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Friction on a mesoscale

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Friction on a mesoscale



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Abstract

Nanofriction on a mesoscopic scale is considered with the help of an earthquakelike (EQ) model. Kinetics of the EQ model with a distribution of static thresholds is reduced to a master equation which can be considered analytically. This approach naturally describes stick-slip and smooth sliding regimes of tribological systems within a framework which separates the calculation of the friction force from the studies of the properties of the contacts. The role of physical parameters which determine stick-slip against smooth sliding is clarified. The model can explain tribological experiments in considerable detail without the need of any special properties of the lubricant film such as, e.g., its huge viscosity.

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I. Introduction



Standard experimental technique



Modern experimental techniques

Surface Force Apparatus (SFA)

Tabor and Winterton (1969); Israelaschvili

- atomically flat mica plates
- thickness is controlled optically (with accuracy of $\sim 1\text{\AA}$)

Friction Force Microscope (FFM)

Quartz-crystal microbalance



Regimes:

- Hydrodynamic lubrication (Reynolds 1886) for a thick liquid layer (> 0.01 mm)
 - Navier–Stokes equations with appropriate boundary conditions
- ▶ **<u>Boundary lubrication</u>** for a thin (few Å) lubricant film
 - > at stop/start, (almost) always the regime of **boundary lubrication** occurs
- Wearing (destroying of surfaces)

١.

Static vs kinetic friction:

- **Static friction** to start motion
- Kinetic friction to keep the slider moving smoothly

Main laws (da Vinci, Amontons, Euler, Coulomb):

of v

(1)
$$\mu = F_{\text{friction}}/F_{\text{load}} \approx \text{constant} < 1$$

(2) $\mu_{\text{kinetic}} < \text{or} << \mu_{\text{static}}$, and μ_{kinetic} is approximately independent
(3) stick-slip and smooth sliding:



Some results

 $\mu = F_{\text{friction}}/F_{\text{load}} \approx \text{constant} < 1$

Bowder & Tabor 1950: Even a surface which appears to be flat on a millimeter scale may contain micrometer-scale asperities, i.e., **the surfaces are rough**



A real (actual) contact area $A_{real} \sim F_{load}$, and A_{real} grows until the external loading force will be balanced by the contact pressure integrated over A_{real}

Let $P_{\text{real load}} = P_{\text{load}} A / A_{\text{real}}$ is the real pressure at the contact. Then:

- at low $P_{\text{real load}} < P_{\text{vield}}$ (elastic regime) the number of contacts increases with load
- at high $P_{\text{real load}} > \dot{P}_{\text{yield}}$ (plastic regime) the area of a contact increases with load

A thin film (less than 10 molecular diameters) is almost always layered, because the substrates induce crystalline order in the film

(solidify / freeze the lubricant, Thompson et al 1995).

When the width is less than about three layers, most films behave like solid

"Memory / age" effects: frictional forces depend on the previous dynamical history of the solid–solid contact(s), e.g., $\mu_{\text{static}}(t) \approx a_s + b_s \ln(t)$ and $\mu_{\text{kinetic}}(v) \approx \mu_{\text{static}}(a_{\varphi}/v)$ with the characteristic length $a_{\varphi} \sim 1 \ \mu \text{m}$ (plasticity of the system)

I.

II. Simulation Microscopic 3D MD model

the MD model must be three-dimensional!



Langevin equations:

Due to the driving force, an energy is pumped into the system This energy must finally be removed from the driven system

A standard approach is to use Langevin equations for only few layers far from the interface. But: a competition "large system \leftrightarrow long times",

while the most important is a detailed modelling of the interface itself.

