

SHORT
COMMUNICATIONS

Melting of Ultrathin Lubricant Film Due to Dissipative Heating of Friction Surfaces

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Abstract—Melting of an ultrathin lubricant film during friction between atomically smooth surfaces is studied. Additive noise of shear stress and strain as well as of film temperature is introduced and the phase diagram is constructed. On the diagram, the noise intensity for this temperature and the temperature of friction surfaces determine the regions of sliding, dry, and stick-slip friction. As a result of numerical analysis of the Langevin equation for various regions of the diagram, time series of stresses are constructed, which make it possible to explain the experiment on friction, in which intermittent motion is observed. Lubricant melting due to dissipative heating of friction surface is considered and the experimental time dependences of friction force are interpreted.

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Melting of an ultrathin lubricant film in the course of friction between atomically smooth solid surfaces with allowance for additive noise of shear stress and strain as well as of temperature is described by the Langevin equation [1, 2]

$$\tau_\sigma \dot{\sigma} = f(\sigma) + \sqrt{I(\sigma)} \xi(t), \quad (1)$$

where σ is the shear stress (which is an order parameter) and τ_σ is its relaxation time. For $\sigma = 0$, the lubricant is solidlike, while the case $\sigma \neq 0$ corresponds to its liquidlike state [3]. In accordance with the new friction chart for the boundary regime [4], an increase in stress,

$$\sigma = \frac{F}{A}, \quad (2)$$

leads to an increase in the viscous friction force,

$$F = \frac{\eta_{\text{eff}} VA}{h}, \quad (3)$$

where V is the velocity of a block, h is the film thickness, η_{eff} is the effective viscosity, and A is the contact area. Comparing relations (2) and (3), we obtain the following expression for velocity in terms of stress:

$$V = \sigma \frac{h}{\eta_{\text{eff}}}; \quad (4)$$

in other words, the total friction force decreases upon an increase in stresses since the velocity of the moving surfaces increases (the lubricant melts).

Generalized force $f(\sigma)$ and effective noise intensity $I(\sigma)$ are given by the equalities

$$\begin{aligned} f(\sigma) &\equiv -\sigma + g\sigma[1 - (2 - T_e)d(\sigma)], \\ I(\sigma) &\equiv I_\sigma + (I_\varepsilon + I_T \sigma^2)g^2 d^2(\sigma), \\ d(\sigma) &\equiv (1 + \sigma^2)^{-1}. \end{aligned} \quad (5)$$

Here, T_e is the temperature of friction surfaces; $g(\sigma) = G/G_0 \equiv \text{const}$ is the ratio of the shear modulus to its characteristic value; and I_σ , I_ε , and I_T are the intensities of stress, strain, and temperature noise, respectively. Function $\xi(t)$ in Eq. (1) is a δ -correlated stochastic source (white noise). Its moments are defined as

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = 2D\delta(t-t'), \quad (6)$$

where D is the integral of the correlation function, which plays the role of the source intensity. The distribution of the values of $\xi(t)$ over ξ is Gaussian [5]:

$$P(\xi) = \frac{1}{\sqrt{2\pi\mu}} \exp\left\{-\frac{\xi^2}{2\mu^2}\right\}. \quad (7)$$

Here, μ^2 is the second moment of the source,

$$\mu^2 \equiv \langle \xi^2(t) \rangle = 2D\delta(0), \quad (8)$$

which diverges as D/τ , where $\tau \rightarrow 0$ is the width of the δ function, which assumes a nonzero value for all real physical systems.

