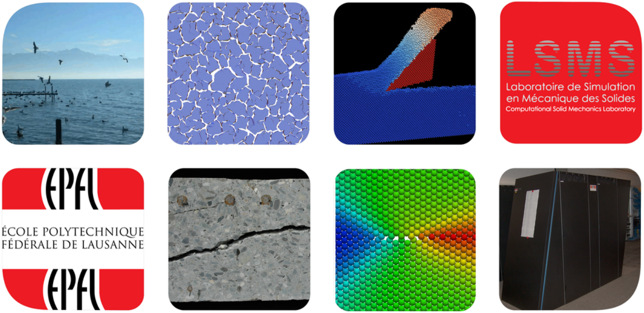
Plastic activity in nanoscratch molecular dynamics simulations of pure aluminum

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



Outline

- MD modeling of friction
  - Brief History of Friction Modeling
  - MD scratching

- Parametric study
  - General setup
  - Parameter space

- Single phase polycrystals
  - Real polycrystals
  - MD polycrystals

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

Outline

MD modeling of friction
  Brief History of Friction Modeling
  MD scratching

Parametric study

Single phase polycrystals

Results

MD modeling of friction

Brief History of Friction Modeling

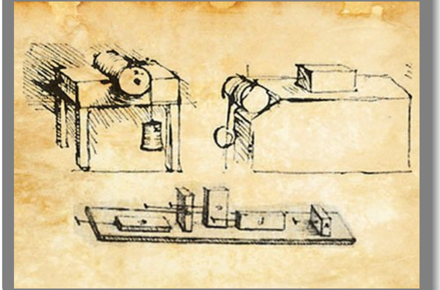
Roughness Hypothesis

Leonardo da Vinci (1495), Later Coulomb, Amontons

Observation

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

Da Vinci Friction Experiments



MD modeling of friction

Brief History of Friction Modeling

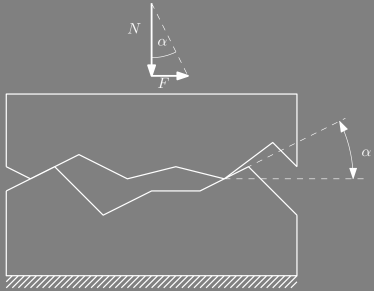
Roughness Hypothesis

Leonardo da Vinci (1495), Later Coulomb, Amontons

Observation

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

Geometric Solution



MD modeling of friction

Brief History of Friction Modeling

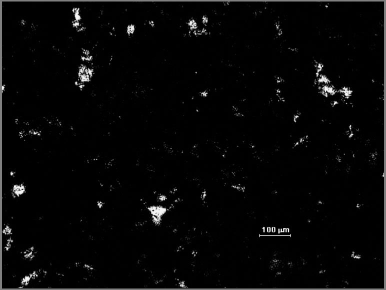
Shear Hypothesis

Bowden and Tabor (1942)

Observation

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

Contact Area *Dieterich et al. (1996)*



calcite at $30\ \mathrm{MPa}$

MD modeling of friction

Brief History of Friction Modeling

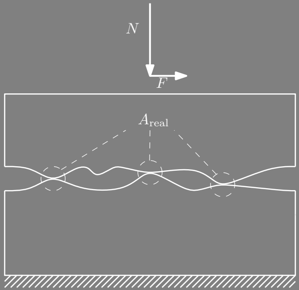
Shear Hypothesis

Bowden and Tabor (1942)

Observation

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

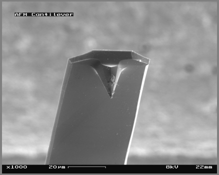
Continuum Mechanics Solution



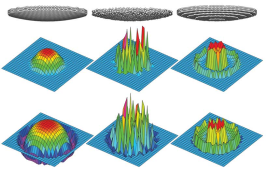
Towards the atomic scale: Luan and Robbins (2005)

Observation

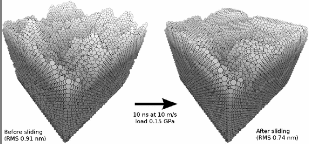
Continuum mechanics break down at contacts