Solution: to use Langevin equations for all lubricant and substrate atoms

O.M.Braun & M.Peyrard, *Phys. Rev. E* **63** (2001) 046110 "Friction in a solid lubricant film" O.M.Braun & A.G.Naumovets, *Surf. Sci. Reports* **60** (2006) 79 "Nanotribology:

Microscopic mechanisms of friction"

II.2. Simulation results

LoLS (Layer over Layer Sliding) ("soft" lubricant, *f*=0.008)



Perfect sliding ("superlubricity") ("hard" lubricant)



"Amorphous" lubricant structure ("hard" lubricant, *T*=0.3, *f*=0.008)



LS (Liquid Sliding) ("hard" lubricant, T=0.4, f=0.01, $v_{top}=0.6$)





O.M.Braun, M.Peyrard, V.Bortolani, A.Franchini, A.Vanossi, *Phys. Rev. E* **72** (2005) 056116 "Transition from smooth sliding to stick-slip motion in a single frictional contact"

II. II.4. "Viscosity" of a thin film (smooth sliding)



Experiments (Granick et al, 1991? Thompson et al? 1995; etc):?

the viscosity of a thin film is many orders of magnitude higher than the bulk viscosity

III. EQ & ME

The earthquakelike (EQ) model



 $P_{c}(x_{s})$ – probability distribution of <u>the thresholds</u> $x_{si}=f_{si}/k_{i}$ at which the contacts break Q(x;X) – distribution of the stretchings x_{i} when the top substrate is at a position X

As the top stage moves, the surface stress at any junction increases, $f_i(t) = k_i x_i(t)$, where $x_i(t)$ is the shift of the *i*-th junction from its unstressed position. A single junction is pinned whilst $f_i(t) \le f_{si}$, where f_{si} is the static friction threshold for it. When the force reaches f_{si} , a rapid local slip takes place, during which the local stress in the block drops to the value $f_{bi} \sim 0$. Then the junction is pinned again, and the whole process repeats itself.

R. Burridge and L. Knopoff, *Bull. Seismol. Soc. Am.* 57 (1967) 341
Z. Olami, H.J.S. Feder, K. Christensen, *Phys. Rev. Lett.* 68 (1992) 1244
B.N.J. Persson, *Phys. Rev. B* 51 (1995) 13568
O.M. Braun and J. Röder, *Phys. Rev. Lett.* 88 (2002) 096102

III.

III.2. The master equation (ME)

Q(x;X) - the distribution of the stretchings x_i when the bottom of the slider is at X. $P_c(x_s)$ - probability distribution of values of the thresholds x_{si} at which contacts break. R(x) - probability distribution of values of the displacements x for "newborn" contacts.

Consider a small displacement $\Delta X > 0$ of the bottom of the solid block. It induces a variation of the stretching x_i of the asperities which has the same value ΔX . The displacement X leads to three kinds of changes in the distribution, which can be written as a master equation for Q(x;X):

$$Q(x; X + \Delta X) = Q(x - \Delta X; X) - \Delta Q_{-}(x; X) + \Delta Q_{+}(x; X)$$

(1) the first term is just the shift due to the global increase of the stretching;(2) some contacts break because the stretching exceeds the maximum that they can stand:

$$\Delta Q_{-}(x;X) = P(x) \Delta X Q(x;X), \quad P(x) = \frac{P_{c}(x)}{\int_{x}^{\infty} d\xi P_{c}(\xi)}$$

(3) those broken contacts form again after a slip: to be broken $=N_cP_c(x)\Delta X$ the number of still $\Delta Q_+(x;X) = R(x) \int_{-\infty}^{\infty} d\xi \,\Delta Q_-(\xi;X)$ unbroken contacts (/N_c)

Finally, with $\Delta X \rightarrow 0$ we get the integro-differential equation:

$$\frac{\partial Q(x;X)}{\partial x} + \frac{\partial Q(x;X)}{\partial X} + P(x) Q(x;X) = R(x) \int_{-\infty}^{\infty} d\xi P(\xi) Q(\xi;X)$$





III.4. The steady state



IV. Generalizations IV.1. Friction loop

if
$$\Delta X < 0$$
, then $\Delta Q_{-}(x;X) = -P_{b}(x) \Delta X Q(x;X)$
and $\Delta Q_{+}(x;X) = R_{b}(x) \int_{-\infty}^{\infty} dx' \Delta Q_{-}(x';X)$ so that

$$\frac{\partial Q(x;X)}{\partial x} + \frac{\partial Q(x;X)}{\partial X} - P_b(x) Q(x;X) = R_b(x) \int_{-\infty}^{\infty} dx' P_b(x') Q(x';X)$$

where for the symmetric case (the forward-backward symmetry) $P_b(x) = P(-x)$ and $R_b(x) = R(-x)$



