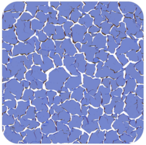
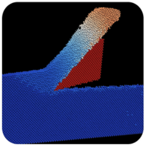
Plastic activity in nanoscratch molecular dynamics simulations of pure aluminum

Till Junge, J.F. Molinari, G. Anciaux

LSMS
Laboratoire de Simulation en Mécanique des Solides
Computational Solid Mechanics Laboratory

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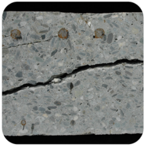
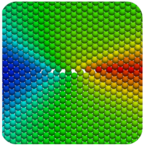




Outline

Outline

MD modeling of friction

Brief History of Friction Modeling

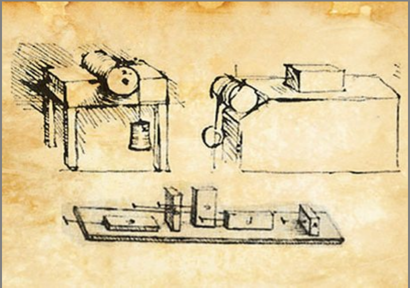
Roughness Hypothesis

Leonardo da Vinci (1495), Later Coulomb, Amontons

Observation

$$F = \mu N \qquad \forall A_{\text{app}}$$

Da Vinci Friction Experiments



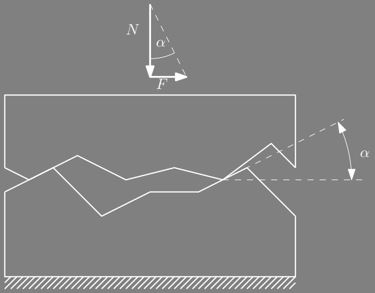
Roughness Hypothesis

Leonardo da Vinci (1495), Later Coulomb, Amontons

Observation

$$F = \mu N \qquad \forall A_{\mathrm{app}}$$

Geometric Solution



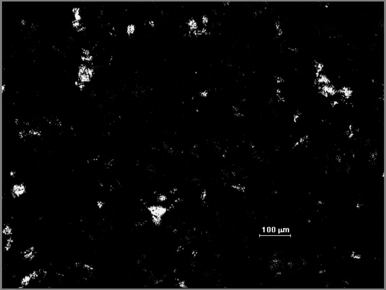
Shear Hypothesis

Bowden and Tabor (1942)

Observation

$A_{\mathrm{app}} \neq A_{\mathrm{real}}(N)$

Contact Area *Dieterich et al. (1996)*



calcite at 30 MPa

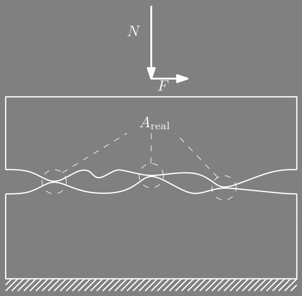
Shear Hypothesis

Bowden and Tabor (1942)

Observation

$A_{\text{app}} \neq A_{\text{real}}(N)$

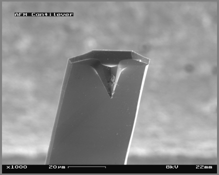
Continuum Mechanics Solution

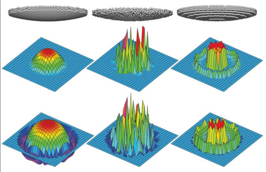


Towards the atomic scale: Luan and Robbins (2005)

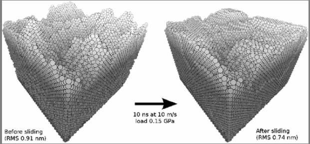
Observation

Continuum mechanics break down at contacts





Atomic force microscopy *Luan, Robbins (2005)*



Spijker et al. (2011)

Towards the atomic scale: Luan and Robbins (2005)

Observation

Continuum mechanics break down at contacts

Continuum Mechanics Solution

? (Scale too small)

Molecular Dynamics Solution

? (problems too big)

Involved Mechanisms

- Elasticity
- Plasticity
- Heating
- Asperity Locking
- Lattice Vibrations
- . . .

Involved Mechanisms

- Elasticity
- **Plasticity**
- Heating
- Asperity Locking
- Lattice Vibrations
- ...