Atomic force microscopy



Luan, Robbins (2005)



Spijker et al. (2011)

MD modeling of friction

Brief History of Friction Modeling

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)

MD modeling of friction

Brief History of Friction Modeling

Involved Mechanisms

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

MD modeling of friction

Brief History of Friction Modeling

Involved Mechanisms

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

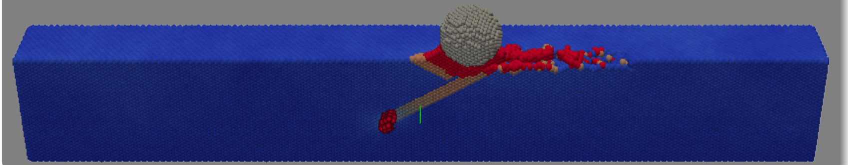
Plasticity in friction is

- poorly investigated
- atomic scale

MD modeling of friction

MD scratching

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



Advantages

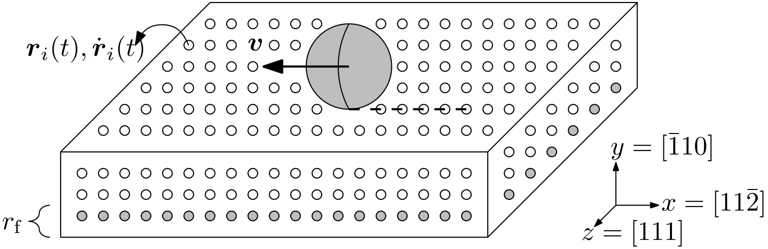
- Very few a priori assumptions (Semi-empirical potentials)
- Deep understanding because of complete knowledge of each atom in the simulation box
- Dislocation nucleation and motion handled accurately

MD modeling of friction

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

Setup

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

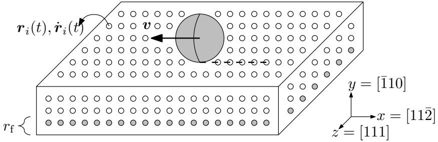


During simulation

- 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

MD modeling of friction

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

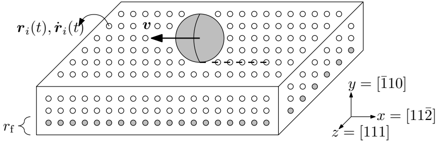


Energy influx

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

MD modeling of friction

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



Energy influx

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

Stored as

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

MD modeling of friction

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

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:

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

Kinetic Energy

- Classical mechanics:

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

- summed over all atoms

MD modeling of friction

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

Stored Energy

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

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~~Kinetic Energy~~

- ~~Classical mechanics:~~

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

- ~~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 $0\,\mathrm{K}$: $\Delta E_{\mathrm{pot}}(0\,\mathrm{K}) = E_{\mathrm{pl}}$

Problem

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

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:

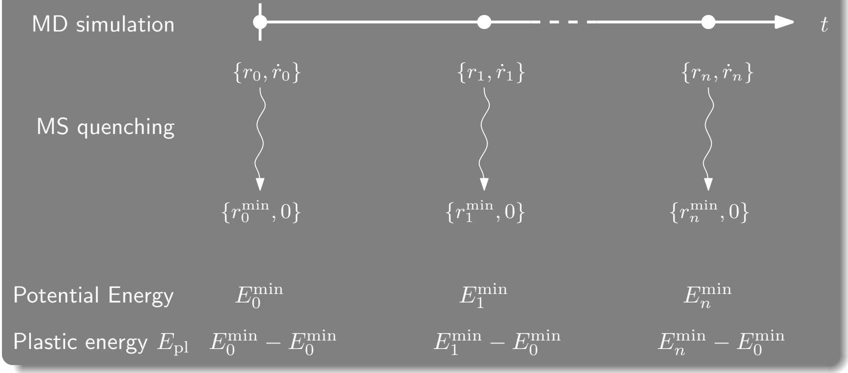
$$E_{\mathrm{pot}}^{\mathrm{min}}(t) = \min_{\boldsymbol{R}=(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N)} E_{\mathrm{pot}}(\boldsymbol{R}(t))$$