IV.2. Delay in contact formation

 $\Delta Q_+ \rightarrow \Delta Q_+(x; X + \Delta X_m)$, where $\Delta X_m = v\tau_m$ (v is the driving velocity) and τ_m is a "delay" time, i.e., the time of break-formation (melting-freezing) of a new contact

$$\frac{\partial \widetilde{Q}(x;X)}{\partial x} + \frac{\partial \widetilde{Q}(x;X)}{\partial X} + P(x) \,\widetilde{Q}(x;X) = R(x) \int_{-\infty}^{\infty} dx' \, P(x') \,\widetilde{Q}(x';X - \Delta X_m)$$



IV.

IV. IV.3a. Aging of contacts: $P_c(x)$ changes with time

Let $P_{ci}(x)$ be the threshold distribution for "newborn" contacts characterized by the average value \bar{x}_{si} and the dispersion σ_{si} . Typically \bar{x}_s grows while σ_s decreases with time, and finally at $t \to \infty$ $P_c(x)$ approaches $P_{cf}(x)$ with $\bar{x}_{sf} > \bar{x}_{si}$ and $\sigma_{sf} < \sigma_{si}$. If the evolution of $P_c(x)$ corresponds to a stochastic process, then it can be described by the Smoluchowsky equation

$$\partial P_c / \partial t = D \, \widehat{L}_x P_c$$
, where $\widehat{L}_x \equiv \frac{\partial}{\partial x} \left(B(x) + \frac{\partial}{\partial x} \right)$,

the "diffusion" parameter D defines the rate of aging, the "potential" U(x) is defined by the final distribution, $P_{cf}(x) \propto \exp\left[-U(x)\right]$ so that $B(x) = \frac{dU(x)}{dx} = -\frac{dP_{cf}(x)/dx}{P_{cf}(x)}$.

An interplay of two processes: the aging which moves $P_c(x)$ to $P_{cf}(x)$, and the breaking/reborn process which returns $P_c(x)$ to $P_{ci}(x)$

$$\begin{cases} \frac{\partial Q(x;X)}{\partial x} + \frac{\partial Q(x;X)}{\partial X} + P(x;X) Q(x;X) = \delta(x) \int_{-\infty}^{\infty} dx' P(x';X) Q(x';X) \\ \frac{\partial P_c(x;X)}{\partial X} - D_X \hat{L}_x P_c(x;X) + P(x;X) Q(x;X) = P_{ci}(x) \int_{-\infty}^{\infty} dx' P(x';X) Q(x';X) \\ P_c(x;X) = P(x;X) \exp\left[-\int_0^x d\xi P(\xi;X)\right] \end{cases}$$

where $D_X = D/v$ and v = dX(t)/dtThe case of fast driving $(v \to \infty, D_X \to 0)$: $P_c(x) = P_{ci}(x)$ The case of slow driving $(v \to 0, D_X \to \infty)$: $P_c(x) = P_{cf}(x)$



IV.4. Slider dynamics: Elastic instability

The force at the substrate/lubricant interface $F = K(X_d - X)$ (*) must be equal to the force F(X) from friction contacts. When X_d and X increase, the substrate remains stationary as long as $dX_d/dX > 0$.

 $dX_d/dX = 0$, or $F'(X) \equiv dF(X)/dX = -K$ (**) just defines the maximal displacement X_m which the contacts can sustain; a larger displacement will broke all the contacts simultaneously, and at this moment all contacts will reborn.