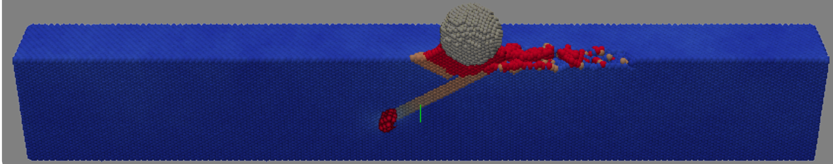
Plasticity in friction is

- poorly investigated
- atomic scale

MD modeling of friction

MD scratching

Molecular dynamics scratching simulation at $\sim 0\,\mathrm{K}$



Advantages

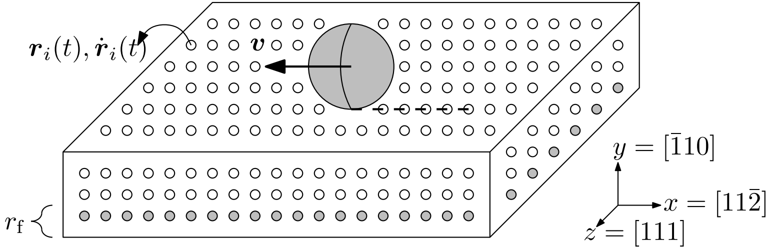
- Very few a priori assumptions (Semi-empirical potentials)
- Deep understanding because of complete knowledge of each atom in the simulation box
- Dislocation nucleation and motion handled accurately

MD modeling of friction

Computation of plastic work E_{pl} — Part I: MD Simulation

Setup

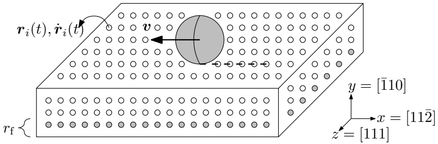
- fixed boundary conditions for bottom atoms
- prescribed indenter path $x(t)$



During simulation

- Evaluate force $F(t)$ acting on the indenter at every time step,
- Save positions $\boldsymbol{r}_i(t)$ and velocities $\dot{\boldsymbol{r}}_i(t)$ periodically

Computation of plastic work $E_{\rm pl}$ — Part II: Energy Balance

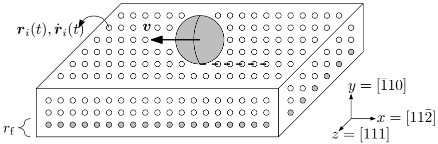


Energy influx

$$E_{\rm in}(t) = \int_0^t \boldsymbol{F}(\tau) \cdot \boldsymbol{v} \, \mathrm{d}\tau$$

MD modeling of friction

Computation of plastic work E_{pl} — Part II: Energy Balance



Energy influx

$$E_{\text{in}}(t) = \int_0^t \boldsymbol{F}(\tau) \cdot \boldsymbol{v} \, \mathrm{d}\tau$$

Stored as

$$\begin{aligned} E(t) &= E\left[\boldsymbol{r}_1, \dots, \boldsymbol{r}_N, \dot{\boldsymbol{r}}_1, \dots, \dot{\boldsymbol{r}}_N\right](t) \\ &= E_{\text{pot}}\left[\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \dots\right](t) \\ &+ E_{\text{kin}}[\dot{\boldsymbol{r}}_1, \dot{\boldsymbol{r}}_2, \dot{\boldsymbol{r}}_3, \dots](t) \end{aligned}$$

Stored Energy

$$E = E_{\mathrm{pot}}\left[\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \ldots\right] + E_{\mathrm{kin}}[\dot{\boldsymbol{r}}_1, \dot{\boldsymbol{r}}_2, \dot{\boldsymbol{r}}_3, \ldots]$$

Potential Energy

- empirical interatomic potential function
- e.g., EAM:

$$E_{\mathrm{pot}_i} = \tfrac{1}{2}\sum_{i\neq j} V(r_{ij}) + \sum_i \Phi\left(\sum_{i\neq j} \rho(r_{ij})\right)$$

