

Nonequilibrium Kinetics of Phase Transitions in the Boundary Friction Mode

I. A. Lyashenko^{a,*}, L. S. Metlov^b, A. V. Khomenko^a, and S. N. Chepul'skiy^a

^aSumy State University, ul. Rymkogo-Korsakova 2, Sumy, 40007 Ukraine

^bDonetsk Institute for Physics and Engineering named after A.A. Galkin, National Academy of Sciences of Ukraine,
ul. Rozy Lyuksemburg 72, Donetsk, 83114 Ukraine

*e-mail: nabla04@ukr.net

Received January 19, 2012

Abstract—A nonequilibrium evolution thermodynamic model is presented, which describes the processes developing in the boundary friction mode. The excessive volume parameter is introduced to describe the lubricant state; it has a minimum value in the case of the solid-like structure of the lubricant and increases during melting. The source of entropy growth which results from the external energy inleak during the deformation of the lubricant owing to the shear of the rubbing surfaces, is taken into account. It is shown that the stick-slip mode of motion occurs within wide ranges of the parameters; this is caused by periodic phase transitions of the first-order between the structural states of the lubricant. The effect of the shear velocity, load, and temperature on the pattern of stick-slip friction is studied.

Keywords: lubricant, friction force, shear stresses and strains, entropy, internal energy, phase transition, stick-slip mode

DOI: 10.3103/S106836661204006X

INTRODUCTION

One of the applied interdisciplinary directions in science is nanotribology [1], which relates to study of the processes of the adhesion, friction, wear, and fracture of rubbing solids at the atomic level. The explanation and modeling of the friction processes at nanoscales is an important problem in this field. The subjects of study in nanotribology are the processes of the adhesion and sliding of surfaces in contact [2, 3], the influence of a nanometer lubricating film on friction [1, 2, 4], mechanical properties of contacts [5, 6], and others.

The effects of the periodic stick and the subsequent slip of rubbing surfaces present great interest to tribologists; they lead to the nonuniformity of the relative motion of the surfaces (stick-slip) [7–9]. This sliding mode occurs mainly during dry friction [10–12], as well as during boundary friction, when the lubricating film is about a few atom diameters thick [1, 2, 4, 5, 7–9, 13]. If asperities separate the rubbing surfaces, the stick-slip mode of boundary friction is explained as follows: at some moment of time the asperities on the rubbing surfaces stick together because of adhesion or capillary forces and their subsequent tear-off requires that the arising mechanical stresses exceed their critical value. The stick-slip mode parameters depend considerably, as a rule, on factors including the velocity of motion, the lubricant temperature, and the load applied to the surfaces. For example, when a critical sliding velocity

is reached, the effect vanishes and the friction force becomes regular.

The experimentally observed processes evolving in the boundary friction mode are more diverse than the processes developing in bulk systems and show a variety of cardinally new phenomena, which cannot be explained from the viewpoint of classical science [7]. A boundary lubricant provides, as a rule, several kinetic modes, between which stepwise phase transitions occur during friction; the transitions yield a complex pattern of the kinetic dependences of the system parameters [7, 14]. The following three basic modes are generally distinguished: sliding at slow shear velocities, the regular stick-slip mode, and sliding at high shear velocities. These modes were determined experimentally [2, 7, 15] and then explained theoretically [13].

Earlier we proposed a model based on the conception of viscoelastic medium to describe boundary friction [16–20]. We used it to describe thermodynamic and shear melting. Consideration of the fluctuations of the basic parameters of the system [16–19] made it possible to explain the causes of hysteresis [20] observed experimentally [21–23] and describe the periodical stick-slip friction mode [17]. However, according to the model, this regime has a pronounced stochastic or trend component, while in experiments it has, as a rule, a periodic pattern with constant frequency and amplitude. To eliminate this “drawback,” we proposed the deterministic theory describing the

friction of atomically smooth solid surfaces separated by an ultrathin lubricating film [24–26]. It involves the excessive volume parameter or the disorder parameter to describe the state of the lubricant; the parameter characterizes the chaotization of the lubricant structure during melting. This allowed us to describe universally thermodynamic and shear melting and analyze the dependence of the stationary friction force on the lubricant temperature and the relative shear velocity of the rubbing surfaces during their uniform shear at a constant shear velocity, as well as to describe the stick-slip friction mode within the framework of the mechanical analog of a simple tribosystem. The current work is aimed at the subsequent development of the above-mentioned theory to describe the nonequilibrium processes which evolve in such tribosystems. To take into account the nonequilibrium processes we introduce the nonequilibrium entropy describing the share of thermal motion which results from the nonequilibrium pattern of the thermal distribution. It is assumed that the equilibrium entropy increases continuously owing to the transition of the nonequilibrium entropy to the equilibrium subsystem. The paper deals with analysis of the effect of the external normal pressure on the pattern of lubricant melting. The stick-slip melting mode observed experimentally is described. It is shown that with increasing shear velocity the frequency of stick peaks in the stick-slip mode grows and then diminishes; subsequently, the sliding mode with a constant friction force occurs.