OR:

The total potential energy of the sliding interface plus the elastic substrate is $V(X) = \int_0^X dX' F(X') + \frac{1}{2}K(X - X_d)^2;$ then Eq.(*) $\leftrightarrow V'(X) = 0;$ it is stable if V''(X) > 0, so that the unstable displacement is defined by $V''(X) = 0 \leftrightarrow \text{Eq.}(^{**})$



$$K^* = -\max F'(X) \approx Nk \left(f_s - f_b\right) / \Delta f_s$$



IV.5. Elastic instability + delay → stick-slip





Spring force $F_d(t)$ for different values of the delay time τ_d (parameters from: J.Klein, *PRL* **98** (2007) 056101)

Despite the soft spring constant K=97 N/m << $K^*=4.34 \times 10^4$ N/m, stick-slip is only found for sufficiently large τ_d IV. IV.6a. "Viscosity" of the confined film (stick-slip)



experiment:

Jacob Klein, Phys.Rev.Lett. 98 (2007) 056101 *"Frictional dissipation"* in stick-slip sliding"

$\eta \approx 10^4 \eta_{\text{OMCTS}}$

Confined film thickness D

FIG. 1. Friction-force traces between mica surfaces sliding across a film of OMCTS of thickness $D = 35 \pm 2$ Å (n = 4 molecular layers), under a load $L = 16 \mu N$ (for details of OMCTS preparation see Ref. [14]). The lower and upper traces, taken directly from the X-t chart recorder, show, respectively, the applied uniform motion (at velocity v_s) of the end of the shear spring, and the extension of the spring in response to stickslip motion between the upper and lower surfaces. The cartoon illustrates schematically the geometry in the SFB (for details see Ref. [22]). Motion of the spring end (lower trace) commences at the point O, and the initial stick spike (upper trace) is characteristically larger than subsequent stick spikes (the slight downward trend of the stick-slip cycles is due to thermal drift). The points y and s, indicated for clarity only for one (circled) cycle, are the vield and solidification points of the confined film.

(region similar to the marked cycle in Fig. 1, but from a different experiment recorded via a LeCroy 9310M recording oscilloscope) for friction between mica surfaces across a 35 ± 3 Å film of OMCTS (n = 4 monolayers) under a load of 42 μ N. The contact area A at this load, evaluated from Johnson-Kendall-Roberts contact mechanics expression [14], is $A = (4 \pm 0.4) \times$ 10⁻¹⁰ m². Traces (b) and (c) focus on the slip region of the same cycle at magnified time scales, where a and b are, respectively, stick and slip regions, x_0 and Δx_0 are, respectively, the spring bending at the yield point y and the extent of slip from y to s. The SFB shear-spring constant K = 97 N/m, while the mass of the moving surface and its mount is M = 1.47 g. The dashed curve (red online) is the predicted variation x(t) given by Eq. (2) in the text, with a value of B corresponding to an effective viscosity of the OMCTS film given by $\eta_{\rm eff} = 27$ Pas. The dotted curve (red online) corresponds to the predicted variation of x(t) with the viscosity of the OMCTS film given by its bulk value $\eta_{\text{bulk}} =$ 2.5×10^{-3} Pa s.

Problem II: the viscosity of a thin confined film is many orders of magnitude higher than the bulk viscosity

IV.6b. Solution: Earthquakelike model



IV.

IV.6d. Role of threshold's dispersion

details...



The system behavior (either stick-slip or smooth sliding) is controlled by the dispersion Δf_s : $K^* = -\max F'(X) \approx Nk (f_s - f_b) / \Delta f_s$

If Δf_s is so small that $K^* > K$, then the motion corresponds to stick-slip;

otherwise the smooth sliding regime is achieved.

In the stick-slip regime, an increase of Δf_s leads to the decrease of the period τ_{ss} of stick-slips. The ratio $\Delta f_s/f_s$ should decrease with the time of stationary contact due to aging of contacts; namely this aging is responsible for the transition from stick-slip to smooth sliding with the increase of driving velocity.

IV.6e. Role of slider elasticity



Slider of N_l layers, each of mass $M_l = M/N_l$, coupled by springs of the constant $K_l = KN_l$ (fix the bottom, and apply F to the top; then the top will shift on $\Delta X = \sum_{l=1}^{N} \Delta X_l$, where $\Delta X_l = F/K_l$, so that $\Delta X = F/K$ as before). Let the top layer be driven with the velocity v_d , while the bottom layer be in frictional contact with the bottom substrate.

The slip kinetics is almost independent of the number of layers N_l and is determined by the minimal slider mechanical frequency Ω_s .

