Plastic activity in nanoscratch molecular dynamics simulations of pure aluminum

Till Junge, J.F. Molinari, G. Anciaux
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 $\mu$
   Thermal sensitivity $s$
Outline

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Brief History of Friction Modeling

Roughness Hypothesis
Leonardo da Vinci (1495), Later Coulomb, Amontons

Observation

\[ F = \mu N \quad \forall A_{\text{app}} \]

Da Vinci Friction Experiments
MD modeling of friction

Brief History of Friction Modeling

Roughness Hypothesis
Leonardo da Vinci (1495), Later Coulomb, Amontons

Observation

\[ F = \mu N \quad \forall A_{\text{app}} \]

Geometric Solution
MD modeling of friction

Brief History of Friction Modeling

Shear Hypothesis
Bowden and Tabor (1942)

Observation

\[ A_{\text{app}} \neq A_{\text{real}}(N) \]

Contact Area Dieterich et al. (1996)

calcite at 30 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
MD modeling of friction

Brief History of Friction Modeling

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
- ...

Plasticity in friction is poorly investigated on the atomic scale.
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 \( \sim 0 \text{K} \)

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 $r_i(t)$ and velocities $\dot{r}_i(t)$ periodically
Energy influx

\[ E_{\text{in}}(t) = \int_0^t F(\tau) \cdot \nu \, d\tau \]
MD modeling of friction

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

Energy influx

$$E_{in}(t) = \int_{0}^{t} F(\tau) \cdot v \, d\tau$$

Stored as

$$E(t) = E[\mathbf{r}_1, \ldots, \mathbf{r}_N, \mathbf{\dot{r}}_1, \ldots, \mathbf{\dot{r}}_N](t)$$
$$= E_{pot}[\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \ldots](t)$$
$$+ E_{kin}[\mathbf{\dot{r}}_1, \mathbf{\dot{r}}_2, \mathbf{\dot{r}}_3, \ldots](t)$$
MD modeling of friction

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

**Stored Energy**

$$E = E_{pot}[r_1, r_2, r_3, \ldots] + E_{kin}[\dot{r}_1, \dot{r}_2, \dot{r}_3, \ldots]$$

**Potential Energy**

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

$$E_{pot_i} = \frac{1}{2} \sum_{i \neq j} V(r_{ij}) + \sum_i \Phi \left( \sum_{i \neq j} \rho(r_{ij}) \right)$$

**Kinetic Energy**

- Classical mechanics:

$$E_{kin_i} = \frac{1}{2} m_i \dot{r}_i^2$$

- summed over all atoms
MD modeling of friction

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

**Stored Energy**

$$E = E_{pot} [r_1, r_2, r_3, \ldots] + E_{kin} [\dot{r}_1, \dot{r}_2, \dot{r}_3, \ldots]$$

**Potential Energy**

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**Kinetic Energy**

- Classical mechanics:

$$E_{kin_i} = \frac{1}{2} m_i \dot{r}_{i}^2$$

- 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 K: $\Delta E_{pot}(0 \text{ K}) = E_{pl}$

Problem
MD snapshots $\{r_i, \dot{r}_i\}(t)$ are close to static equilibrium ($\sim 0 \text{ K}$)
MD modeling of friction

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

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

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

Solution
Molecular Statics:

$$E_{pot}^{\text{min}}(t) = \min_{R=(r_1, \ldots, r_N)} E_{pot}(R(t))$$

$$E_{pl}(t) = E_{pot}^{\text{min}}(t) - E_{pot}^{\text{min}}(0)$$
MD modeling of friction

Computation of plastic work $E_{pl}$

Using molecular statics (MS)

MD simulation

MS quenching

Potential Energy

Plastic energy $E_{pl}$

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:
Outline

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Single phase polycrystals

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Parametric study

General setup

Setup

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- Evaluate force $F(t)$ acting on the indenter at every time step,
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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: \( \Delta y \in \{0, 1, 2, 5, 10\} \text{ Å} \)
- rigid indenter
- Mendelev EAM Aluminum potential

Substrate thickness
\[ h \in \{22.9, 45.8, 91.5, 183.1, 366.1\} \text{ Å} \]
at \( v = 10 \text{ m/s} \)

Scratch speed
\[ v \in \{2.5, 5, 10, 20, 40, 80, 1000\} \text{ m/s} \]
at \( h = 45.8 \text{ Å} \)

Microstructure
- 40 or 200 grains
- 2 different random seeds
- \( h = 91.5 \text{ Å}, v = 10 \text{ m/s} \)

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
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:
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

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- Stored plastic energy $E_{pl}$
- Microscopic friction coefficient $\mu$
- Thermal sensitivity $s$
Results

Stored plastic energy $E_{pl}$

Effect of substrate thickness $h$

![Graph showing the effect of substrate thickness on stored plastic energy.](image)