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

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			
	$\{r_0^{\mathrm{min}}, 0\}$	$\{r_1^{\mathrm{min}}, 0\}$	$\{r_n^{\mathrm{min}}, 0\}$
Potential Energy	E_0^{min}	E_1^{min}	E_n^{min}
Plastic energy E_{pl}	$E_0^{\mathrm{min}} - E_0^{\mathrm{min}}$	$E_1^{\mathrm{min}} - E_0^{\mathrm{min}}$	$E_n^{\mathrm{min}} - E_0^{\mathrm{min}}$

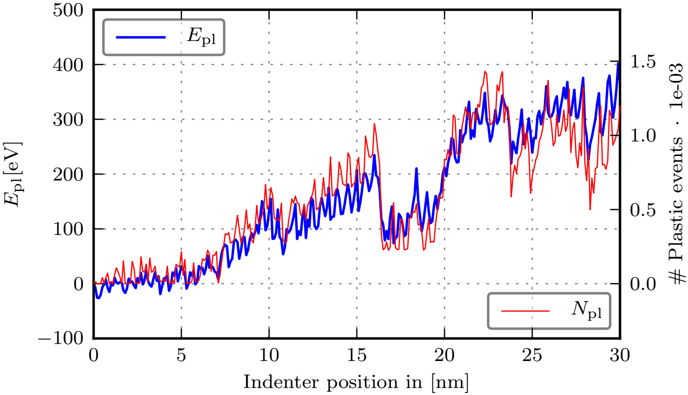
Paper in review

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

MD modeling of friction

Computation of plastic work E_{pl}

Plastic count vs. stored plastic energy



Compare:

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

Outline

MD modeling of friction

Parametric study

- General setup
- Parameter space

Single phase polycrystals

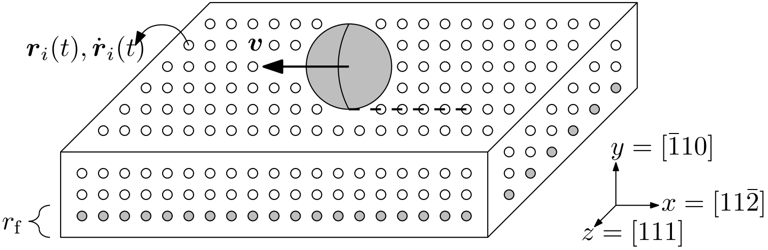
Results

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

MD modeling of friction

Parametric study

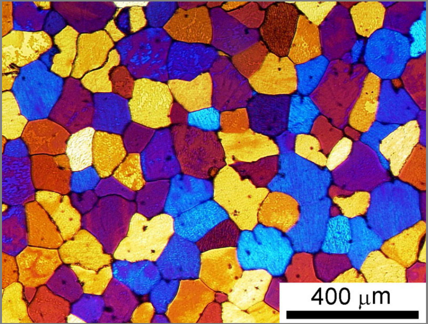
Single phase polycrystals
  Real polycrystals
  MD polycrystals

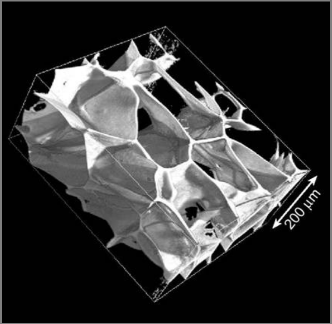
Results

Single phase polycrystals

Real polycrystals

Single phase aluminum





Sources:

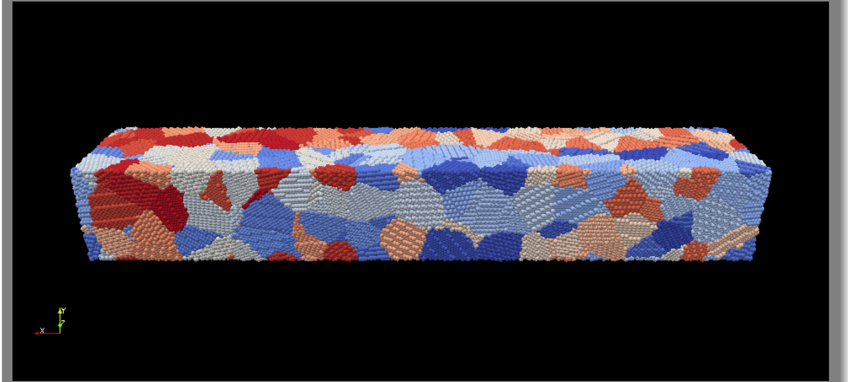
T. Quested, DoITPoMS, Micrograph 712

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

Single phase polycrystals

MD polycrystals

Voronoi tessellation

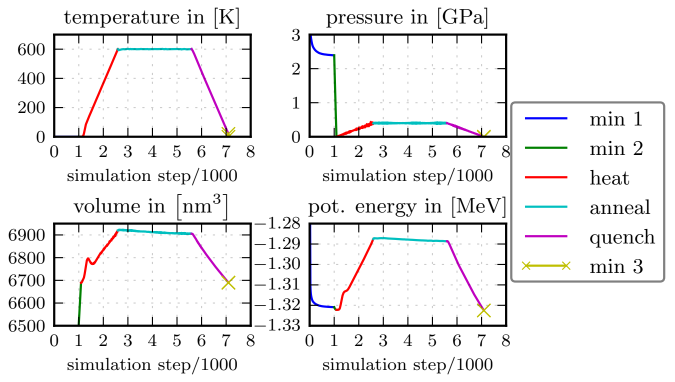


- Voronoi nuclei randomly positioned
- Periodic boundary conditions in all directions
- Random lattice orientation assigned to each cell

Single phase polycrystals

MD polycrystals

Annealing and relaxation of microstructure (heuristic)



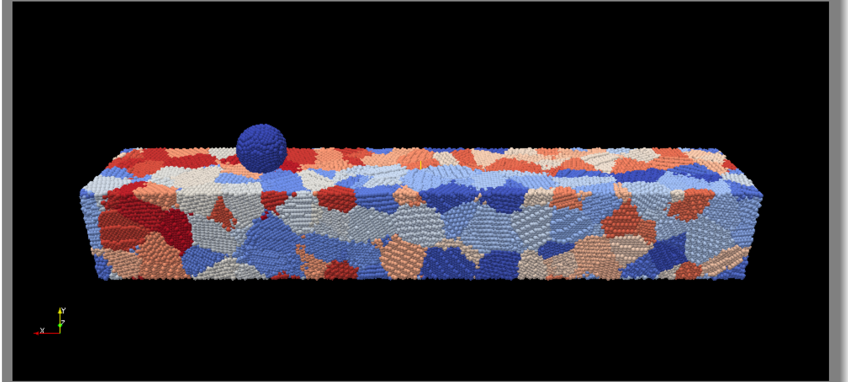
Similar:

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

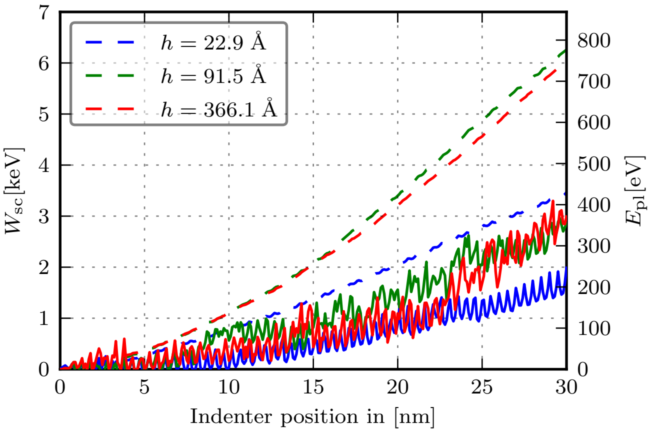
Single phase polycrystals

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

Results

Stored plastic energy E_{pl}

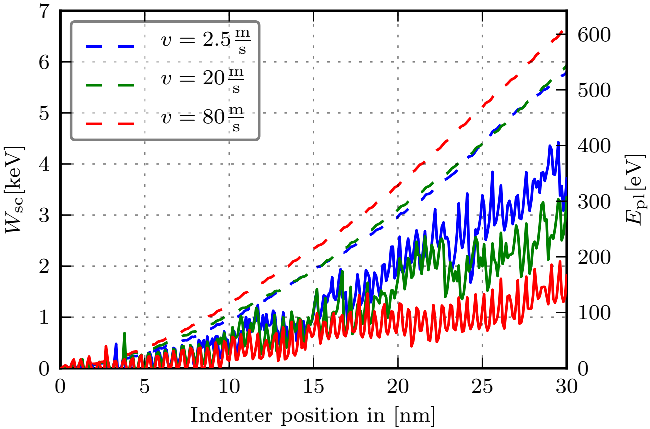
Effect of substrate thickness h



Results

Stored plastic energy E_{pl}

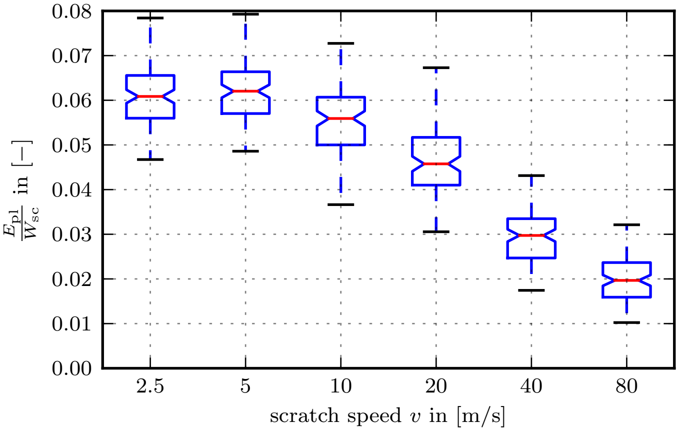
Effect of scratch speed v



Results

Stored plastic energy E_{pl}

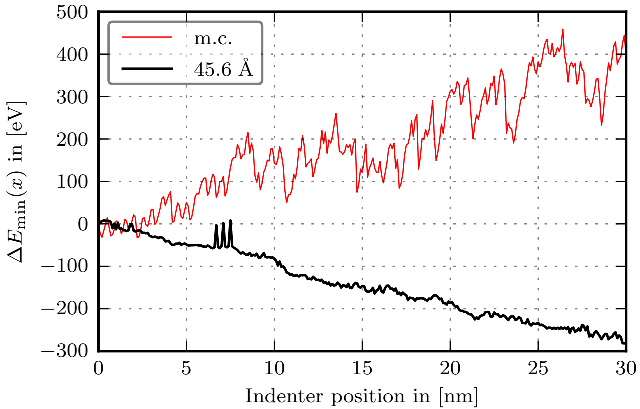
Relative plastic contribution $E_{\mathrm{pl}}/W_{\mathrm{sc}}$ decreases with speed



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:

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

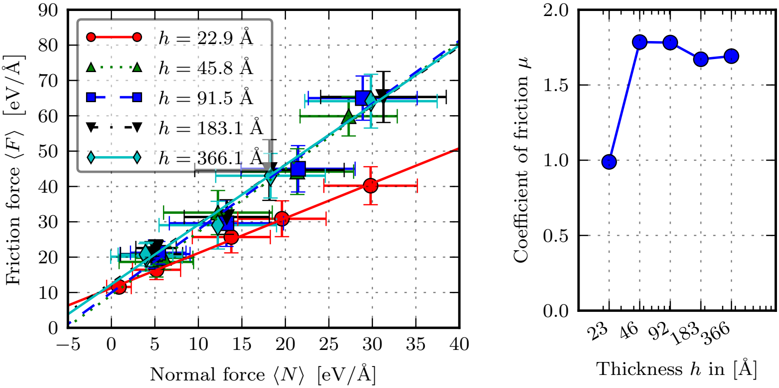
Least–squares–fit the coefficient

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

Results

Microscopic friction coefficient μ

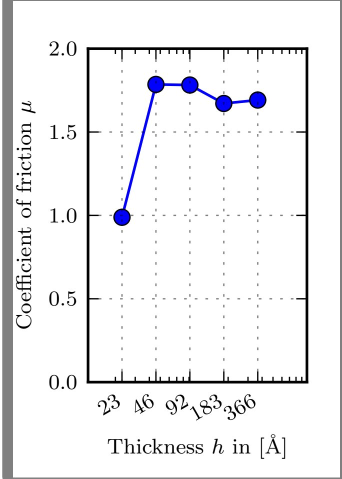
Effect of substrate thickness h



Results

Microscopic friction coefficient μ

Thickness h

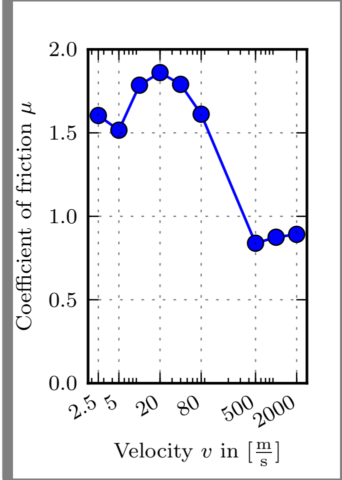


- Linearity!
- Coefficient large by continuum standards
- No simulation box size dependence for thick substrates
- Suppressed plasticity for thin substrate leads to lower μ

Results

Microscopic friction coefficient μ

Scratch speed v

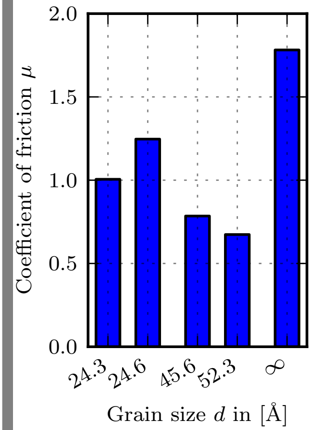


- Bell shape with trailing plateau:
  - Found in nano-machining sims
    P. A. Romero et al. Modelling Simul. Mater. Sci. Eng. 20 (2012)
  - Found in steel friction experiments
    S. Philippon et al. Wear 257 (7-8) (2004)
  - Analytically explained
    A. Molinari et al. Journal of Tribology 121/35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

Results

Microscopic friction coefficient μ

Grain size d



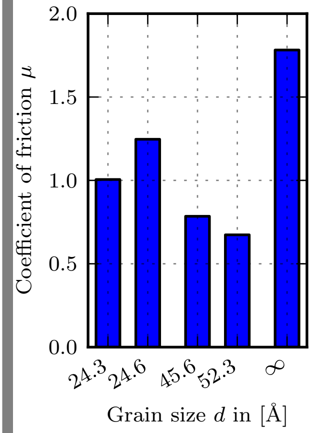
- Coefficient not explained by the grain size

  Not enough grains to average orientation effects?

Results

Microscopic friction coefficient μ

Grain size d



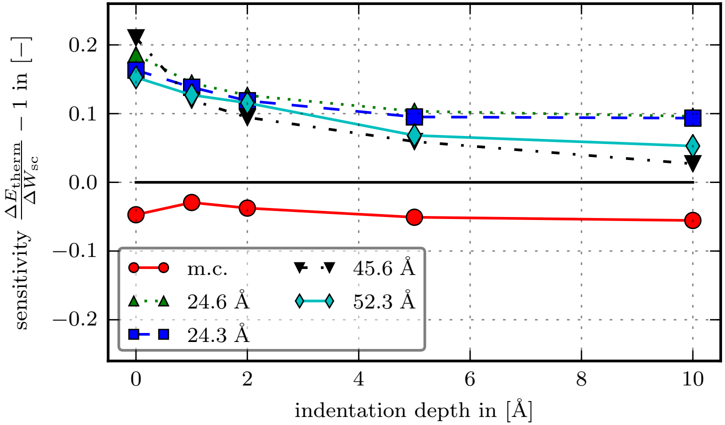
- Coefficient not explained by the grain size

