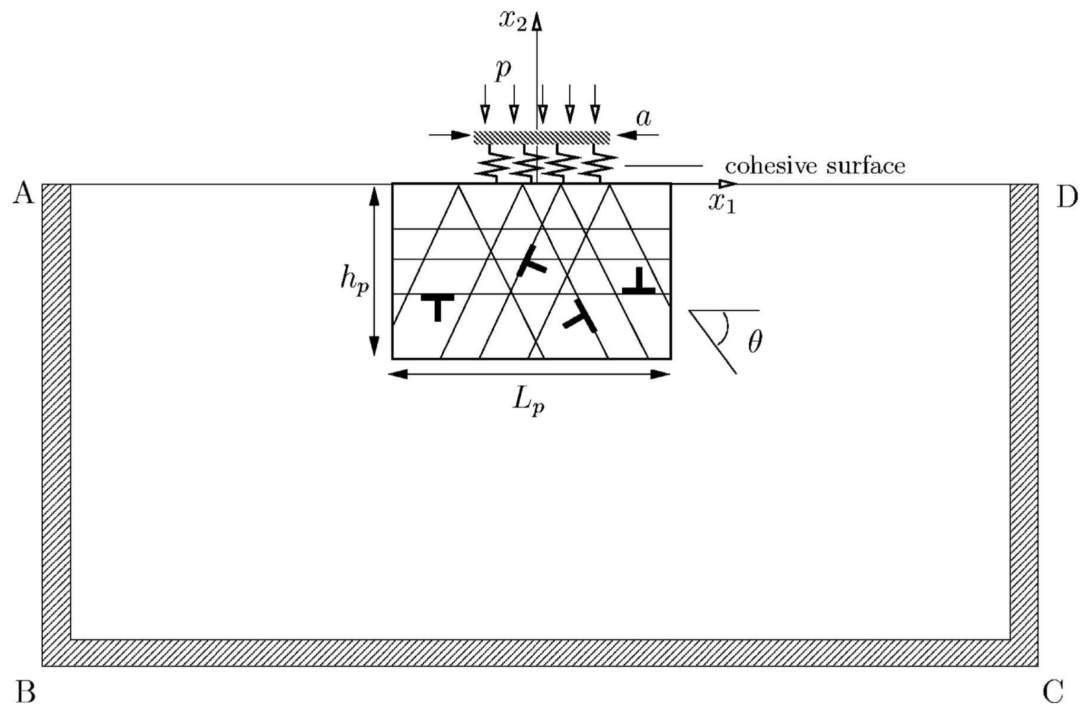


Total



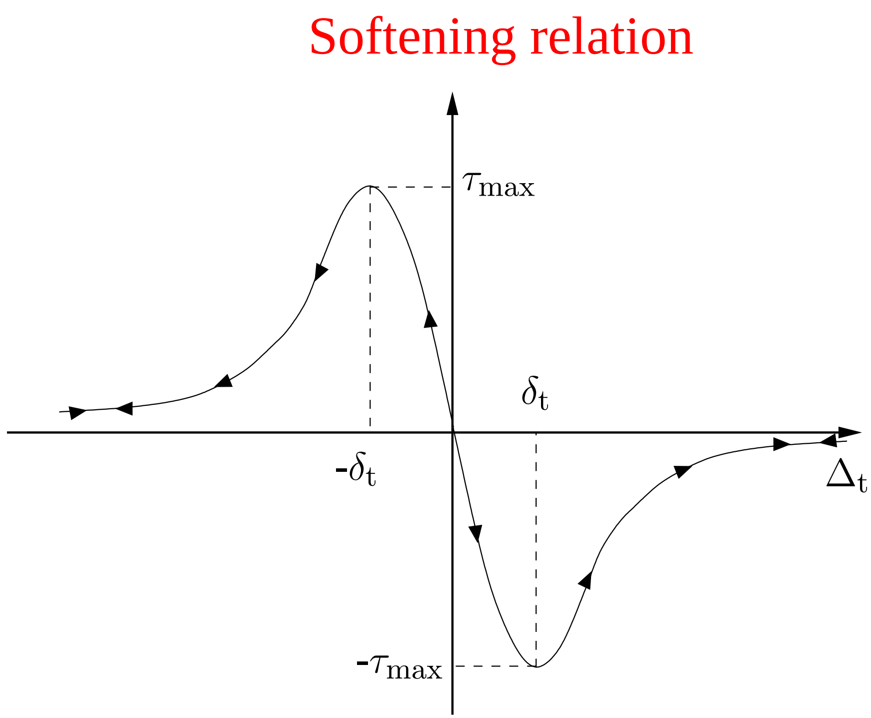
(ˆ) field

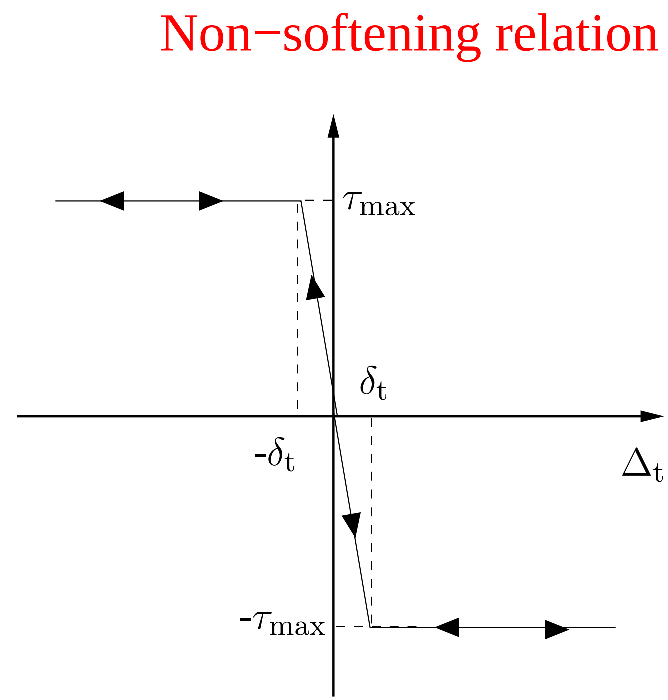
Single Contact – Initiation of Sliding



- Single crystal, three slip systems specified by $\theta = \pm 60°$, $0°$.
- First, prescribe monotonically increasing p (but in most cases $p = 0$).
- Second, $u_1 = U(t)$ and $u_2 = 0$ on AB, BC and CD.
- No restriction on normal displacements where p prescribed.

