Numerical modeling of sliding contact

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1) Atomistic modeling of sliding contact; P. Spijker, G. Anciaux
2) Continuum modeling; D. Kammer, V. Yastrebov, P. Spijker

ICTP/FANAS Conference on Trends in Nanotribology, 2011
Motivation

Friction: one of the great unsolved mystery

- Can we explain the microscopic origins of friction? (nm)
- What happens inside an earthquake? (km) (rated by livescience as top mystery)
- Challenge of scales (time and length)
- Complex physics (plasticity, surface roughness, third body interactions, adhesion, chemistry...)

\[ F = \mu N \]
A quick introduction

According to Da Vinci, Amontons, and Coulomb, **friction** is ...
- ... proportional to load
- ... independent of contact area
- ... independent of sliding speed

- Bowden and Tabor (1950)
  - real vs. apparent contact area
  - contact surface is rough
  - number of contacting asperities increases with load (confirmed by Dieterich)

- Theoretical models:
  - Greenwood and Williamson
  - Persson
Toward the atomistic scale

Nanotribology

- Magnification until atomic level
- Domain of nanotribology
- Elucidate molecular origins of friction
- Experimental techniques include AFM

[Diagram of nanotribology with labels for normal force, displacement, friction, and experimental setup including AFM and lateral force images.]
Influence of roughness

Open questions...

- Roughness generally not included in Molecular Dynamics modeling (flat on flat, or single tip on flat)

- Computed friction coefficients tend to be low

- Roughness, plasticity (wear) dominate at the engineering scale

- Objective: investigate atomic scale roughness
  - Existence?
  - How does it influence friction?
Self-affine fractal surfaces

Random mid-point displacement algorithm with different Hurst exponents

- Random mid-point displacement algorithm

(Also known as Voss algorithm, diamond-square algorithm, plasma fractal)

\[ C(q) = \frac{1}{2\pi} \int h(x)h(0)e^{-iq\cdot x}dx \]

\[ C(q) \sim q^{-2(H+1)} \]

\( H = 0.8 \)

Increasing Hurst exponent: smoother surface / larger asperities / less asperities
Elastic or J2 elasto/perfectly-plastic solid with a rough surface contacting a rigid surface

$L = 512$ nodes per side; periodic BCs
Full range of H and roughness amplitude

No Frictional Force
No plasticity (Johnson, 1985)

$1 - \nu' = \frac{1 - \nu_1^2}{E_1} + \frac{1 - \nu_2^2}{E_2}$

$H=0.7$ ($D = 3 - H = 2.3$), 256x256 grid; generated by successive Random Addition Rule (RF Voss)

Complex contact morphology

Elastic contact with $A=0.0125$

Elasto-plastic contact, $A=0.0335$
Perfectly plastic (more contact area for fixed $W$)

Overlap or cut-off model, $A=0.03$

Overlap model way off:
asperities elastic (long range) interactions matter!

Morphology dominated by small contact clusters
Atomic rough surfaces

Top a mesoscale asperity

Characteristics:
• Hurst = 0.5
• Grid size = 128
• Peak-valley = 30 Å
• $R_A = 3.92$ Å
• RMS = 4.96 Å

Atom representation:
• $N_{\text{atoms}} = 485,368$
• $r_{\text{atom}} = 1.0$ Å
• dims. = 250 x 250 Å
MD simulation set-up

Material
- aluminium (FCC structure)
- diameter: 0.291 nm / mass: 27 g/mol
- Young’s modulus: 68 GPa / ν: 0.35

Potential
- Lennard-Jones
- bulk-energy: 10.3 kJ/mol
- gap-energy: 0.103 kJ/mol (weak adhesion)

System set-up
- 6 different regions
- dimensions: 13 x 13 x 26 nm (periodic)
- 185,000 to 240,000 particles
- top domain rotated by 21 degrees
- Langevin thermostat close to 0 K

Simulations (all 10 ns with 5 fs time step)
- 3 rough surfaces (0.2, 0.5, 1.0 nm)
- for every RMS 3 different surfaces
- 5 applied pressures (0.05 – 0.25 GPa)
- 3 high sliding speeds (2, 10, 50 m/s)
Simulation analysis

Global forces
- decompose forces per region
- allows to compute global $\mu = \frac{F}{F_N}$

Change of surface characteristics
- RMS roughness / RMS slope
- Skewness, flatness

Statistics and height distribution
- Height profile
- Height distribution

Contact area
- retype particles if necessary
- projected on xy-plane
- compute 'true' contact area
Animation
Simulation results

Friction coefficient vs. time (RMS roughness 0.5 nm / load 0.20 GPa)

\[
\mu = \frac{F_e}{F_N}
\]

- Red: Sliding at 2 m/s
- Pink: Sliding at 10 m/s
- Orange: Sliding at 50 m/s
- Blue diamond: Average at 10 m/s
- Blue triangle: Average at 50 m/s
Simulation results

Friction coefficient vs. roughness

- 0.05 GPa
- 0.10 GPa
- 0.15 GPa
- 0.20 GPa
- 0.25 GPa

RMS 1.0 nm
RMS 0.5 nm
RMS 0.2 nm

Time

10 m/s
Simulation results

Surface roughness vs. contact area

Contact area (A/A₀) vs. Surface RMS roughness (nm)