- $h = 22.9\,\text{Å}$
- $h = 91.5\,\text{Å}$
- $h = 366.1\,\text{Å}$
Results

Stored plastic energy $E_{pl}$

Effect of scratch speed $v$

![Graph showing the effect of scratch speed on stored plastic energy $E_{pl}$]
Results

Stored plastic energy $E_{pl}$

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

![Graph showing the relative plastic contribution $E_{pl}/W_{sc}$ decreases with scratch speed $v$ in [m/s].]
Results

Stored plastic energy $E_{pl}$

Effect of microstructure is non-trivial/counterintuitive

![Graph showing the change in energy $\Delta E_{min}(x)$ with indenter position in [nm]. The graph includes lines for m.c. and 45.6 Å.]
Results

Microscopic friction coefficient $\mu$

Macroscopic friction model

$$\mu \equiv \frac{dF}{dN} \Leftrightarrow F(N; \mu, f_a) = f_a + \mu N$$

Microscopic translation

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

$$\langle F \rangle_i = \frac{1}{N_w} \sum_{j}^{N_w} F(t_i+j)$$

Least-squares-fit the coefficient

$$\mu = \arg \min_{\hat{\mu}} \left( [F(\langle N \rangle, \hat{\mu}) - \langle F \rangle]^2 \right)$$
Results

**Microscopic friction coefficient $\mu$**

**Effect of substrate thickness $h$**

![Graph showing the effect of substrate thickness on friction force and normal force](image)

- For $h = 22.9$ Å, the friction force is around 50 eV/Å.
- For $h = 45.8$ Å, the friction force is around 70 eV/Å.
- For $h = 91.5$ Å, the friction force is around 100 eV/Å.
- For $h = 183.1$ Å, the friction force is around 150 eV/Å.
- For $h = 366.1$ Å, the friction force is around 200 eV/Å.

The graph also shows the normal force $\langle N \rangle$ in eV/Å as a function of thickness $h$. The coefficient of friction $\mu$ increases with increasing thickness $h$. For example, $\mu$ is approximately 0.5 for $h = 22.9$ Å, and it increases to around 2 for $h = 366.1$ Å.
Results

Microscopic friction coefficient $\mu$

Thickness $h$

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

Microscopic friction coefficient $\mu$

Scratch speed $v$

- Bell shape with trailing plateau:
  - Found in nano-machining sims
  - 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 $\mu$

Grain size $d$

- Coefficient not explained by the grain size
- Not enough grains to average orientation effects?
Results

Microscopic friction coefficient $\mu$

Grain size $d$

- Coefficient not explained by the grain size
- Not enough grains to average orientation effects?
- Consistently lower friction for polycrystal

<table>
<thead>
<tr>
<th>Grain size $d$ in [Å]</th>
<th>Coefficient of friction $\mu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.3</td>
<td>1.0</td>
</tr>
<tr>
<td>24.6</td>
<td>1.5</td>
</tr>
<tr>
<td>45.6</td>
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<tr>
<td>52.3</td>
<td>2.5</td>
</tr>
<tr>
<td>$\infty$</td>
<td>3.0</td>
</tr>
</tbody>
</table>
Results

Thermal sensitivity $s$

Thermal Sensitivity for different Microstructures

![Graph showing thermal sensitivity for different indentation depths and microstructures. The graph plots the change in thermal energy ($\Delta E_{\text{therm}}$) and work of adhesion ($\Delta W_{\text{sc}}$) normalized by the work of adhesion ($\Delta W_{\text{sc}}$) against indentation depth in Å. The different microstructures are represented by various markers and lines, with labels for 24.3 Å, 24.6 Å, 45.6 Å, and 52.3 Å.](image-url)
Results

Sensitivity $s$ – vertical centrosymmetry distribution

Growing disorder in single crystal

Coarsening of microstructure

Plastic energy is stored

Grain boundary energy is released

Darker means higher disorder
Conclusions

1.) Computation of $E_{pl}$

- Novel method to analyze and quantify MD friction simulations

![Graph showing the computation of $E_{pl}$](image)
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

![Graph showing correlation between scratch speed and $E_{pl}/W_{sc}$]
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
2.) Regression-based computation of $\mu$

- Recovered simple linear continuum friction model
2.) Regression-based computation of $\mu$

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

![Graph showing coefficient of friction $\mu$ vs. velocity $v$]

- Apparent strong link between $E_{pl}$ and $\mu$
- Sim box size independent for thick substrates
- Plastic zones not resolved!
Conclusions

2.) Regression-based computation of $\mu$

- Recovered simple linear continuum friction model
- Recovered bell-shaped speed dependence observed in machining
- Apparent strong link between $E_{pl}$ and $\mu$

![Graph showing coefficient of friction against velocity and thickness]
Conclusions

2.) Regression-based computation of $\mu$

- Recovered simple linear continuum friction model
- Recovered bell-shaped speed dependence observed in machining
- Apparent strong link between $E_{pl}$ and $\mu$
- 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

seed = 1, nb grains = 200

mean = 29.7
quartiles = 25.6, 28.8, 32.6