Kinetic Energy

- Classical mechanics:

$$E_{\mathrm{kin}\,i} = \tfrac{1}{2} m_i \dot{\boldsymbol{r}}_i^2$$

- summed over all atoms

Stored Energy

$$E = E_{\mathrm{pot}}\left[\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \ldots\right] + E_{\mathrm{kin}}[\dot{\boldsymbol{r}}_1, \dot{\boldsymbol{r}}_2, \dot{\boldsymbol{r}}_3, \ldots]$$

Potential Energy

- empirical interatomic potential function
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~~Kinetic Energy~~

- ~~Classical mechanics:~~

$$\require{cancel}\cancel{E_{\mathrm{kin}_i} = \tfrac{1}{2} m_i \dot{\boldsymbol{r}}_i^2}$$

- ~~summed over all atoms~~

But we won't use this!

MD modeling of friction

Computation of plastic work E_{pl} — Part III: Minimizing Potential Energy

Main Idea

Monitor variation of potential energy at $0\,\mathrm{K}$: $\Delta E_{\text{pot}}(0\,\mathrm{K}) = E_{\text{pl}}$

Problem

MD snapshots $\{\boldsymbol{r}_i, \dot{\boldsymbol{r}}_i\}(t)$ are **close** to static equilibrium ($\sim 0\,\mathrm{K}$)

MD modeling of friction

Computation of plastic work E_{pl} — Part III: Minimizing Potential Energy

Main Idea

Monitor variation of potential energy at $0\,\mathrm{K}$: $\Delta E_{\mathrm{pot}}(0\,\mathrm{K}) = E_{\mathrm{pl}}$

Problem

MD snapshots $\{\boldsymbol{r}_i, \dot{\boldsymbol{r}}_i\}(t)$ are **close** to static equilibrium ($\sim 0\,\mathrm{K}$)

Solution

Molecular Statics:

$$E_{\mathrm{pot}}^{\mathrm{min}}(t) = \min_{\boldsymbol{R}=(\boldsymbol{r}_1,\dots,\boldsymbol{r}_N)} E_{\mathrm{pot}}(\boldsymbol{R}(t))$$

$$E_{\mathrm{pl}}(t) = E_{\mathrm{pot}}^{\mathrm{min}}(t) - E_{\mathrm{pot}}^{\mathrm{min}}(0)$$

MD modeling of friction

Computation of plastic work E_{pl}

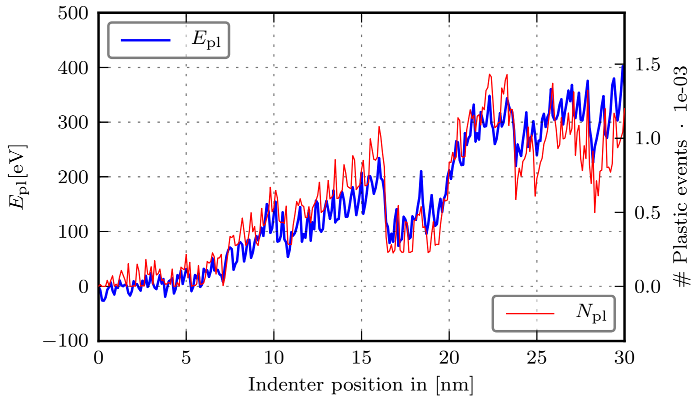
Using molecular statics (MS)

MD simulation				t
	$\{r_0, \dot{r}_0\}$	$\{r_1, \dot{r}_1\}$	$\{r_n, \dot{r}_n\}$	
MS quenching	↓	↓	↓	
	$\{r_0^{\text{min}}, 0\}$	$\{r_1^{\text{min}}, 0\}$	$\{r_n^{\text{min}}, 0\}$	
Potential Energy	E_0^{min}	E_1^{min}	E_n^{min}	
Plastic energy E_{pl}	$E_0^{\text{min}} - E_0^{\text{min}}$	$E_1^{\text{min}} - E_0^{\text{min}}$	$E_n^{\text{min}} - E_0^{\text{min}}$	

Paper in review

T. Junge et al., *Plastic activity in nanoscratch molecular dynamics simulations of pure aluminium*, submitted for publication

Plastic count vs. stored plastic energy



Compare:

B. Luan, Ph.D. thesis, Johns Hopkins University (2006)

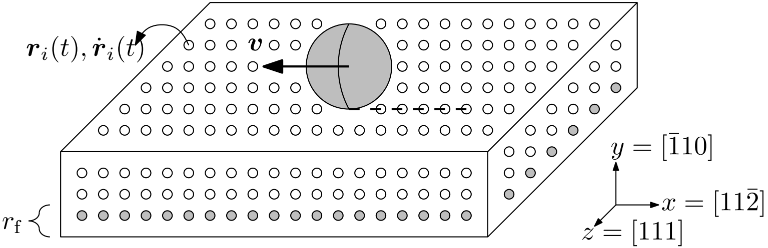
Outline

Parametric study

General setup

Setup

- fixed boundary conditions for bottom atoms
- prescribed indenter path $x(t)$



During simulation

- Evaluate force $F(t)$ acting on the indenter at every time step,
- Save positions $\boldsymbol{r}_i(t)$ and velocities $\dot{\boldsymbol{r}}_i(t)$ periodically

Parametric study

Parameter space

Space is split in three groups

In common:

- substrate thickness and width
- scratch path length
- every scratch performed at the same five indentation depths:

  $\Delta y \in \{0, 1, 2, 5, 10\}$ Å
- rigid indenter
- Mendelev EAM Aluminum potential

Substrate thickness

$h \in \{22.9, 45.8, 91.5, 183.1, 366.1\}$ Å
at $v = 10$ m/s

Scratch speed

$v \in \{2.5, 5, 10, 20, 40, 80, 1000\}$ m/s
at $h = 45.8$ Å

Microstructure

- 40 or 200 grains
- 2 different random seeds
- $h = 91.5$ Å, $v = 10$ m/s

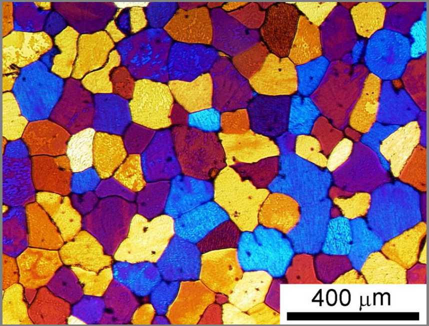
M. I. Mendelev et al., Philosophical Magazine 88 (12), 1723-1750

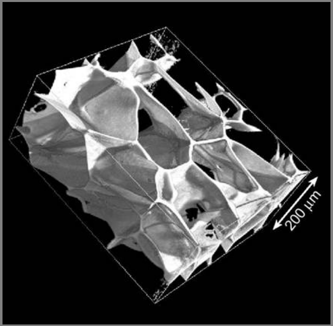
Outline

Single phase polycrystals

Real polycrystals

Single phase aluminum





Sources:

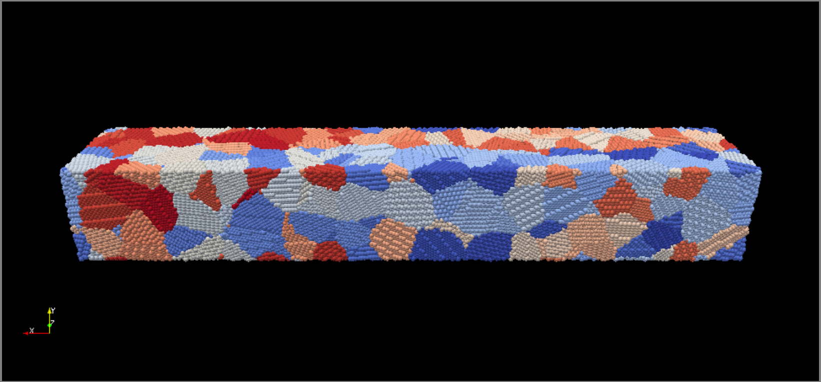
T. Quested, DoITPoMS, Micrograph 712

K. M. Döbrich et al., Metall. Trans. A 35, 1953–1961, (2004).

Single phase polycrystals

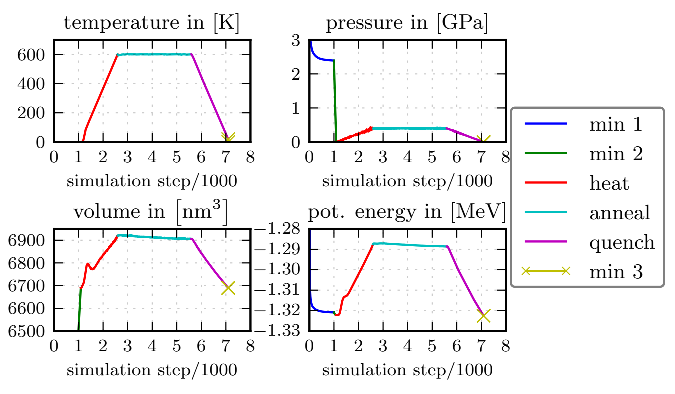
MD polycrystals

Voronoi tesselation



- Voronoi nuclei randomly positioned
- Periodic boundary conditions in all directions
- Random lattice orientation assigned to each cell

Annealing and relaxation of microstructure (heuristic)



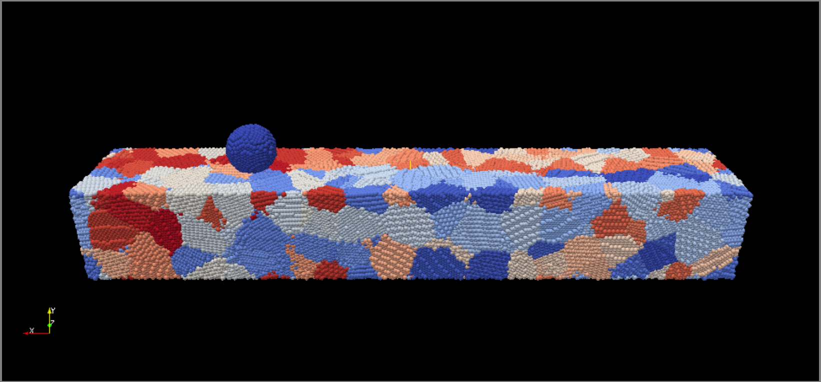
Similar:

H. van Swygenhoven, Acta Materialia 54 (7), 1975, (2006)

Single phase polycrystals

MD polycrystals

Final structure



- split microstructure, insert indenter
- fix bottom layer and indenter
- constrained minimisation of potential energy

Outline

MD modeling of friction

Parametric study

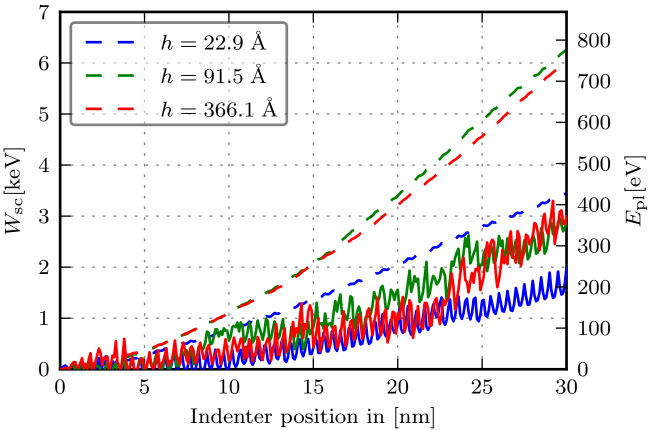
Single phase polycrystals

Results
- Stored plastic energy E_{pl}
- Microscopic friction coefficient μ
- Thermal sensitivity s