- RMS 0.2 nm
- RMS 0.5 nm
- RMS 1.0 nm

Time

- 10 m/s

- 0.05 GPa
- 0.10 GPa
- 0.15 GPa
- 0.20 GPa
- 0.25 GPa
Simulation results

Flattening of surfaces; threshold = 20% difference in height between points

RMS 0.2 nm

RMS 0.5 nm

RMS 1.0 nm

RMS 0.2 nm

RMS 0.5 nm

RMS 1.0 nm
Simulation results

Flatness vs. friction; exponential decay

$R^2 = 0.87$
Influence of temperature

Change in roughness; 1 nm RMS roughness

- 0.05 GPa
- 0.10 GPa
- 0.15 GPa
- 0.20 GPa
- 0.25 GPa

RMS roughness (nm)

Sliding distance (nm)
Simulation results

Thermal effect – Friction coefficient vs. temperature

Friction coefficient vs. temperature for different roughness levels:
- Atomically flat
- RMS 0.2 nm
- RMS 0.5 nm
- RMS 1.0 nm

The graph shows the relationship between friction coefficient and temperature for various roughness conditions, indicating how friction decreases as temperature increases.
Discussion

View on friction of rough surfaces

A 2D depiction of the sliding plane

Top surface + Bottom surface = Resultant surface
Summary 1

- Rough deformable on rough deformable MD model
- Key role of roughness
  - Gives « realistic » friction coefficients
  - Geometric effect: friction proportional to number of atom direct collisions (scales with RMS roughness)

- But roughness decreases quickly (exp decay of friction with flatness)
- What is roughness at atomic scale?
  - Reserve of « fresh » (i.e. rough asperities)
  - Mechanisms for roughness creation? (ex: third bodies)

Publications:
Tribol. Int., submitted (2011)
Large scale sliding

Mode II Fracture vs. Initiation of Dynamic Sliding

- Continuum scale
- Onset of sliding
- Friction or Fracture?
Lab earthquakes
Experimental results for quasi-static shear loading

PMMA Interface under Quasi-static Shear Loading

Coker, Lapusta, Rosakis
JMPS 2005

Lu et al.
PNAS 2007

Ben-David, Cohen, Fineberg, Science 2010
Lab earthquakes

Experimental results for quasi-static shear loading

Coker et al. JMPS 2005

Lu et al. PNAS 2007

Ben-David et al. Science 2010

Real Contact Area Indicates Interface Rupture Propagation

Stress Distributions

A

Time (μsec)

0 1000 2000

0 0.04C_s

Slow rupture

Stress (MPa)

Shear τ

Normal σ

0 5 10

0 2.5 5

x (mm)

0 50 100 150 200
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Experimental results for quasi-static shear loading

Rupture velocity, $V(x)$ (m/s)

$\tau(x) / \sigma(x)$

Coker et al.
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Experimental results for quasi-static shear loading

Features:
All modes of rupture velocity reproduced
Local friction can be much higher than macroscopic value
Key role of heterogeneities

Fracture energy analogy:
More energy needed to break interface
→ higher local interface strength
→ more real contact area
→ more local normal stress
Numerical model

Explicit FE; energy-conserving contact
Problem setup

(a) 

(b)
Problem setup
Problem setup
Velocity weakening friction law

Tangential resistance is proportional to the contact pressure

\[ \mu = \mu_s + (\mu_k - \mu_s)(1 - \exp(-|v| \sqrt{\frac{\mu_s - \mu_k}{\alpha}})) \]

\( v \) is the material slip velocity, \( \mu_s, \mu_k \) are the static and the kinetic friction coefficients, \( \alpha \) is the transition parameter
Comparison with experiments

Matches but... non uniqueness of V_{tip}
Spontaneous and triggered slip initiations

Directionality effect?

Diagram showing slip front and velocity components with graphs of velocity as a function of distance.
Spontaneous and triggered slip initiations

Directionality effect?
In front of the slip front

Things change ...

Tip of the slip front

Mach cone

P-wave

\( l^* \)

\( t^i \)

\( t^{i+1} \)

\( t_d \)

\( p_d \)
In front of the slip front

Dynamic effects help
Slip velocity as a function of local energy

Back to fracture mechanics analogy

$$\Delta E / E = \frac{E_{\text{needed}} - E_{\text{stored}}}{E_{\text{stored}}}$$

![Graph showing slip velocity as a function of local energy with different markers for spontaneous rupture and triggered on the left and right. The graph includes a fit range highlighting the data points.](image-url)
Conclusions

• Simple model gives consistent observations (with Ben-David et al. 2010 Science paper)
  – Tau-Sigma ratio exceeds global friction coefficient
  – **Rupture velocity depends on local tau-sigma ratio**

• Additional observations
  – Different rupture modes
  – Non uniqueness of Vtip
  – Explained by energy flux (dynamics)

• Perspectives
  – More sophisticated friction law
  – Deformable-deformable contact
  – Interface heterogeneity
  – Access dynamic fields experimentally

• Adding roughness would be nice
  – At what scale roughness breaks down?
  – Challenge for multiscale modeling