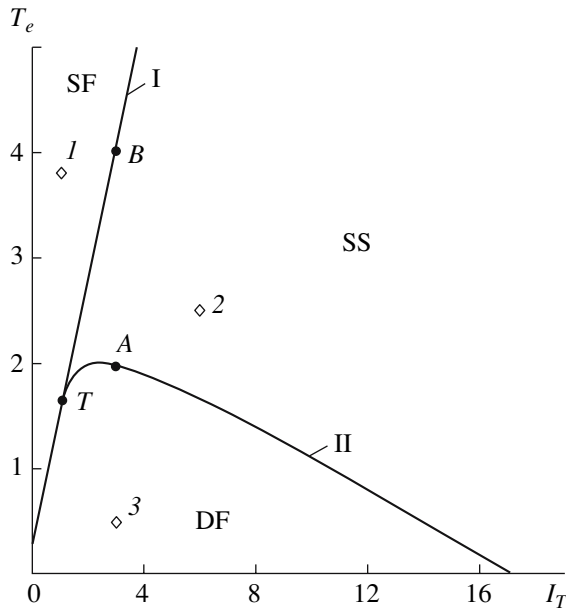


Fig. 1. Phase diagram for $g = 0.8$, $I_\varepsilon = 0.8$, and $D = 0.8$ with the regions of sliding (SF), dry (DF), and stick-slip (SS) friction (T is the tricritical point).

Langevin equation (1) is in one-to-one correspondence with the Fokker–Planck equation (FPE) in the Ito form [6],

$$\tau_\sigma \frac{\partial P(\sigma, t)}{\partial t} = -\frac{\partial}{\partial \sigma} f(\sigma) P(\sigma, t) + D \frac{\partial^2}{\partial \sigma^2} I(\sigma) P(\sigma, t). \quad (9)$$

The distribution of solutions to Eq. (1) becomes stationary after some time and its explicit form can be found from Eq. (9) for $\partial P(\sigma, t)/\partial t = 0$:

$$P(\sigma) = Z^{-1} \exp\{-U(\sigma)\}. \quad (10)$$

The resultant distribution is controlled by the normalization constant

$$Z = \int_{-\infty}^{+\infty} d\sigma \exp\{-U(\sigma)\} \quad (11)$$

and the effective potential¹

$$U(\sigma) = \ln I(\sigma) - \frac{1}{D} \int_{-\infty}^{\sigma} \frac{f(\sigma')}{I(\sigma')} d\sigma'. \quad (12)$$

The equation defining the positions of maxima of function $P(\sigma)$ has the form

$$\begin{aligned} (1-g)x^3 + g(2-T_e)x^2 - 2g^2DI_Tx \\ + 4g^2D(I_T - I_\varepsilon) = 0, \quad (13) \\ x \equiv 1 + \sigma^2. \end{aligned}$$

¹ In contrast to [1], the lower integration limit in our case is $-\infty$ and not 0 since negative stresses will also be considered below.

Thus, the shape of the $P(\sigma)$ distribution is independent of noise intensity I_σ .

For a fixed intensity I_ε , the phase diagram has the form shown in Fig. 1, where curves I and II correspond to stability loss limits for the system. Above straight line I defined by the equation

$$T_e = 1 + g^{-1} + 2gD(I_T - 2I_\varepsilon), \quad (14)$$

the most probable value of stress $\sigma \neq 0$ and the lubricant is in the liquidlike phase ensuring stable sliding friction (SF) state. Below curve II, which is tangential to straight line I at tricritical point T with coordinates

$$\begin{aligned} T_e^c &= \frac{2}{3}(1 + 2g^{-1} - 2gDI_\varepsilon), \\ I_T^c &= \frac{1}{6gD}(g^{-1} - 1 + 8gDI_\varepsilon), \end{aligned} \quad (15)$$

function $P(\sigma)$ has a peak only at point $\sigma = 0$ and dry friction (DF) typical of solidlike lubricant takes place. Between these curves, the peaks of $P(\sigma)$ correspond to zero and nonzero value of stresses; i.e., this is the region of stick-slip (SS) friction, where periodic transitions between these dynamic friction regimes occur. This is typical of the intermittent conditions during lubricant melting, where a mixture of solidlike and liquidlike states exists. In accordance with expressions (15), lubricant can melt even at zero temperature T_e of the friction surfaces if the intensity of strain fluctuations exceeds the critical value

$$I_\varepsilon = (1 + 2g^{-1})/2gD.$$

It follows hence that this value decreases upon an increase in the stochastic source intensity D .