BASIC EQUATIONS AND PHASE DIAGRAM

Let us write the expansion for the volume density of the internal energy u by the parameter f with account for the contributions from the elastic components of shear strains ε_{ij}^e , the equilibrium entropy s , and the nonequilibrium entropy \tilde{s} in the following form [4, 27]:

$$u = u_0 + t_0 \tilde{s} - \frac{1}{2} t_1 \tilde{s}^2 + \phi_0 f^2 - \frac{1}{4} \phi_1 f^4 + \frac{1}{6} \phi_2 f^6, \quad (1)$$

where the variable f^2 is the excessive volume, the zero value of which corresponds to the solid-like structure of the lubricant and the nonzero value of which corresponds to the fluid-like structure [4, 24, 27]. Here, the minor expression parameters u_0 , ϕ_0 , and t_0 are the functions of the first two invariants of the elastic strain tensor ε_{ii}^e and $\varepsilon_{ij}^e \varepsilon_{ji}^e$, as well as the entropy s :

$$u_0 = u_0^* + \frac{1}{2} \lambda (\varepsilon_{ii}^e)^2 + \mu \varepsilon_{ij}^e \varepsilon_{ji}^e + \alpha s^2, \quad (2)$$

$$\phi_0 = \phi_0^* - \frac{1}{2} \bar{\lambda} (\varepsilon_{ii}^e)^2 - \bar{\mu} \varepsilon_{ij}^e \varepsilon_{ji}^e - \alpha_\phi s^2, \quad \text{and} \quad (3)$$

$$t_0 = t_0^* + \frac{1}{2} \tilde{\lambda} (\varepsilon_{ii}^e)^2 + \tilde{\mu} \varepsilon_{ij}^e \varepsilon_{ji}^e. \quad (4)$$

The elastic stresses σ_{ij}^e arising in the lubricating film can be presented in the following form using expression (1) for the internal energy:

$$\frac{\partial u}{\partial \varepsilon_{ij}^e} \equiv \sigma_{ij}^e = \lambda \varepsilon_{ii}^e \delta_{ij} + 2\mu \varepsilon_{ij}^e - \left(\bar{\lambda} \varepsilon_{ii}^e \delta_{ij} + 2\bar{\mu} \varepsilon_{ij}^e \right) f^2 + \left(\tilde{\lambda} \varepsilon_{ii}^e \delta_{ij} + 2\tilde{\mu} \varepsilon_{ij}^e \right) \tilde{s}, \quad (5)$$

where ε_{ij}^e is the shear component of the elastic strain. Expression (5) is reduced to the effective Hooke's law [24, 28]

$$\sigma_{ij}^e = 2\mu_{\text{eff}} \varepsilon_{ij}^e + \lambda_{\text{eff}} \varepsilon_{ii}^e \delta_{ij} \quad (6)$$

with the effective elastic parameters

$$\mu_{\text{eff}} = \mu - \bar{\mu} f^2 + \tilde{\mu} \tilde{s}, \quad \text{and} \quad (7)$$

$$\lambda_{\text{eff}} = \lambda - \bar{\lambda} f^2 + \tilde{\lambda} \tilde{s}, \quad (8)$$

which diminish during the melting of the lubricant owing to the growth of the excessive volume f^2 . Since the elastic constant cannot take negative values, one should assume $\mu_{\text{eff}} = 0$ if the inequality $f^2 > (\mu + \tilde{\mu} \tilde{s}) / \bar{\mu}$ is true; if $f > (\lambda + \tilde{\lambda} \tilde{s}) / \bar{\lambda}$, one should assume $\lambda_{\text{eff}} = 0$.

For the plane strain state of the lubricant wherein $\varepsilon_{22} = 0$, the strain tensor invariants are determined as follows [25, 29]:

$$\varepsilon_{ii}^e = \frac{n}{\lambda_{\text{eff}} + \mu_{\text{eff}}}, \quad \text{and} \quad (9)$$

$$\varepsilon_{ij}^e \varepsilon_{ji}^e = \frac{1}{2} \left[\left(\frac{\tau}{\mu_{\text{eff}}} \right)^2 + (\varepsilon_{ii}^e)^2 \right], \quad (10)$$

where n and τ are the normal and tangential components of the stresses applied to the lubricant by the rubbing surfaces. The shear stress τ is found from expression (6), which yields the following dependence at $i \neq j$ or $\delta_{ij} = 0$:

$$\tau = 2\mu_{\text{eff}} \varepsilon_{ij}^e. \quad (11)$$

The stationary states of the lubricant are determined by the condition $\partial u / \partial f = 0$, which yields

$$\bar{\mu} \varepsilon_{ij}^e \varepsilon_{ji}^e + \alpha_\phi s^2 = \phi_0^* - \frac{1}{2} \bar{\lambda} (\varepsilon_{ii}^e)^2 - \frac{1}{2} \phi_1 f^2 + \frac{1}{2} \phi_2 f^4 + \frac{n^2 (\bar{\lambda} + \bar{\mu})}{(\lambda_{\text{eff}} + \mu_{\text{eff}})^2}. \quad (12)$$