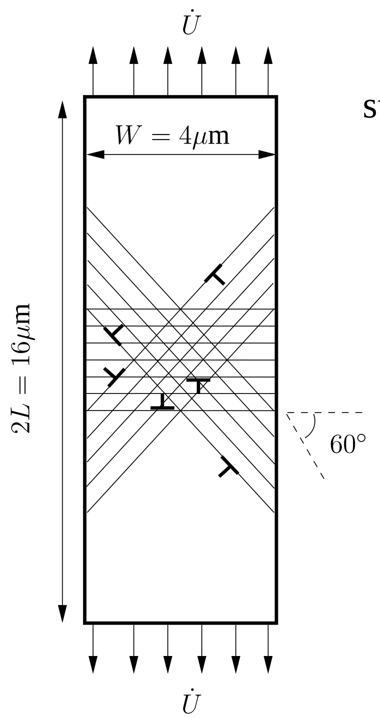
Cohesive Relations

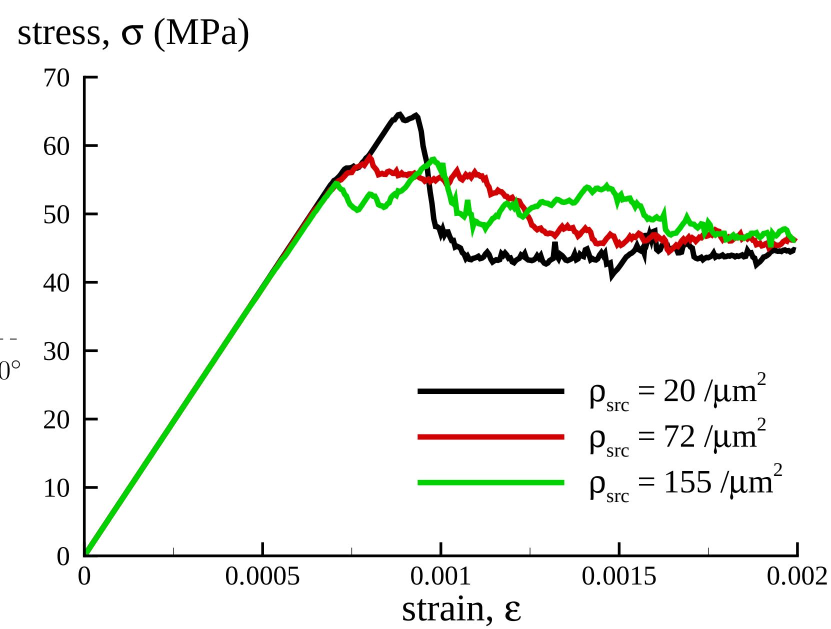




Parameters and Stress-Strain Response

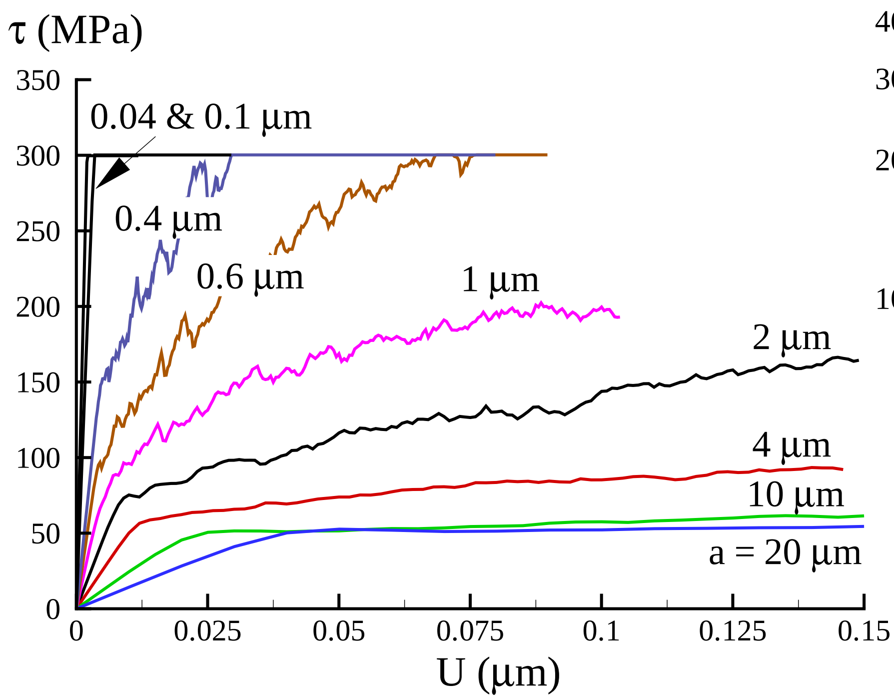
- $E = 70$ GPa, $\nu = 0.33$.
- $b = 0.25$ nm, active slip plane spacing $100b$, $B = 10^{-4}$ Pa s, $L_e = 6b$.
- mean $\bar{\tau}_{\rm nuc} = 50$ MPa with standard deviation 10 MPa, $t_{\rm nuc} = 10$ ns, $\tau_{\rm obs} = 150$ MPa.
- $\rho_{\rm src} = 72\ /\mu{\rm m}^2$, $\rho_{\rm obs} = 124\ /\mu{\rm m}^2$.

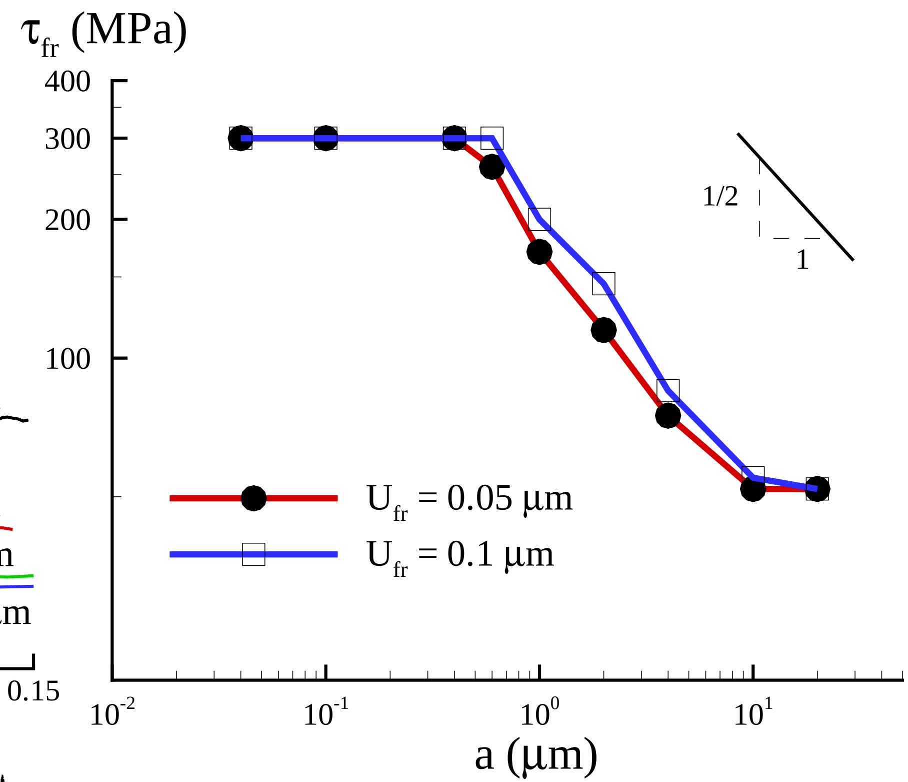


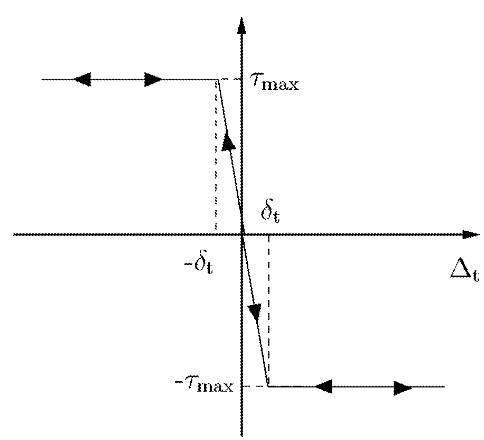


Effect of Contact Size

- Non-softening cohesive relation; $\tau_{\max} = 300$ MPa.
- $p = 0$.