The phase diagram of states of the system is constructed in accordance with the analytically determined distribution $P(\sigma)$. We will carry out such a procedure analyzing Eq. (1) numerically. This is due to the fact that time dependences of physical quantities are usually measured in experiments. In addition, this procedure makes it possible to demonstrate once again that the FPE was chosen correctly.

Multiplying Eq. (1) by dt , we obtain the Langevin differential equation

$$\tau_\sigma d\sigma = f(\sigma)dt + \sqrt{I(\sigma)}dW(t), \quad (16)$$

where $dW(t) = W(t+dt) - W(t) \equiv \xi(t)dt$ is a Wiener process exhibiting the properties of white noise [7]:

$$\langle W(t) \rangle = 0, \quad \langle (W(t))^2 \rangle = 2Ddt. \quad (17)$$

To solve Eq. (16) numerically, we will employ the Euler method. Having measured time in the τ_σ units and taking into account the definition of a discrete analog of

random force differential $dW(t) \equiv \sqrt{\Delta t} W_n$, we obtain the iterative procedure for calculating the time series of stresses:

$$\sigma_{n+1} = \sigma_n + f(\sigma_n)\Delta t + \sqrt{I(\sigma_n)}\Delta t W_n. \quad (18)$$

The equation is solved on time interval $t \in [0, T]$. For a preset number N of iterations (number of points of the time series), the time increment is defined as $\Delta t = T/N$. Force W_n possesses the following properties:

$$\langle W_n \rangle = 0, \quad \langle W_n W'_n \rangle = 0, \quad \langle W_n^2 \rangle \rightarrow 2D. \quad (19)$$

A random force possessing the properties of white noise can be correctly defined using the Box–Muller model [8]:

$$W_n = \mu \sqrt{-2 \ln r_1} \cos(2\pi r_2), \quad r_i \in (0, 1], \quad (20)$$

where $\mu = \sqrt{2D}$ and W_n is an absolutely random number with properties (19) and (7). Pseudorandom numbers r_1 and r_2 are repeated after a certain interval.

Trajectories $\sigma(t)$ for various regions on the phase diagram are shown in Fig. 2. The upper part of the figure corresponds to point 1 in Fig. 1 (SF). One can see periodic transitions between positive and negative stable values of stress of the same absolute magnitude. This regime corresponds to the liquidlike structure of the lubricant and a small value of friction force. We must assume that reverse motion (motion of surfaces displaced in the opposite direction) takes place for negative values of stress; strain in this case is also negative. We can disregard the negative region, assuming that it is deprived of physical meaning, and suppose that stresses begin to increase after attaining zero value, which allows us to analyze the behavior of $|\sigma|$. The middle part of the figure corresponds to point 2 in Fig. 1 (SS). It shows frequent transitions between zero and nonzero values of stress, which corresponds to stick-slip friction, in which the friction force changes abruptly during motion. Since these transitions are very frequent, this situation corresponds to the intermittent conditions, when a mixture of liquidlike and solidlike phases exists in the lubricant [2]. The lower part of the figure corresponds to point 3 in Fig. 1 (DF). In this case, oscillations occur in the vicinity of $\sigma = 0$, which corresponds to the solidlike structure of the lubricant and the highest value of the friction force.

Figure 3a shows probability distribution (10) for the points indicated on the phase diagram, while Fig. 3b shows analogous distributions obtained numerically by solving the Langevin equation and corresponding to the trajectories in Fig. 2. It can be seen that the corresponding dependences $P(\sigma)$ perfectly match in both cases, which confirms the correspondence of the FPE in Ito form (9) to iterative procedure (18). Curve 1 corresponds to the region of sliding friction on the phase diagram, where only the nonzero maximum of $P(\sigma)$ exists;