It is convenient to present this equation as the function $\varepsilon_{ij}^e \varepsilon_{ji}^e(f, n, s, \tilde{s})$ or $s(f, n, \varepsilon_{ij}^e \varepsilon_{ji}^e, \tilde{s})$. When analyzing equation (12), we determine the elastic shear strain ε_{ij}^e in accordance with (9), (10), and (11) through the invariants as follows:

$$\varepsilon_{ij}^e = \frac{1}{2} \sqrt{2\varepsilon_{ij}^e \varepsilon_{ji}^e - (\varepsilon_{ii}^e)^2}. \quad (13)$$

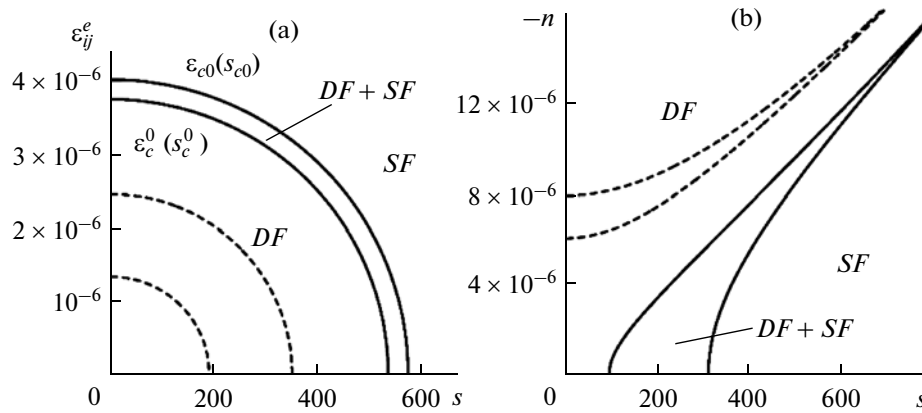


Fig. 1. Phase diagrams with areas of sliding (*SF*) and dry (*DF*) friction at parameters $\phi_0^* = 2 \text{ J/m}^3$, $\phi_1 = 8.5 \text{ J/m}^3$, $\phi_2 = 5.0 \text{ J/m}^3$, $\lambda = 5 \times 10^{11} \text{ Pa}$, $\bar{\lambda} = 10^9 \text{ Pa}$, $\mu = 10^{12} \text{ Pa}$, $\bar{\mu} = 2 \times 10^{11} \text{ Pa}$, $\alpha = 0.95 \text{ K}^2 \text{ m}^3/\text{J}$, $\alpha_\phi = 2 \times 10^{-5} \text{ K}^2 \text{ m}^3/\text{J}$, and $\bar{s} = 0$: (a) solid lines correspond to stress $n = -10^7 \text{ Pa}$, dashed lines to $n = -3 \times 10^6 \text{ Pa}$; (b) solid lines correspond to strain $\varepsilon_{ij}^e = 0$, dashed lines to $\varepsilon_{ij}^e = 3 \times 10^{-6}$.

Analysis of the above equations shows that there are critical values of the strain ε_{c0} and entropy s_{c0} at which lubricant melting follows the mechanism of the first-order phase transition. In this case, ε_{c0} is the function of the entropy s and s_{c0} depends on the strain ε_{ij}^e . The lubricant solidifies at other values of the strain ε_c^0 and the entropy s_c^0 . Since potential (1) proposed for the description of the melting process is symmetrical, we can distinguish the following cases [27]: 1) within the range of values $\varepsilon_{ij}^e < \varepsilon_c^0$ (or $s < s_c^0$) the lubricant is in the solid-like state that corresponds to the occurrence of the sole minimum of energy (1) at $f^2 = 0$; 2) within the range of values $\varepsilon_{ij}^e > \varepsilon_{c0}$ (or $s > s_{c0}$) the lubricant has the fluid-like structure (in this case, potential (1) has two symmetric nonzero minima separated by a single maximum); 3) within the intermediate range of values of the governing parameters $\varepsilon_c^0 < \varepsilon_{ij}^e < \varepsilon_{c0}$ ($s_c^0 < s < s_{c0}$) the potential has two symmetric minima, which are separated from the zero minimum by two symmetric maxima, the state of the lubricant being dependent on the initial conditions [8].

The stationary states of the lubricant (at $\bar{s} = 0$) on the phase diagrams plotted by equations (12) and (13) are separated by the curves $\varepsilon_{c0}(s_{c0})$ and $\varepsilon_c^0(s_c^0)$ (Fig. 1a). Above the line $\varepsilon_{c0}(s_{c0})$ the lubricant is in the fluid-like state and the sliding friction mode occurs (the area *SF*). The potential in this area has the form described above as case 2. Below the curve $\varepsilon_c^0(s_c^0)$ the lubricant is in the solid-like state that corresponds to the form of the internal energy $u(f)$ described in case 1. In the area between these curves the state of the lubricant depends