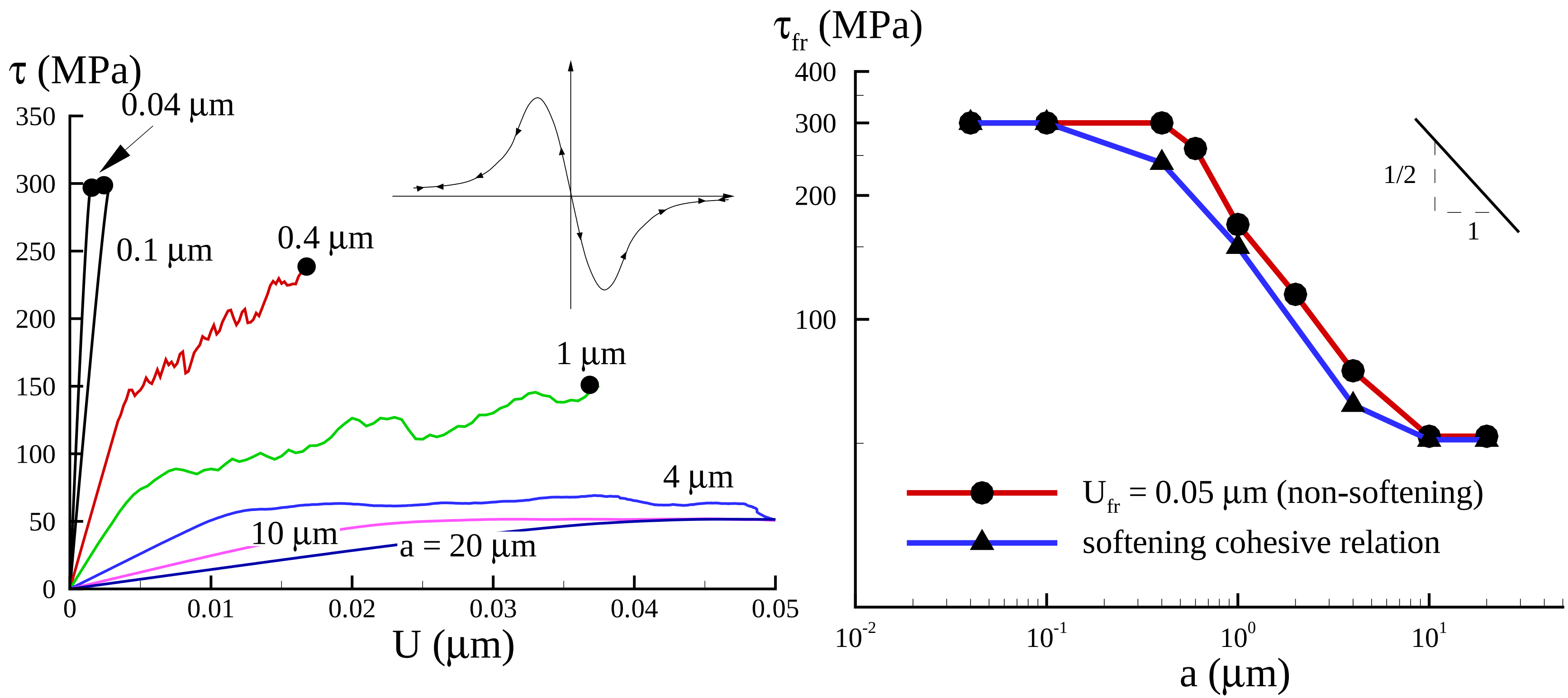






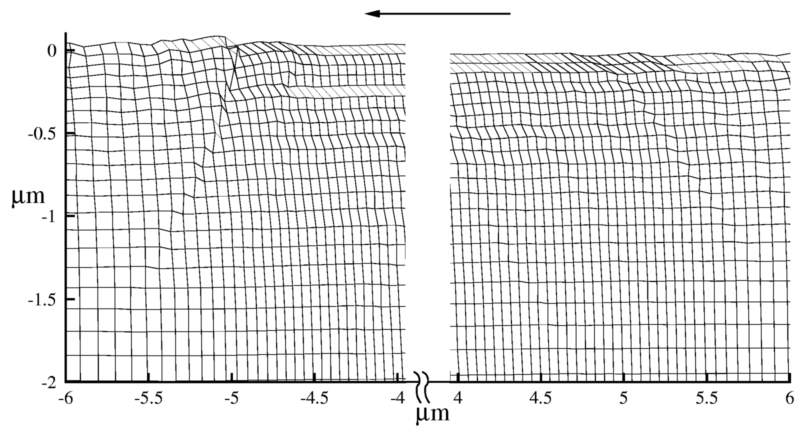
Effect of Contact Size

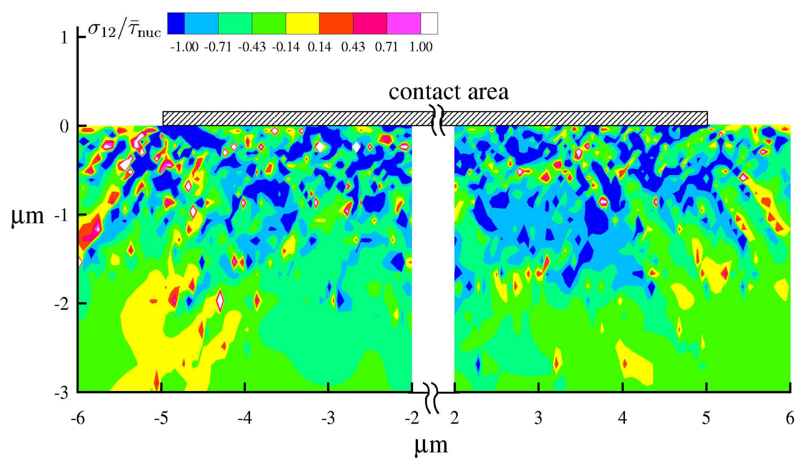
- Softening cohesive relation; $\tau_{\max} = 300$ MPa.
- $p = 0$.