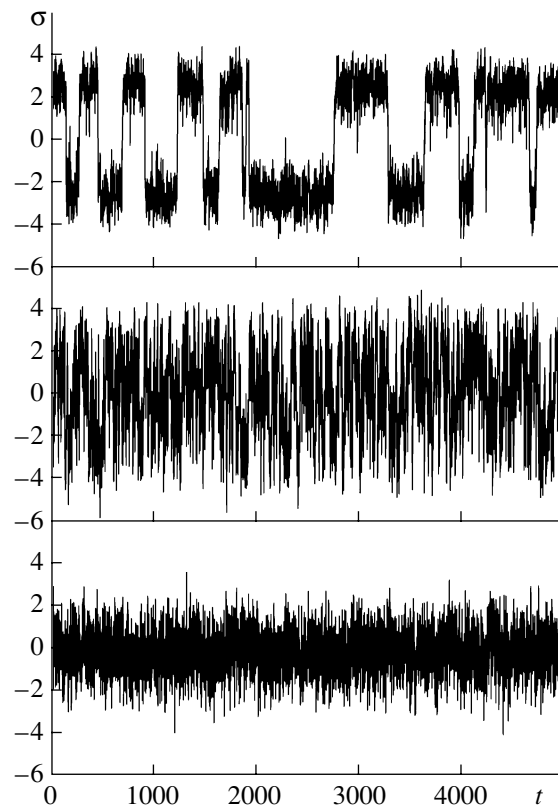


Fig. 2. Time series of stresses $\sigma(t)$ corresponding to the regimes represented by points in Fig. 1 for $I_\sigma = 0.1$. The upper part corresponds to point 1 ($I_T = 1, T_e = 3.8$, SF), the middle part corresponds to point 2 ($I_T = 6, T_e = 2.5$, SS), and the lower part corresponds to point 3 ($I_T = 3, T_e = 0.5$, DF).

curve 2 corresponds to the stick-slip friction region, where zero and nonzero maxima exist; and curve 3 corresponds to the region of dry friction with a single zero maximum of $P(\sigma)$.

The experimental dependences of the friction force on the velocity of mica surfaces being displaced, between which hydrocarbon and silicon liquids (cyclohexane, octamethyl cyclotetrasiloxane, *n*-octane, *n*-tetradecane, and branched isoparaffin-2-methyl octadecane) were placed, are given in [9]. According to these curves, the friction force first increases linearly and then the stick-slip regime sets in, in which the friction force varies periodically, ensuring intermittent motion. In the approach proposed in [9], such a behavior can be explained as follows. At the first stage of motion, the elastic component of stress σ predominates and the lubricant is solidlike (the lower part of Fig. 2). In this region, Hooke's law is observed and the total friction force increases. For a certain critical value of velocity, transitions between the solidlike and liquidlike structures (in the latter structure, the viscous component of stress dominates) of the lubricant take place due to the "shear melting" effect [10] (middle part of Fig. 2).

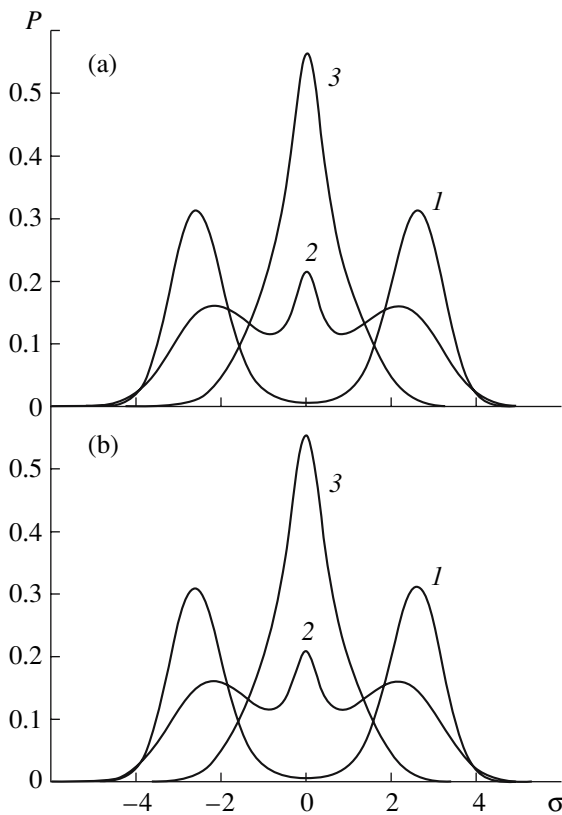


Fig. 3. Probability distributions: (a) determined by expression (10) and corresponding to points in Fig. 1; (b) determined from numerical analysis of Eq. (18) with parameters $N = 10^8$, $T = 10^6$, $\Delta t = 0.01$ and corresponding to trajectories in Fig. 2.