on the initial conditions and the potential takes on the form described by case 3. The dashed lines show the areas of the phase diagram at smaller values of the normal stresses. It is seen from the figure that with increasing contact load the dry friction area widens, while the hysteresis area, which separates it from the fluid-like state area, narrows. The external load described in our model by the normal stresses n often has a determining effect on nanosized tribosystems. For example, it is shown in experimental work [7] that the growth of the load increases the critical melting shear velocity for some types of lubricants, while for other types of lubricants it diminishes the melting shear velocity. Such pressure variations lead to changes in the frequency of phase transitions, etc. The phase diagram in the pressure–entropy coordinates presented in Fig. 1b serves to elucidate the effect of the external stresses on the state of the lubricant. It follows from the diagram that with increasing contact load the transition of the lubricant from the solid-like state (area *DF*) to the fluid-like one (area *SF*) occurs, omitting the hysteresis area (*DF + SF*). Thus, when the external load applied to the friction surfaces exceeds its critical value, the first-order phase transition does not occur; instead of it, the continuous melting of the lubricant evolves by the second-order phase transition mechanism. Earlier we showed that the growth of the normal component of the stresses causes the solidification of the lubricant and increases the total friction force; depending on the value of n , either the first-order or second-order phase transition can occur [25]. Under light external pressures this model describes only the first-order phase transition.

Such phase diagrams are also plotted when generalizing the experimental data [7]. One of the common methods of plotting phase diagrams is analysis of the

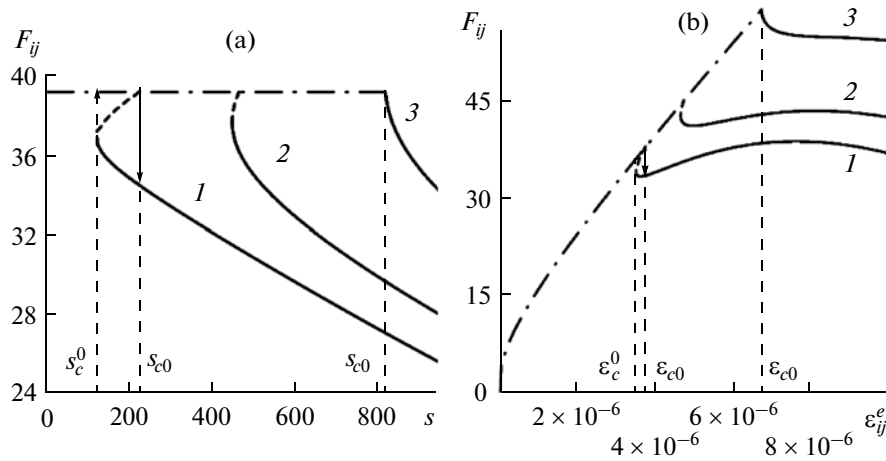


Fig. 2. Dependences of friction force F_{ij} (mN) (14) on elastic strains ε_{ij}^e and entropy s ($\text{J K}^{-1} \text{m}^{-3}$) at parameters presented in Fig. 1, as well as at $\tau_\varepsilon = 10^{-8} \text{ s}$, $\gamma = -2/3$, $k = 7 \times 10^5 \text{ Pa s}^{1/3}$, and $A = 3 \times 10^{-9} \text{ m}^2$: (a) $\varepsilon_{ij}^e = 4 \times 10^{-6}$; (b) $s = 300 \text{ J K}^{-1} \text{m}^{-3}$. Curves 1–3 in both figures correspond to values $n = -1.1 \times 10^7 \text{ Pa}$, $-1.4 \times 10^7 \text{ Pa}$, and $-2 \times 10^7 \text{ Pa}$.

time dependences of the friction force $F(t)$ at various temperatures, shear velocities, lubricant film thicknesses, etc. The friction force is determined by the expression [4, 8, 24, 25]

$$F_{ij} = \left[\tau + k \text{sgn}(V_{ij}) \left(\frac{|V_{ij}|}{h} \right)^{\gamma+1} \right] A, \quad (14)$$

where the first summand in the square brackets found from expression (11) gives the elastic component of the friction force and the second summand gives the viscous component. In expression (14) we introduced the area of the contact between the surfaces being sheared A and the phenomenological coefficients k , γ , which allowed us to take into account the type of the lubricant [24]. Expression (14) includes the velocity of the relative shear of the friction surfaces V_{ij} , whose value in the stationary case $d\varepsilon_{ij}^e/dt = 0$ depends on the lubricating film thickness h and the relaxation time of the internal stresses τ_ε [8, 26]

$$V_{ij} = \frac{h\varepsilon_{ij}^e}{\tau_\varepsilon}. \quad (15)$$

With account for formula (15) for positive values of ε_{ij}^e , expression (14) becomes

$$F_{ij} = \left[\tau + k \left(\frac{\varepsilon_{ij}^e}{\tau_\varepsilon} \right)^{\gamma+1} \right] A. \quad (16)$$

Dependence (16) is shown in Fig. 2, where, as above, we assume $\tilde{s} = 0$. Here, the dash-dot portion corresponds to the solid-like lubricant and the portions shown by the dashed lines correspond to the unstable

stationary solutions. It is seen in Fig. 2a that at $s > s_{c0}$ the melting of the lubricant is accompanied by a discrete decrease in the friction force, while at $s < s_c^0$ the lubricant solidifies and the friction force increases again. These transitions are not shown for curve 2 to avoid needless details in the figure. When the lubricant is in the solid-like state (the dash-dot portion), the friction force does not depend on the entropy since in this case the stationary value $f = 0$ is reached. Curves 1–3 are plotted with gradually increasing contact pressure. For curves 1 and 2, hysteresis is observed since the first-order phase transition occurs, during which shear modulus (7) varies abruptly; with increasing pressure the hysteresis area narrows, as was shown in Fig. 1. At the parameters of curve 3 the continuous second-order phase transition occurs, when the critical value of the entropy s_{c0} at which the lubricant melts coincides with the value at which it solidifies.