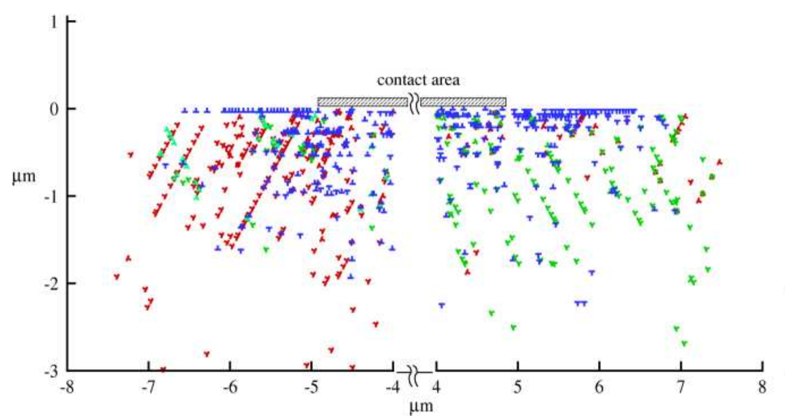


- Overall behavior is the same for both cohesive relations.
- Qualitative features are the same as in the Hurtado-Kim (1999) model even though the physics is very different.

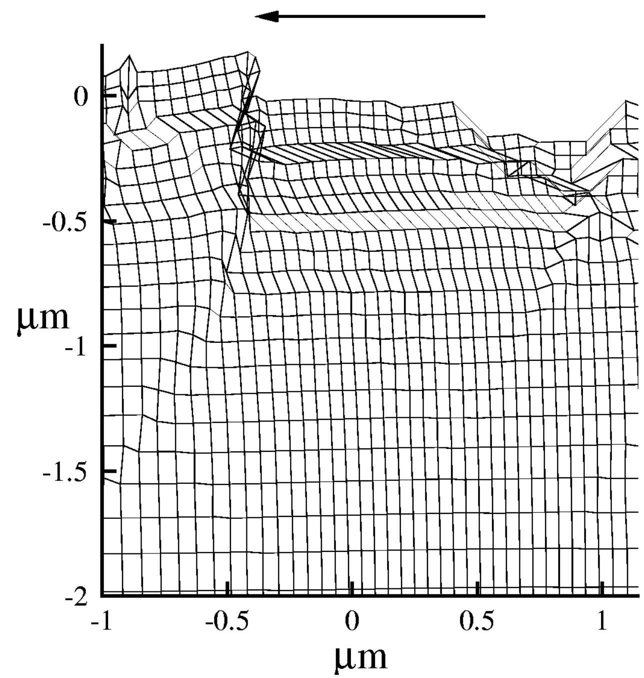
10 μm Contact

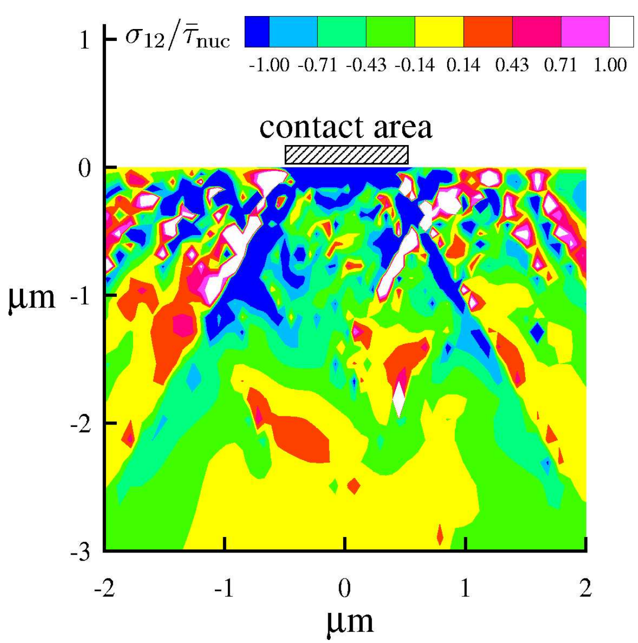


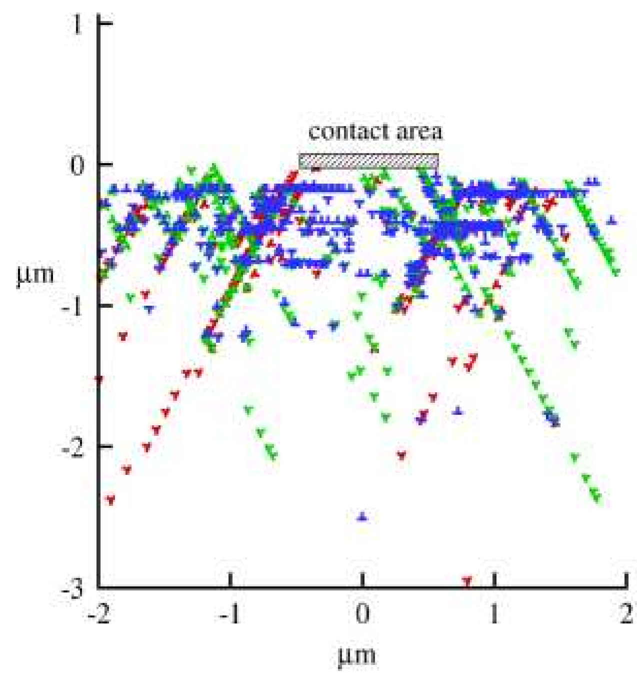




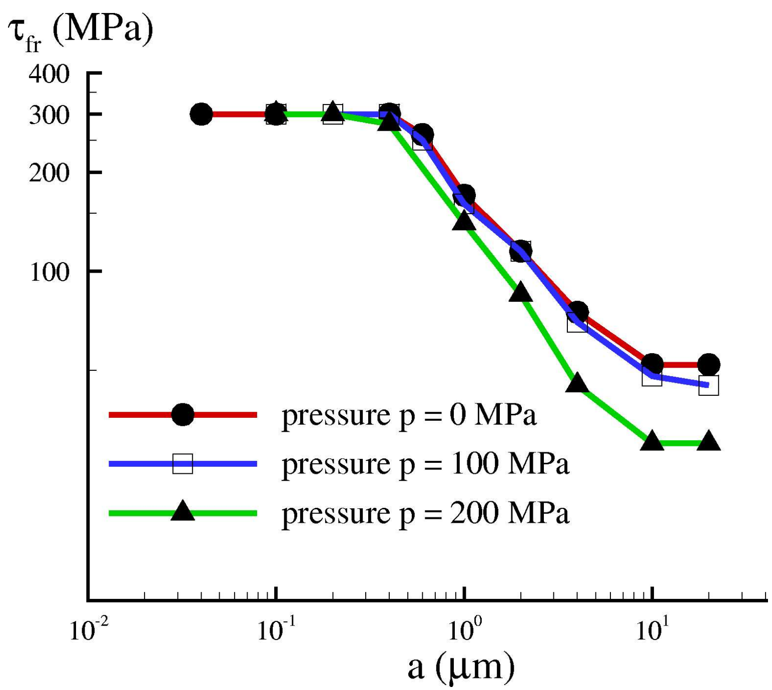
1 μm Contact

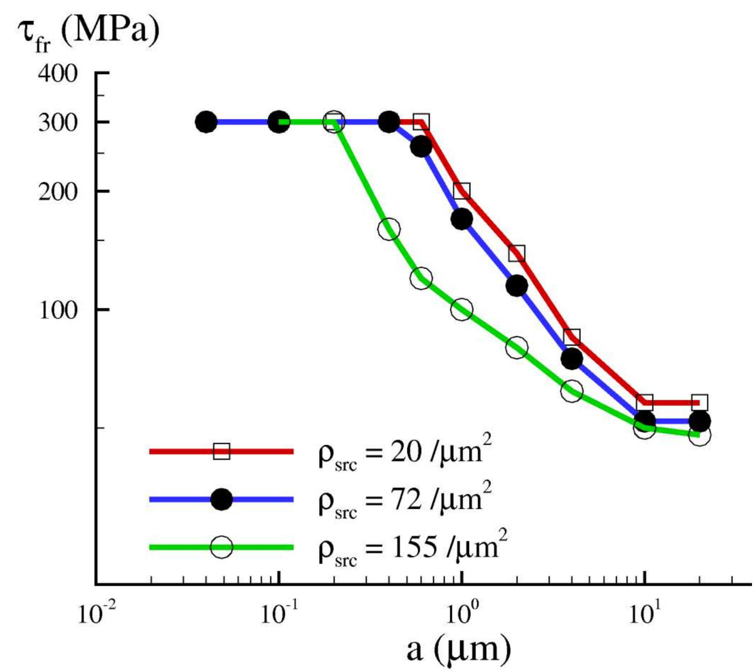