The frequency Ω_s can be found with the help of elastic theory:

Let the slider have a cylinder shape of height L and radius r, and is characterized by the section $S=\pi r^2$, inertial momentum $I=\pi r^4/4$, mass density ρ and Young modulus E.

If the cylinder foot is fixed and a force F is applied to its top,

the latter will be shifted on the distance $\Delta X = FL^3/3EI$.

Thus, the effective elastic constant of the slider is $K=3EI/L^3$.

The minimal frequency of bending vibration of the pivot with one fixed end and one free end is given by $\Omega_S = (3.52/L^2)(EI/\rho S)^{1/2}$.

Taking $M = \rho SL$, we finally obtain $\Omega_S \approx 2.03 \sqrt{(K/M)}$.

IV.6f. Role of lubricant viscosity



details...

IV. IV.6g. Role of interaction between the contacts

The elastic interaction between the contacts is described by the potential $V(r)=g/r^3$. The interaction becomes important, when $g/a^3 \sim f_s a$, where *a* is the distance between NN contacts. How the system behavior changes with the dimensionless parameter $\xi = g/(f_s a^4)$? The interaction between the contacts works roughly in the same way as the dispersion Δf_s : the stronger is the interaction, the wider is the range of model parameters where stick-slip operates. Fig: system kinetics with increasing interaction ($\xi = 0$ to 0.3) for kN=200 N/m, $\Delta f_s/f_s=0.3$. The system quickly goes to smooth sliding for noninteracting contacts (a), but demonstrates stick-slip for a strong interaction $\xi=0.3$ (d).



IV.7a. Nonzero temperature

When T > 0, the contact may relax due to a thermally activated jump before the threshold x_s is reached. The rate of this process is

$$dQ(t)/dt = h(x; x_s) Q(t) \quad (x < x_s)$$

For the set of contacts, this equation is to be generalized to

IV.

$$dQ(t)/dt = H(x)\,Q(t)$$
 with $H(x) = \int_x^\infty dx'\,h(x;x')\,P_c(x')$

If X = vt, then $P(x) \to P_T(x) = P(x) + H(x)/v$ in the ME.





 $dF_{\rm k}/dv > 0 \rightarrow$ stable

IV. IV.8. Onset of sliding (soft surface contacts, $K_s = K$)



(b) distribution of
elastic forces in the slider
as a function of
the block number *j*and time *t*.
The unstressed and
stressed regions are
displayed by blue
and red colors.

(d) enlarged view
of the fast detachment
front from (c)
showing an excitation
of a secondary
Rayleigh front
by the slow fronts

experiment: S.M. Rubinstein, G. Cohen & J. Fineberg, *Nature* **430**, 1005 (2004); *Phys. Rev. Lett.* **98**, 226103 (2007)

V. $P_{c}(x)$ Probability distribution of thresholds $P_{c}(x)$

 $\widetilde{P}_c(f_s)$ is the distribution of (static) friction force thresholds of the contacts. If a given contact has an area A, then it is characterized by the static friction threshold $f_s \propto A$ and the elastic constant $k \sim \rho c^2 \sqrt{A}$ (here ρ is the mass density and c is the sound velocity). The displacement threshold for the given contact is $x_s = f_s/k$, so that $f_s \propto x_s^2$, or $df_s/dx_s \propto x_s$. Using the relationship $P_c(x_s) dx_s = \widetilde{P}_c(f_s) df_s$, we obtain

$$P_c(x_s) \propto x_s \widetilde{P}_c[f_s(x_s)]$$

Systems:

dry friction:contact of rough surfaces



- dry or lubricated friction:
 contact of polycrystalline substrates
- > lubricated friction: Lifshitz-Slözov coalescence



V. V.2a. *P*_c(*x*): contact of rough surfaces



Rough surface: hills of heights $\{h_i\}$ distributed with $P_h(h) = \bar{h}^{-1} \exp(-h/\bar{h}) \Theta(h)$, where \bar{h} is the average height. Greenwood and Williamson: all hills have spherical shape of radius r. When this surface is pressed with another rigid flat surface, which takes a position at the level h_0 , then the hills of heights $h > h_0$ will form contacts.