The dependences presented in Fig. 2b show that at low strains the lubricant is in the solid-like state and dry friction occurs (the dash-dot portion of the dependence). The growth of ε_{ij}^e in the dry friction mode causes an increase in friction force (14). At $\varepsilon_{ij}^e > \varepsilon_{c0}$ the lubricant melts and elastic shear stresses (11) drop sharply leading to the abrupt decline of the friction force F_{ij} for curves 1 and 2. As the strain continues increasing, the value of F_{ij} grows and then begins diminishing owing to the decline of the elastic component of the friction force, though the viscous component continues growing with increasing strain. The lubricant solidifies at $\varepsilon_{ij}^e < \varepsilon_c^0$ (for curve 1 the reverse transition is not shown by arrows because for reasons of scaling and for curve 2 the direct transition is also

not shown). According to curve 3, as for Fig. 2a, at great values of the normal stresses or surface pressure, the second-order phase transition occurs, during which the friction force varies continuously. The results presented in Fig. 2b are a kind of Stribeck curve for the boundary mode, which was first proposed in work [30] when generalizing the experimental data.

THE SYSTEM OF KINETIC EQUATIONS

Since the internal energy is assigned in form (1), the current temperature of the lubricant can easily be found:

$$\frac{\partial u}{\partial s} \equiv T = 2s(\alpha - \alpha_\phi f^2), \quad (17)$$

and the effective temperature of the nonequilibrium subsystem is determined in the same way:

$$\frac{\partial u}{\partial \tilde{s}} \equiv \tilde{T} = t_0 - t_1 \tilde{s}. \quad (18)$$

To continue the study of the kinetic processes, we write the evolution equations for the nonequilibrium parameters f and \tilde{s} in the form of a system of equations like that in the Landau–Khalatnikov system:

$$\tau_f \dot{f} = -\frac{\partial u}{\partial f}, \quad \tau_s \dot{\tilde{s}} = \frac{\partial u}{\partial \tilde{s}}, \quad (19)$$

where the constants τ_f, τ_s are the reciprocals of the kinetic coefficients. According to equations (19), the internal energy by the coordinate f tends to a minimum and the internal energy by the coordinate \tilde{s} tends to a maximum; this corresponds to nonequilibrium processes [27, 31].

Evolution equations (19) in the explicit form become [27]

$$\tau_f \frac{\partial f}{\partial t} = -2\phi_0 f + \phi_1 f^3 - \phi_2 f^5 - \frac{2n^2(\bar{\lambda} + \bar{\mu})f}{(\lambda_{eff} + \mu_{eff})^2}, \quad \text{and} \quad (20)$$

$$\tau_s \frac{\partial \tilde{s}}{\partial t} = t_0 - t_1 \tilde{s}, \quad (21)$$

where the presence of the last summand in (20) is caused by the dependence of invariants (9) and (10) on the value of f . In equation (21) the summand with the sign + describes the increment of the nonequilibrium entropy owing to the external energy sources (the work) and the summand with the sign – describes its transfer to the equilibrium subsystem.

Since we consider the open nonequilibrium system, it is appropriate to introduce the temperature of the friction surfaces T_e to describe the processes of heat exchange between the lubricant and the environment. In the case of the nonuniform heating of the environ-

ment, the heat conduction equation is reduced to the common continuity equation [28]

$$T \frac{\partial s}{\partial t} = \kappa \nabla^2 T, \quad (22)$$

where the thermal conductivity κ is assumed to be constant. To simplify the problem we suppose the lubricating film to be uniform over the plane ($\nabla_x^2 = \nabla_y^2 = 0$). Since the lubricating film is thin, the following approximation for the component ∇_z^2 can be used with a sufficient accuracy [28]:

$$\nabla_z^2 T \approx \frac{T_e - T}{h^2}, \quad (23)$$

where h is the lubricating film thickness or the distance between the rubbing surfaces (see (15)). With account for approximation (23), equation (22) is written in the following simpler form:

$$\frac{\partial s}{\partial t} = \frac{\kappa}{h^2} \left(\frac{T_e}{T} - 1 \right), \quad (24)$$

where the variable h^2/κ plays the role of the relaxation time, during which the temperatures are equalized along the lubricating film thickness owing to thermal conductivity. However, the interaction between the equilibrium and nonequilibrium subsystems is ignored in (24). A decrease in the nonequilibrium entropy is taken into account in the negative summands in evolution equation (21); therefore, these summands should take into account the increment of the equilibrium entropy. With this in mind, we derive the final equation for the equilibrium entropy

$$\tau_s \frac{\partial s}{\partial t} = t_1 \tilde{s} + \tau_s \frac{\kappa}{h^2} \left(\frac{T_e}{T} - 1 \right), \quad (25)$$

where the lubricant temperature T (17) in the stationary state $\partial s/\partial t = 0$ is determined not only by the temperature of the friction surfaces T_e , which plays the role of a thermostat (the environment), like in (24), but also by the value of the nonequilibrium entropy \tilde{s} .