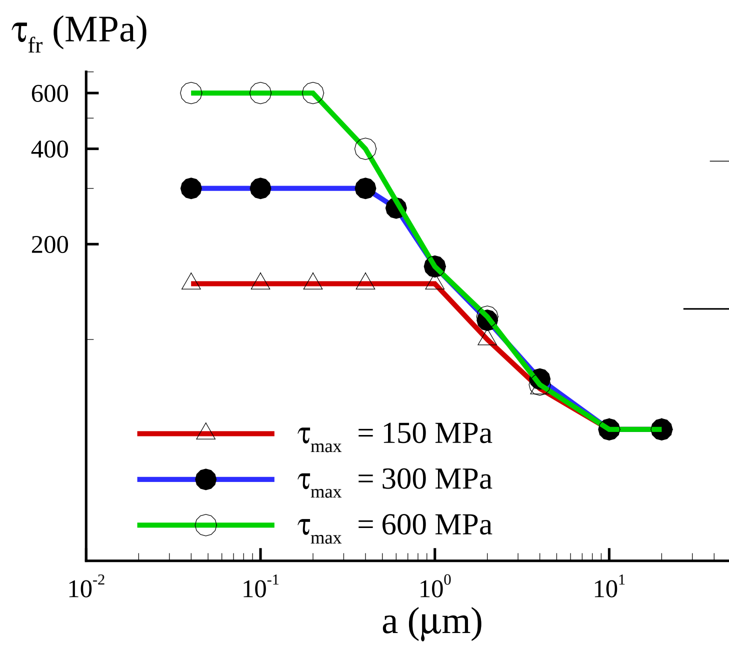




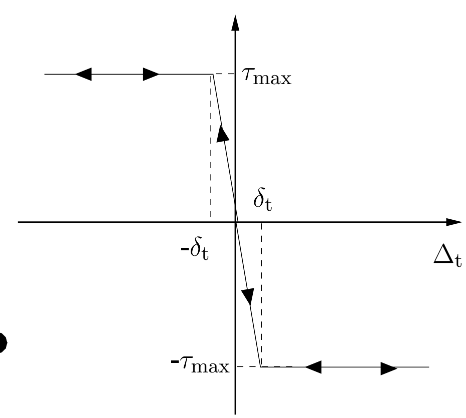
Parameter Studies



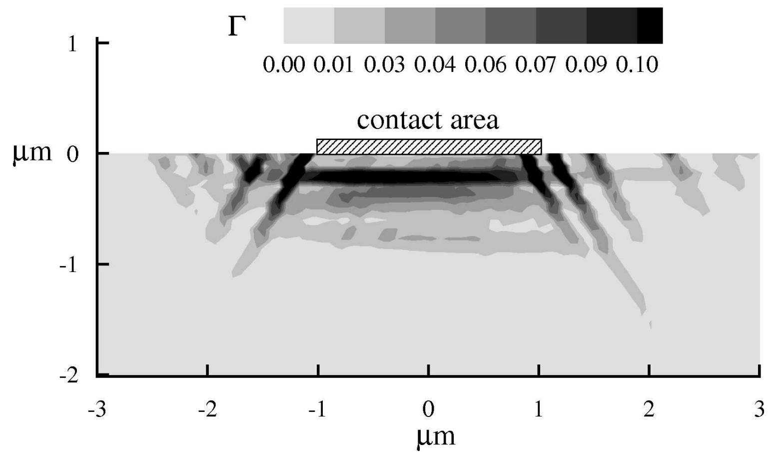




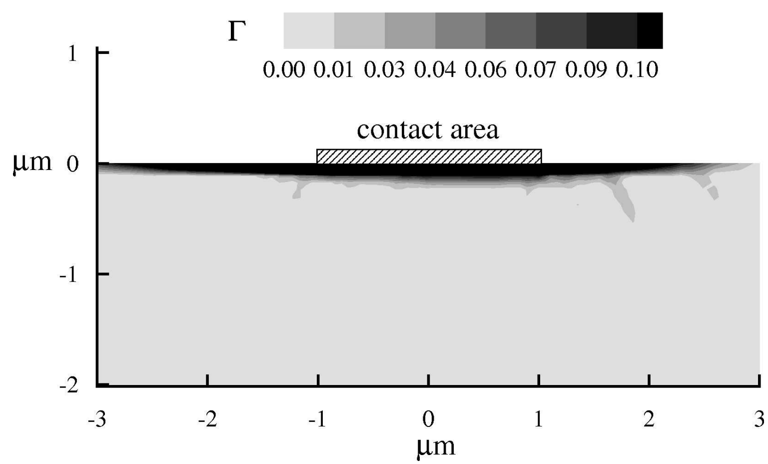
Non−softening relation



Effect of Source Density



$$\rho_{\mathrm{src}} = 72\ /\mu\mathrm{m}^2$$



$$\rho_{\mathrm{src}} = 155\ /\mu\mathrm{m}^2$$

At a sufficiently high source density, the slip mode approaches that of conventional ideal plasticity.