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

Results

Thermal sensitivity s

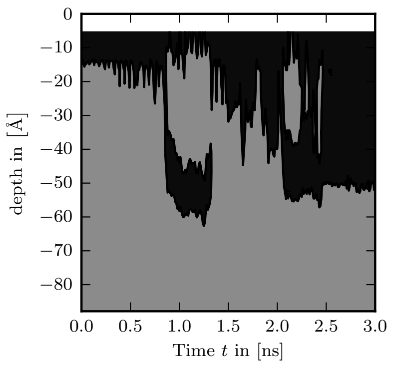
Thermal Sensitivity for different Microstructures



Results

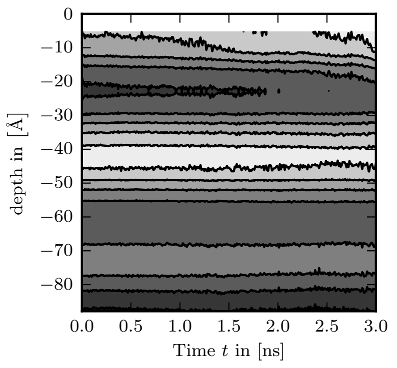
Sensitivity s – vertical centrosymmetry distribution

Growing disorder in single crystal



Plastic energy is stored

Coarsening of microstructure



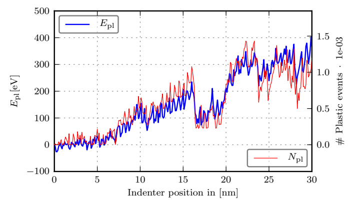
Grain boundary energy is released

Darker means higher disorder

Conclusions

1.) Computation of E_{pl}

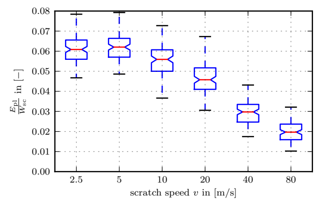
- Novel method to analyze and quantify MD friction simulations



Conclusions

1.) Computation of E_{pl}

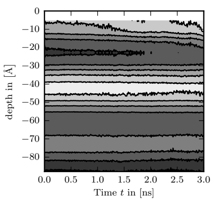
- Novel method to analyze and quantify MD friction simulations
- Showed clear negative rate correlation for high speeds, none for low



Conclusions

1.) Computation of E_{pl}

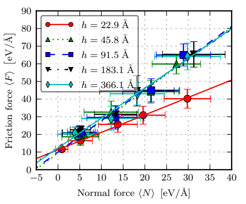
- Novel method to analyze and quantify MD friction simulations
- Showed clear negative rate correlation for high speeds, none for low
- Polycrystals can **release** stored plastic energy during scratching



Conclusions

2.) Regression-based computation of μ

- Recovered simple linear continuum friction model



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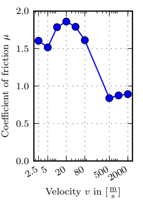
2.) Regression-based computation of μ

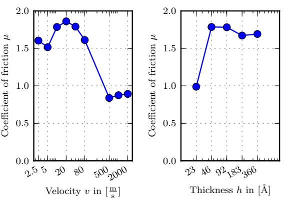
- Recovered simple linear continuum friction model
- Recovered bell-shaped speed dependence observed in machining



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



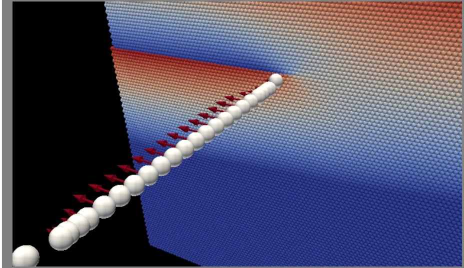
Conclusions

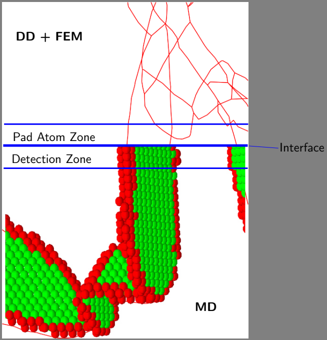
2.) Regression-based computation of μ

- 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

Grain size distributions