In our works [24–26] we derived the kinetic equation for the strain ε_{ij}^e in the following form:

$$\tau_\varepsilon \dot{\varepsilon}_{ij}^e = -\varepsilon_{ij}^e + \frac{V_{ij} \tau_\varepsilon}{h}, \quad (26)$$

where τ_ε is the Maxwell relaxation time of the internal stresses and V_{ij} is the relative shear velocity of the rubbing surfaces introduced in (14). Since the small value of the relaxation time $\tau_\varepsilon = 10^{-8}$ s will be used in the subsequent calculations, we shall stay within the approximation $\tau_\varepsilon \ll \tau_f, \tau_s$ [32, 33], wherein $\tau_\varepsilon \dot{\varepsilon}_{ij}^e \approx 0$ can be assumed. The last equation yields the dependence (compare with (15))

$$\varepsilon_{ij}^e = \frac{V_{ij} \tau_\varepsilon}{h}. \quad (27)$$

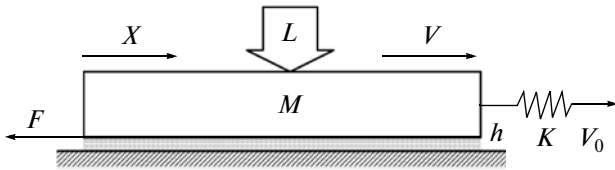


Fig. 3. Mechanical analog of simplest tribosystem.

The study of the kinetics of the system requires the joint numerical solution of kinetic equations (20), (21), and (25) involving the determination of the invariants according to (9) and (10), the shear stresses τ from (11), the elastic constants from (7) and (8), the current lubricant temperature T according to (17), and the strains according to expression (27).

THE KINETICS OF THE TRIBOSYSTEM

The dynamic characteristics of any tribosystem are governed by its properties as a whole. In particular, in the area of the above-considered hysteresis during friction, the stick-slip mode of movement can occur [7, 13]. Figure 3 shows the typical diagram of the mechanical analog of a tribosystem. Here, the spring with the rigidity K is connected to the block of mass M , which experiences the additional normal load L . The block is placed on a smooth surface and they are separated by the lubricating film with the thickness h . The free end of the spring is driven with the constant velocity V_0 . The movement of the block yields friction force F (14), which reacts against the movement. In the general case, the block velocity V and the spring velocity V_0 do not coincide because of the oscillating pattern of the force F ; this results in the stick-slip movement of the block. This mode is similar to dry friction [12]. The load L is related to the normal component of the stresses n considered in this work as $n = -L/A$, where A is the area of contact between the surfaces from expression (14).

Let us designate the current coordinate of the upper block as X ; then the corresponding equation of motion is [7, 34]

$$M\ddot{X} = K\Delta X - F. \quad (28)$$

Here, ΔX is the elongation of the spring, which can be determined as follows:

$$\Delta X = \int_0^t V_0 dt' - X, \quad (29)$$

where $t = t'$ is the time of the movement of the free end of the spring.

To study the kinetic regimes of boundary friction, which occur in the system shown in Fig. 3, we shall act within the above-introduced adiabatic approximation $\tau_\varepsilon \ll \tau_f, \tau_s$. It is sufficient to solve the system of

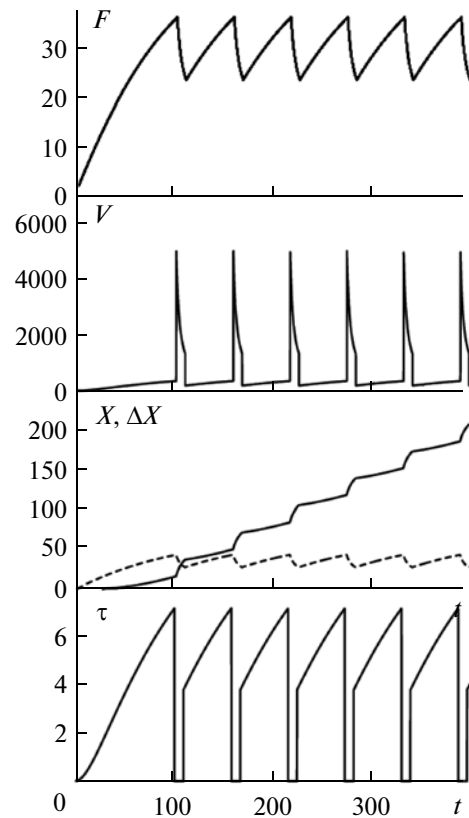


Fig. 4. Dependences of total friction force F (mN) (14), shear velocity of upper friction surface V (nm/s), its coordinate X (μm), elongation of moving spring ΔX (μm), and elastic shear stresses τ (MPa) on time t (s) at parameters of Figs. 1 and 2 and $t_0^* = 600$ K, $t_1 = 200$ K² m³/J, $\tilde{\lambda} = 2 \times 10^9$ K, $\tilde{\mu} = 5 \times 10^9$ K, $\tau_f = 0.1$ J s/m³, $\tau_s = 0.01$ K² s m³/J, $\kappa = 10^{-10}$ W/(K m), $h = 10^{-9}$ m, $K = 800$ N/m, and $M = 0.1$ kg.