Plastic Dissipation

- Conservation of energy:

$$W = a \int_0^U \tau dU = \Phi + W_{\text{plas}} + W_{\text{cohes}}$$

- Elastic energy (excluding a region of radius $4b$ around each dislocation core):

$$\Phi = \int_A \frac{1}{2} \sigma_{ij} \left(\hat{\epsilon}_{ij} + \tilde{\epsilon}_{ij} \right) dA$$

- Cohesive energy:

$$W_{\text{cohes}} = \int_{S_{\text{coh}}} \left[\int T_t d\Delta_t \right] dS$$

Plastic Dissipation

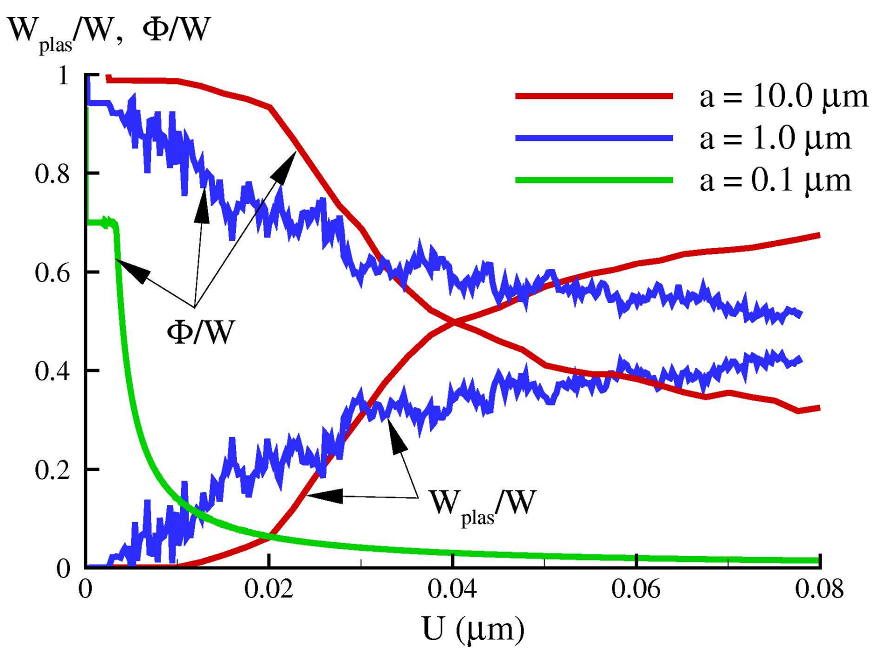
$$W_{\text{plas}} = a \int_0^U \tau dU - \Phi - W_{\text{cohes}}$$

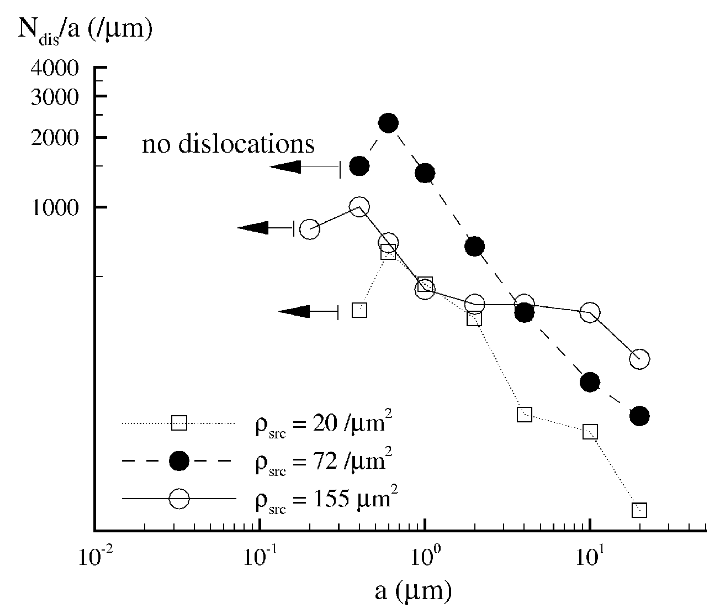
- Direct calculation of W_{plas} is complicated by the fact that the plastic part of the deformation involves displacement jumps across the slip planes so that the displacement gradient field involves delta functions.
- Approximation – introduce a smooth strain rate field, $\dot{\epsilon}^{\text{d}}_{ij}$, in each finite element by differentiating the total displacement rate field $\dot{u}_i$ in that element using the finite element shape functions:

$$W_{\text{plas}} = \int_A w_{\text{plas}} dA \quad w_{\text{plas}} = \int_0^t \sigma_{ij} \dot{\epsilon}^{\text{d}}_{ij} dt - \frac{1}{2} \sigma_{ij} \left(\hat{\epsilon}_{ij} + \tilde{\epsilon}_{ij} \right)$$

Plastic Dissipation

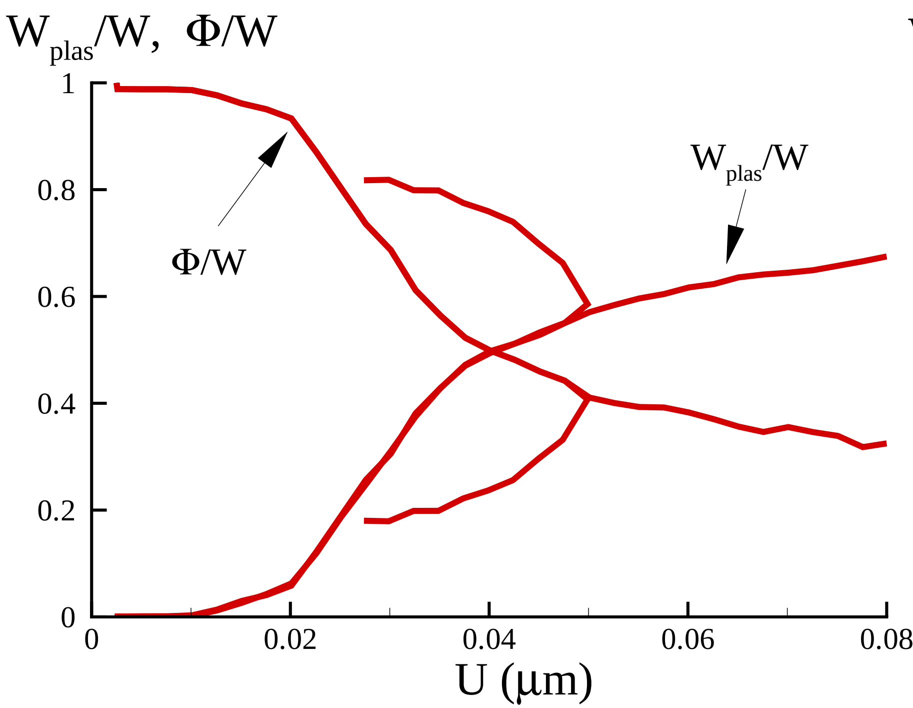
- For a sufficiently large contact size, the energy is mainly partitioned into elastic energy and plastic dissipation.
- The elastic energy involves energy stored in the dislocation structure and the energy associated with the applied loads.
- Below a critical contact size, there are no dislocations and the cohesive energy dominates.