Results

Stored plastic energy E_{pl}

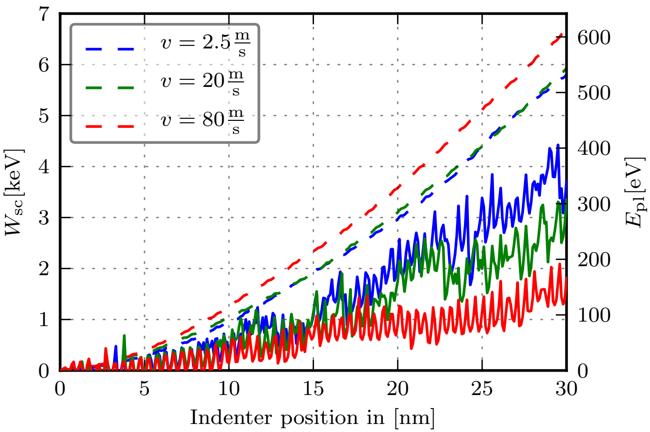
Effect of substrate thickness h



Results

Stored plastic energy E_{pl}

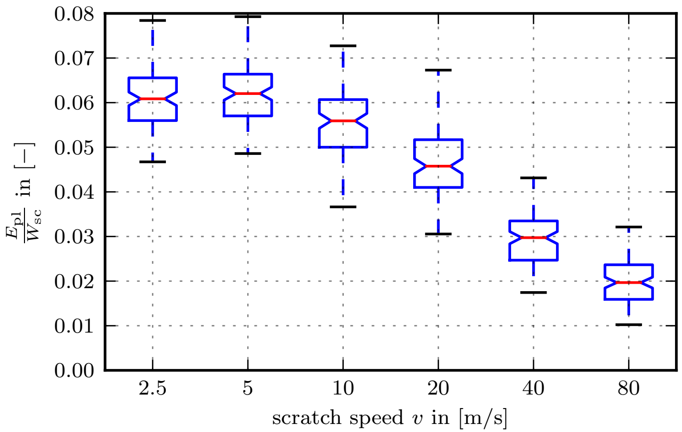
Effect of scratch speed v



Results

Stored plastic energy E_{pl}

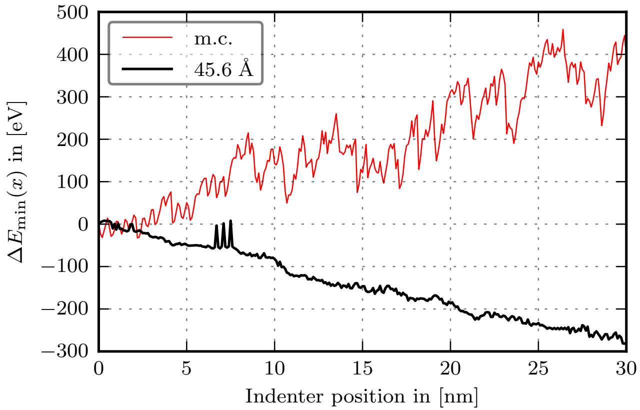
Relative plastic contribution $E_{\text{pl}}/W_{\text{sc}}$ decreases with speed



Results

Stored plastic energy E_{pl}

Effect of microstructure is non-trivial/counterintuitive



Results

Microscopic friction coefficient μ

Macroscopic friction model

$$\mu \equiv \frac{\mathrm{d}F}{\mathrm{d}N} \Leftrightarrow F(N;\mu,f_\mathrm{a}) = f_\mathrm{a} + \mu N$$

Microscopic translation

Large fluctuations at nano-scale $\Rightarrow$ window-average forces:

$$\langle F \rangle_i = \tfrac{1}{N_\mathrm{w}} \textstyle\sum_j^{N_\mathrm{w}} F(t_{i+j})$$

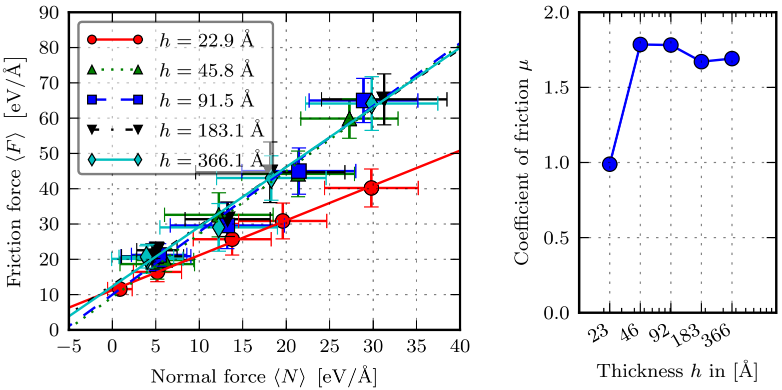
Least–squares–fit the coefficient

$$\mu = \underbrace{\arg\min}_{\hat{\mu}} \left(\left[F(\langle \boldsymbol{N} \rangle, \hat{\mu}) - \langle \boldsymbol{F} \rangle \right]^2 \right)$$