kinetic equations (20), (21), (25), and (28) determining the current strain in accordance with relation (27). Figure 4 shows the result of solving these equations and presents the dependences of the friction force F (14), the shear velocity of the upper rubbing block $V = \dot{X}$, the block coordinate X , the spring elongation ΔX , and the elastic stresses τ , which arise in the lubricant. At the beginning of movement all the parameters presented in the figure increase monotonically since the melting of the lubricant requires either the lubricant temperature T or the shear velocity V to exceed their critical values. As the above dependences are obtained for the temperature of the friction surfaces T_e , which provides the lubricant temperature T below the critical value, in the rest at $t = 0$ the lubricant is in the solid-like state and has a nonzero value of the effective shear modulus. At the initial moment of time the free spring end begins moving at the velocity $V_0 \neq 0$; this causes the elongation of the spring, the

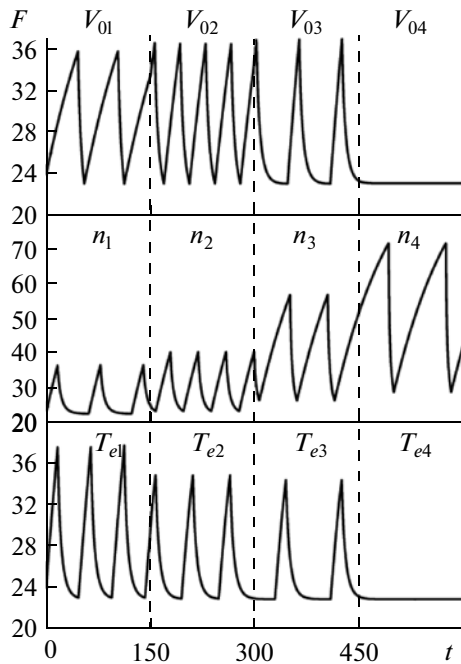


Fig. 5. Dependences of total friction force F (mN) (14) on time t (s) at parameters of Fig. 4. Upper part: $T_e = 280$ K, $n = -0.8 \times 10^7$ Pa, $V_{01} = 600$ nm/s, $V_{02} = 1000$ nm/s, $V_{03} = 1320$ nm/s, and $V_{04} = 1330$ nm/s; middle part: $T_e = 280$ K, $V_0 = 1320$ nm/s, $n_1 = -0.8 \times 10^7$ Pa, $n_2 = -10^7$ Pa, $n_3 = -1.8 \times 10^7$ Pa, and $n_4 = -2.5 \times 10^7$ Pa; lower part: $V_0 = 1300$ nm/s, $n = -0.8 \times 10^7$ Pa, $T_{e1} = 200$ K, $T_{e2} = 600$ K, $T_{e3} = 715$ K, and $T_{e4} = 720$ K.

growth of the shear velocity of the upper surface V , and, according to (14), an increase in the friction force F . As a result, a moment comes when the velocity V exceeds its critical value and the melting of the lubricant follows the “shear melting” mechanism [7]. After melting, the stresses relax rapidly to the zero value and this yields the zero value of the elastic component of the friction force F , but the sharp rise of the shear velocity V increases considerably the viscous component of F ; this does not lead to a sharp drop of the friction force. Subsequently, the shear velocity V diminishes again owing to a decrease in the spring elongation ΔX and the viscous component of the friction force behaves similarly. The situation arises with time when the velocity V becomes smaller than the critical value and fails to retain the lubricant in the melted state. After this moment, the lubricant solidifies and the elastic stresses, and therefore the elastic component of the friction force F , arise in it. Because of this, the upper block moves more slowly (the sharp drop of the velocity V in the figure after its abrupt rise and subsequent relaxation). The described process occurs periodically with time, thus providing the stick-slip mode of movement with the sawtooth time depen-

dence of the friction force. The block coordinate X increases monotonically since the block moves in only one direction. It should be noted that in this case, according to the dependence $\tau(t)$, the elastic stresses in the melted state of the lubricant vanish because the effective shear modulus μ_{eff} (7) takes on the zero value. However, this is not the necessary condition for providing such a regime. A similar behavior was shown earlier within the framework of the simpler equilibrium thermodynamic model [8, 9, 34].