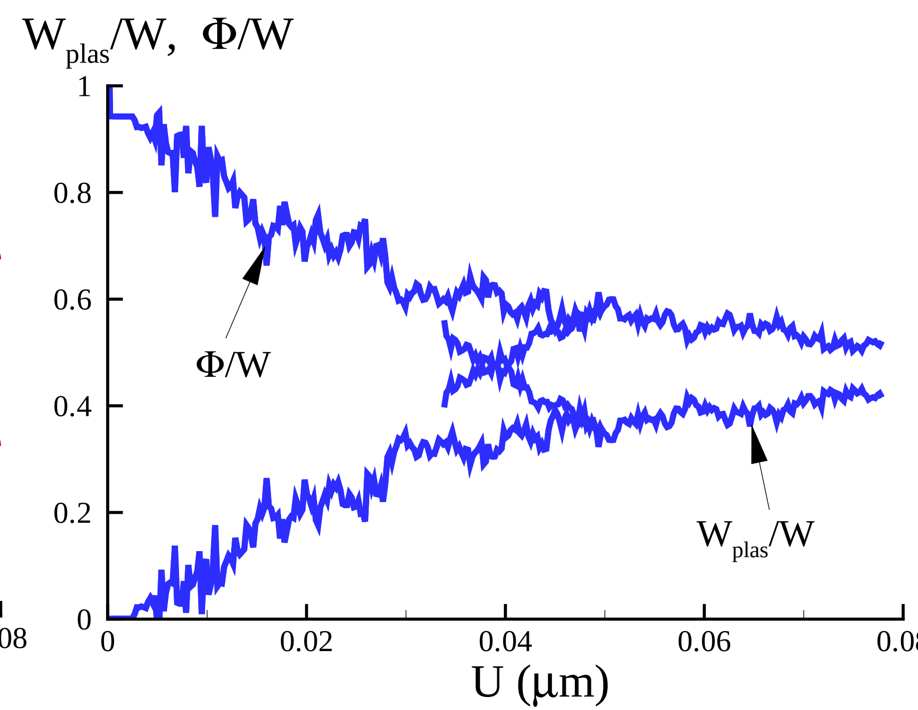


Unloading

- Less than 20 % stored energy for the $a = 10\mu$m contact.
- About 40 % stored energy for the $a = 1\mu$m contact.

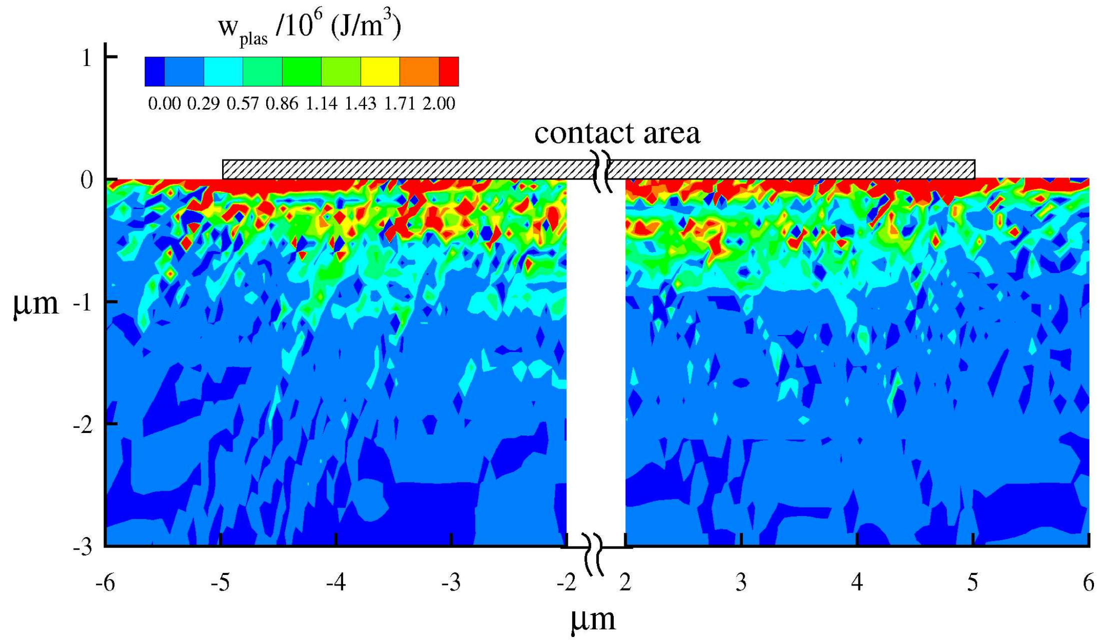


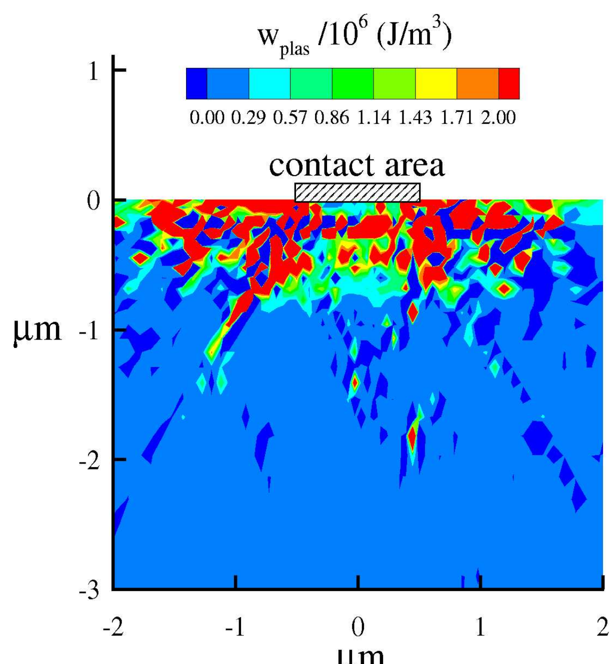
a = 10 μm



a = 1 μm

Local Plastic Dissipation





Contact Interactions

Comparison with conventional crystal plasticity.

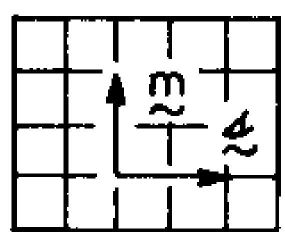
- Geometry changes neglected.

$$\dot{\epsilon}_{ij} = \frac{1}{2}\left(\dot{u}_{i,j} + \dot{u}_{j,i}\right) \qquad \dot{\epsilon}_{ij} = \dot{\epsilon}^{e}_{ij} + \dot{\epsilon}^{p}_{ij}$$

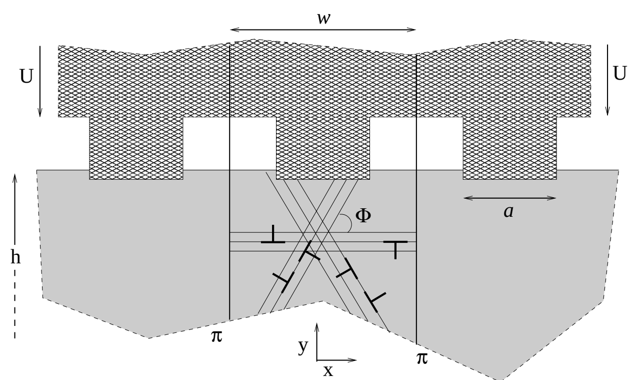
- Slip on discrete slip systems.