In addition, the time dependences of the friction force, on which the melting of the lubricant is shown for constant shear rate are depicted (see, for example, [9, 11]), are measured experimentally. It should be noted that friction is always accompanied by dissipation of energy of translatory motion of rubbing surfaces, which leads to their heating. The dissipation is the stronger the higher the value of the total friction force; consequently, for the solidlike state of the lubricant, the surfaces are heated at a higher rate than in the case of the liquidlike state of the lubricant. The change in the temperature of the surfaces becomes weaker and weaker with time due to the increase in the amount of energy liberated to the environment until the equilibrium value T_e sets in. To approximate the increase in the temperature of rubbing surfaces with time, we can use the exponential dependence, which makes it possible to take into account these peculiarities,

$$T_e(t) = T_e^0(1 - \exp(-Bt)), \quad (21)$$

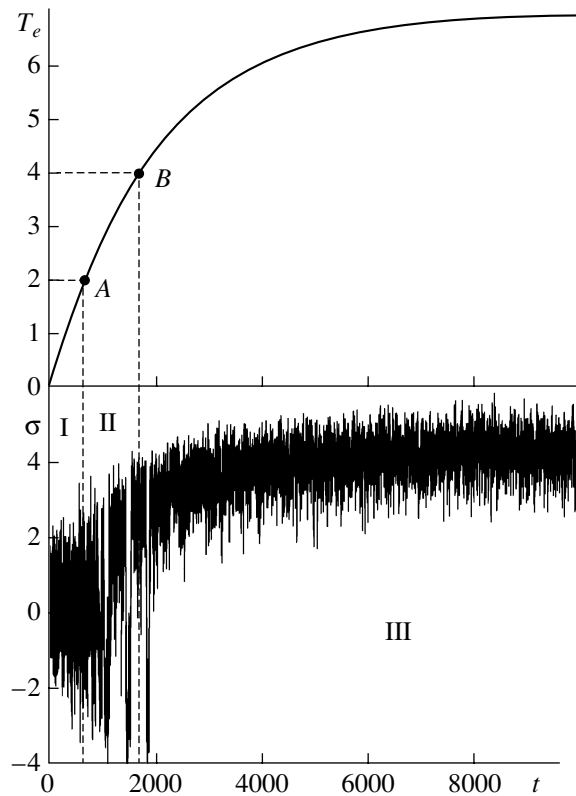


Fig. 4. Upper part shows the time dependence (21) of the temperature of moving surfaces for $T_e^0 = 7.0$ and $B = 0.005$. Points A and B correspond to points in Fig. 1. The lower part shows the time series $\sigma(t)$, corresponding to parameters in Fig. 1 for $I_\sigma = 0$, $I_T = 3.0$, and for varying temperature T_e represented by dependence (21).

where T_e^0 is the value of T_e being stabilized and B is the constant determining the rate of temperature increase at the initial stage.

Figure 4 shows the solution $\sigma(t)$ of the Langevin equation taking formula (21) into account. The upper part shows dependence (21). In accordance with the phase diagram (see Fig. 1), point A corresponds to the temperature of transition from dry friction (DF) to stick-slip (SS) regime. At the temperature depicted by point B, a further transition to sliding friction (SF) takes place. The lower part shows the evolution of stresses $\sigma(t)$, where three temporal regions are singled out: region I (DF), II (SS), and III (SF). In the first region, the friction force assumes the maximal value or increases; in the second region, stick-slip motion takes place; while in the third region, the friction force decreases. The figure is in good agreement with experimental data obtained in [11, 12].

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