Results

Microscopic friction coefficient μ

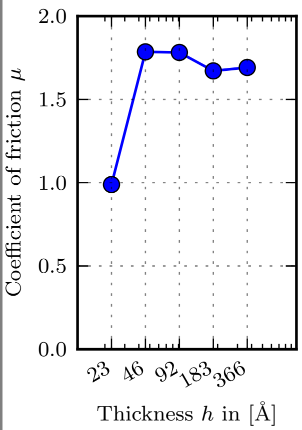
Effect of substrate thickness h



Results

Microscopic friction coefficient μ

Thickness h

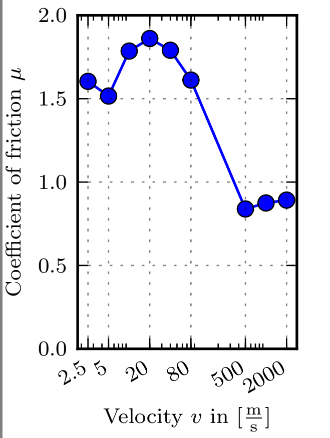


- Linearity!
- Coefficient large by continuum standards
- No simulation box size dependence for thick substrates
- Suppressed plasticity for thin substrate leads to lower μ

Results

Microscopic friction coefficient μ

Scratch speed v

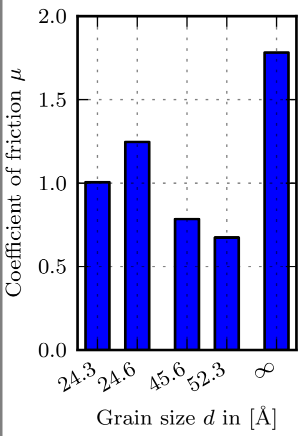


- Bell shape with trailing plateau:
  - Found in nano-machining sims
    P. A. Romero et al. Modelling Simul. Mater. Sci. Eng. 20 (2012)
  - Found in steel friction experiments
    S. Philippon et al. Wear 257 (7-8) (2004)
  - Analytically explained
    A. Molinari et al. Journal of Tribology 121/35 (1999)
- Suppressed plasticity for high speeds leads to same effect as thin substrate

Results

Microscopic friction coefficient μ

Grain size d



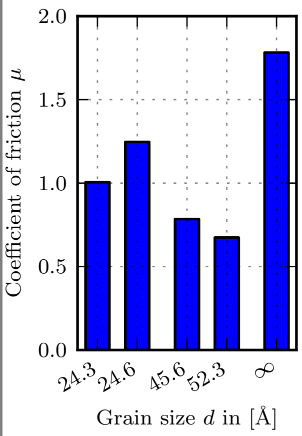
- Coefficient not explained by the grain size

  Not enough grains to average orientation effects?

Results

Microscopic friction coefficient μ

Grain size d



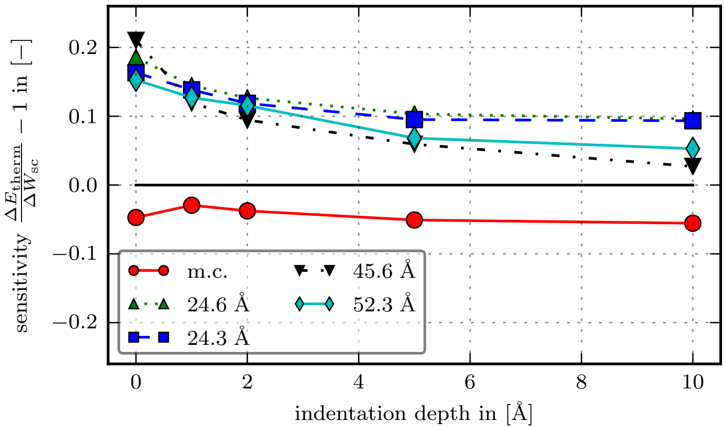
- Coefficient not explained by the grain size

  Not enough grains to average orientation effects?
- Consistently lower friction for polycrystal

Results

Thermal sensitivity s

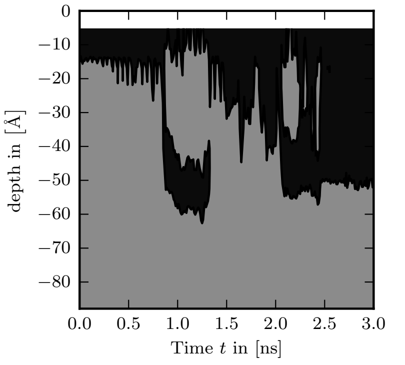
Thermal Sensitivity for different Microstructures