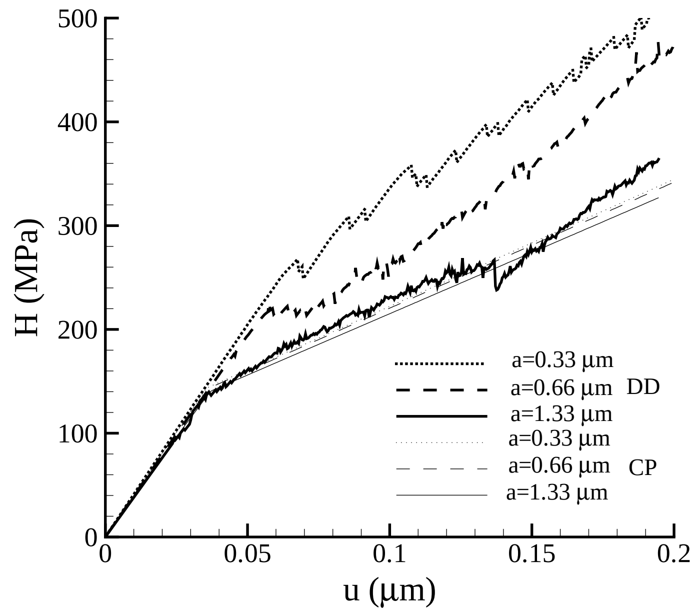
$$\dot{\epsilon}^{p}_{ij} = \sum_{\alpha=1}^{3} \frac{\dot{\gamma}^{(\alpha)}}{2}\left(s_i^{(\alpha)} m_j^{(\alpha)} + s_j^{(\alpha)} m_i^{(\alpha)}\right)$$

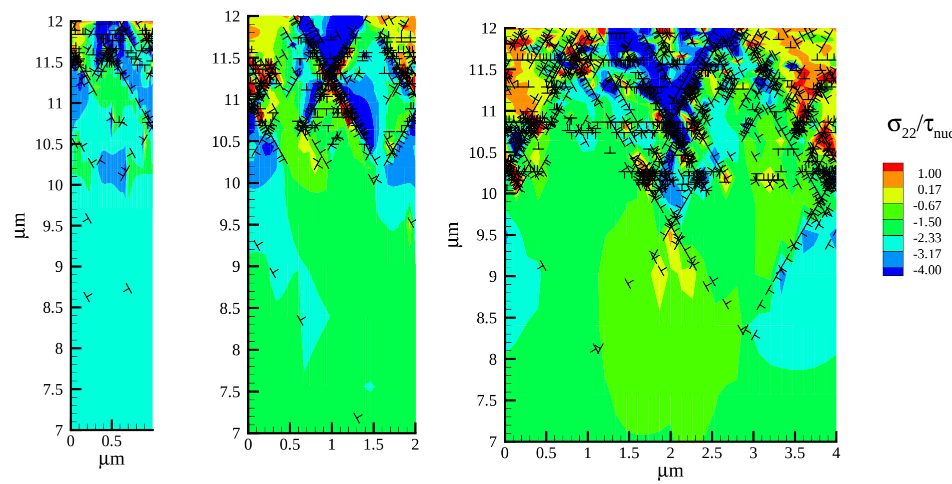
- Equal flow strength on all slip systems; linear hardening.



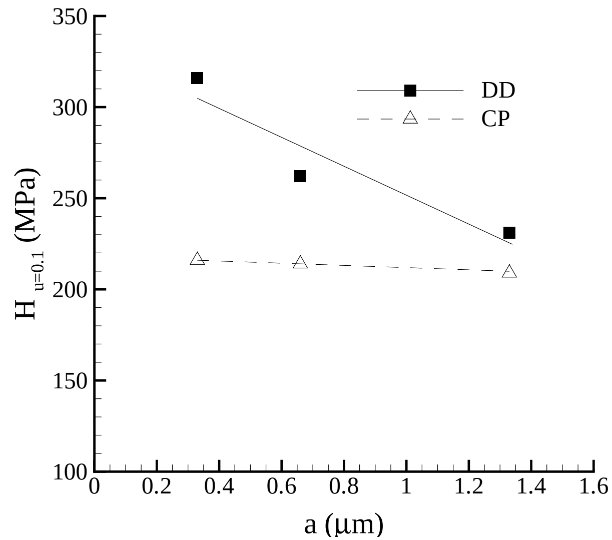
Contact Interactions

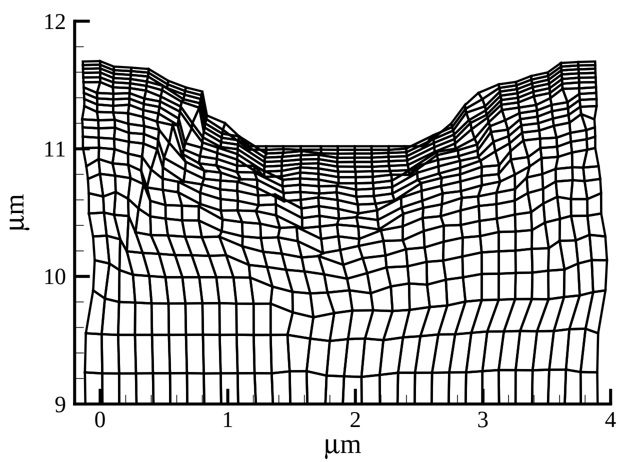


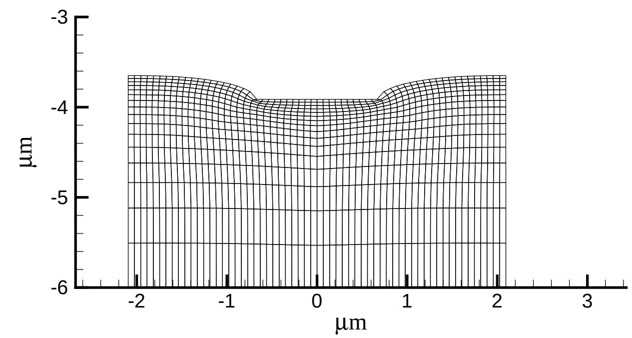




Contact Interactions







Concluding Remarks

- For sufficiently small contact sizes, adhesion dominates, $\tau_{\rm fr} = O(\tau_{\rm max})$; for sufficiently large contacts plasticity dominates, $\tau_{\rm fr} = O(\sigma_Y)$; in the intermediate regime, $\tau_{\rm fr} \propto a^{-1/2}$, but this scaling can be lost for a high source density.
  - For large large contact sizes (and high source densities), slip and plastic dissipation is mainly in a band at the surface and parallel to it.
  - In the intermediate regime, slip is oblique to the surface, creating an asperity ahead of the slider even for an initially flat surface, high plastic dissipation extends further into the material and the relative amount of energy stored in the dislocation structure is greatest.
- The scaling (with both size and material properties) can be quite different from what conventional continuum plasticity predicts.