Elastic contacts: the contact of height $h \to \text{compression } (h - h_0) \to \text{area } \pi r(h - h_0) \to \text{it bears the normal force } f_l(h) \approx (4\pi/3) E^* r^{1/2} (h - h_0)^{3/2}$ (E^* = the effective Young modulus).

Assume that $f_s(h) \approx \mu f_l(h)$, where $\mu < 1$ is a constant. Then $\widetilde{P}_c(f_s)$ is coupled with $P_h(h)$ by $\widetilde{P}_c(f_s) df_s \propto P_h(h) dh$, or

 $\widetilde{P}_c(f) \propto f^{-1/3} e^{-B_1 f^{2/3}}, P_c(x) \propto x^{1/3} \exp(-B' x^{4/3}), B_1 \propto \left[\bar{h} r^{1/3} (\mu E^*)^{2/3}\right]^{-1}$

Plastic contacts: the local pressure on contacts $= p_{\text{load}} = H = \text{hardness}$. The normal force at the contact is $f_l(h) \approx \pi r(h - h_0)H$. Assume: $f_s(h) \approx \mu f_l(h) \rightarrow f_s = \pi r(h - h_0)\mu H$ and $\widetilde{P}_c(f_s) \propto P_h[h(f_s)]$, or $\widetilde{P}_c(f) \propto \exp(-B_2 f)$, or $P_c(x) \propto x \exp(-B'' x^2)$, where $B_2 = (\pi \bar{h} r \mu H)^{-1}$

V.2b. Contact of rough surfaces: $P_{c}(x) \& F_{k}$



 $F_k \propto B^{-3/4} \propto \bar{h}^{3/4}$ for the elastic contacts, and $F_k \propto B^{-1/2} \propto \bar{h}^{1/2}$ for the plastic contacts

V. V.3. $P_c(x)$: contact of polycrystalline substrates



0.00

0

5

х

15

10

the rigid substrate of square lattice

V. V.4. *P*_c(*x*): Lifshitz-Slözov coalescence



Melting/freezing: the lubricant melts during slip and solidifies at stops. Lifshitz-Slözov: grains of solid phase emerge and grow in size, $\bar{r} \propto t^{1/3}$. Distribution: the number of grains with the radius from r to $r + \Delta r$ is equal to $P_{\rm LS}(r/\bar{r}) \Delta r/\bar{r}$, where

$$P_{\rm LS}(u) \propto \frac{u^2 \exp[-1/(1-2u/3)]}{(u+3)^{7/3} \left(\frac{3}{2}-u\right)^{11/3}}$$

When the size of a grain exceeds the film thickness d, it pins the surfaces. Using

 $\widetilde{P}_c(f)df \propto P_{\rm LS}(r/\bar{r}) dr/\bar{r}$, we obtain $\widetilde{P}_c(f) \propto (dr/df) P_{\rm LS}(r/\bar{r})/\bar{r}$.

A single grain: $f_s \propto \pi (r^2 - d^2/4)$ for r > d/2thus $dr/df \propto f^{-1/2}$.

Finally, $P_c(x) = P_{\rm LS}(u)$, where $u = \rho^{-1} (1 + Bx^2)^{1/2}$, $\rho(t) = 2\bar{r}(t)/d$ and B is determined by the system parameters.



Conclusion

The complex problem of behavior of the tribological system is split into two independent subproblems:

(*I*) to find the distribution of static thresholds $P_{c}(x)$ for a given system

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(a separate problem for MD)
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(II) dynamics of the friction contact, if the distribution $P_{c}(x)$ is known

- > EQ model with a distribution of thresholds
- ► EQ model reduces to Master Equation
- ➢ includes: delay effects, aging, *T*>0, interaction (MF)
- \succ describes the dependences of friction on *v* & *T*
- > stick-slip $\leftarrow \rightarrow$ smooth sliding:

macroscopic smooth sliding = uncorrelated microscopic stick-slip; macroscopic stick-slip = correlated microscopic stick-slip

huge "viscosity" of a thin film emerges due to sequential melting/sliding of different domains one by one because of film's non-homogeneity

Perspective:

- certain systems, taking into account all effects simultaneously
- > further development: combine with elastic eqs., X=X(r)

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