Results

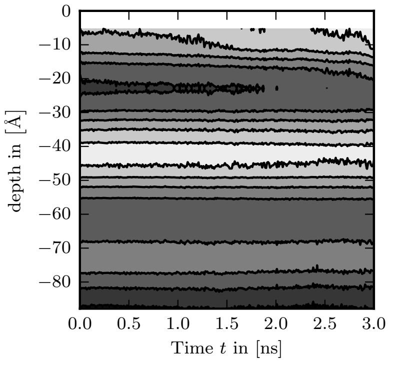
Sensitivity s – vertical centrosymmetry distribution

Growing disorder in single crystal



Plastic energy is stored

Coarsening of microstructure



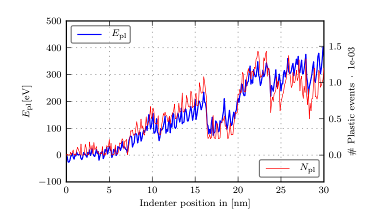
Grain boundary energy is released

Darker means higher disorder

Conclusions

1.) Computation of E_{pl}

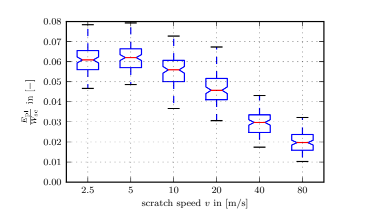
- Novel method to analyze and quantify MD friction simulations



Conclusions

1.) Computation of E_{pl}

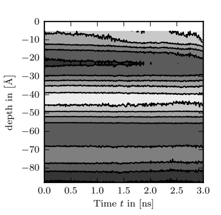
- Novel method to analyze and quantify MD friction simulations
- Showed clear negative rate correlation for high speeds, none for low



Conclusions

1.) Computation of E_{pl}

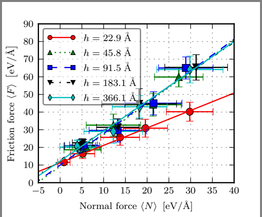
- Novel method to analyze and quantify MD friction simulations
- Showed clear negative rate correlation for high speeds, none for low
- Polycrystals can **release** stored plastic energy during scratching



Conclusions

2.) Regression-based computation of μ

- Recovered simple linear continuum friction model



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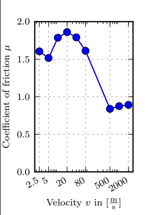
- Recovered bell-shaped speed dependence observed in machining



Conclusions

2.) Regression-based computation of μ

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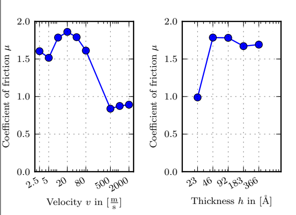
- Apparent strong link between E_{pl} and μ



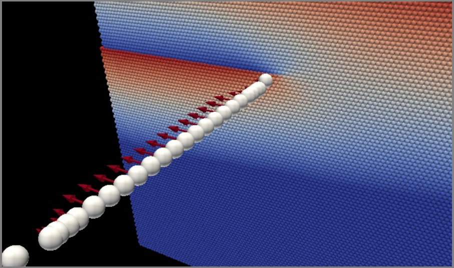
Conclusions

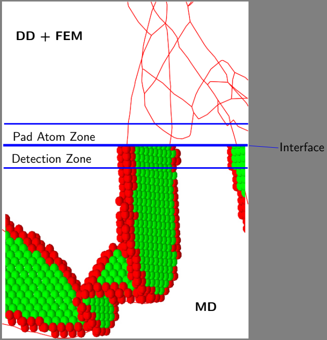
2.) Regression-based computation of μ

- Recovered simple linear continuum friction model
- Recovered bell-shaped speed dependence observed in machining
- Apparent strong link between E_{pl} and μ
- Sim box size independent for thick substrates
  Plastic zones not resolved!

Outlook

Coupled Atomistics and discrete dislocations in 3D





Under development at LSMS

Appendix

MD Polycrystals

Grain size distributions