The friction mode is affected greatly by the governing parameters such as the temperature of the surfaces T_e , the shear velocity V_0 , and the external pressure n . Since this friction mode is one of the main causes of the fracture of rubbing microelectronic components, we carry out an additional micro study of the effect of the above factors on the specific features of the stick-slip mode. The time dependence of the friction force (14) at the increasing shear velocity of the free spring end V_0 and with other parameters constant is shown in the top of Fig. 5. It is seen that velocity growth initially increases the frequency of the phase transitions and then the frequency diminishes owing to the appearance of the kinetic portions on the dependence $F(t)$. We also note that there is a critical value of the velocity, at which the lubricant remains continuously in the fluid-like state and provides the kinetic mode of sliding with the minimal constant friction force ($V_0 = V_{04}$). Such behavior was observed repeatedly in the experiments [7, 35]. As the normal component of the load applied to the upper part of the friction surface (the middle of Fig. 5) increases, the kinetic portion $F = \text{const}$ diminishes and the friction force amplitude grows. According to the figure, the value of the load affects the system in an unusual manner since the frequency of the phase transition initially grows and then declines again. These specific features were demonstrated by the tribosystem studied in detail in experimental work [7]. We note that the observed effect of the load on the behavior of the system as a whole is also explained by the fact that, when the normal external stresses exceed their critical value, the type of the phase transition changes (see Fig. 1 and its description). And, finally, with temperature elevation (the bottom of the figure under consideration) the system tends to melting, which appears as a decrease in the amplitude $F(t)$ and the elongation of the kinetic portions $F = \text{const}$. When the temperature exceeds its critical value ($T_e = T_{e4}$), the lubricant melts fully and this leads to the occurrence of the kinetic sliding mode with the constant velocity V ; this, in turn, provides the value $F = \text{const}$.

We note that, according to experimental work [7], the long kinetic portions $F = \text{const}$ appear on the dependence $F(t)$ when the value of the shear velocity V is close to the critical one, at which the lubricant melts. This behavior is also observed within the framework of our model since the velocities V_{03} and V_{04} on

the top of Fig. 5 have similar values. The bottom of Fig. 5 shows a similar behavior of the temperature of the friction surfaces since the temperatures T_{e3} and T_{e4} , like the velocities on the top of the figure, have close values.

CONCLUSIONS

A model of boundary friction founded on the principles of nonequilibrium thermodynamics has been proposed. We have used it as a basis to describe a number of effects observed during friction of atomically smooth solid surfaces separated by a boundary lubricating film. The stationary states of lubricants at various pressures, shear velocities, and temperatures are considered. The dynamic mode is studied within the framework of the mechanical analog of a tribosystem during the shear of the upper friction surface in one direction. The dependences of the friction force on the shear velocity and temperature are obtained. It is shown that the lubricant melts when these variables exceed their critical values. At a high temperature of the friction surfaces, shear melting occurs at a lower shear velocity and when the temperature elevates ever more the lubricant melts even at the zero shear velocity. The study of the effect of the normal component of the pressure on the friction surfaces shows that the first-order phase transition occurs under small loads on the friction surfaces and when the load exceeds its critical value the transition becomes a continuous second-order phase transition. It is shown that the stick-slip friction mode occurs within a wide range of the parameters. The results agree qualitatively with the known experimental data but quantitative agreements can be achieved, if necessary, for concrete experiments since the model is quantitative and implies a possibility of modification.

ACKNOWLEDGMENTS

The work was supported by the project "Modeling of friction of metal nanoparticles and boundary fluid films interacting with atomically smooth surfaces" (No. 0112U001380) of the Ministry of Education, Science, Youth, and Sport of Ukraine and was partially carried out during the visit of I.A. Lyashenko and A.V. Khomenko to the Jülich Research Center (Forschungszentrum Jülich, Germany) on the invitation of B.N.J. Persson.

DESIGNATIONS

u —internal energy density; f^2 —excessive volume (disorder parameter); ε_{ij}^e —elastic strain tensor; s —equilibrium entropy; \tilde{s} —nonequilibrium entropy; $u_0, t_0, t_1, \phi_0, \phi_1,$ and ϕ_2 —expansion parameters of internal energy; ε_{ii}^e —first invariant of strain tensor; $\varepsilon_{ij}^e \varepsilon_{ji}^e$ —sec-

ond invariant of strain tensor; $u_0^*, \lambda, \mu, \alpha, \phi_0^*, \bar{\lambda}, \bar{\mu}, \alpha_\phi, t_0^*, \tilde{\lambda},$ and $\tilde{\mu}$ —expansion parameters of internal energy; σ_{ij}^e —elastic stress tensor; δ_{ij} —delta symbol; $\mu_{\text{eff}}, \lambda_{\text{eff}}$ —effective elastic constants (Lame constants); ε_{22} —diagonal component of strain tensor; n —normal component of stresses applied to friction surfaces; τ —tangential component of stresses; $\varepsilon_{c0}(s_{c0})$ —critical value of strain (entropy), at which lubricant melts; $\varepsilon_c^0(s_c^0)$ —critical value of strain (entropy), at which lubricant solidifies; F —friction force; t —time; F_{ij} —friction force tensor; k, γ —phenomenological coefficients, which assign dependence of effective viscosity η_{eff} on velocity gradient; V_{ij} —tensor of relative shear velocities of friction surfaces; h —lubricating film thickness; A —area of contact between friction surfaces; τ_e —Maxwell stress relaxation time; T —lubricant temperature; \tilde{T} —nonequilibrium lubricant temperature; τ_f, τ_s —constants being reciprocals of kinetic coefficients in relaxation equations of excessive volume and equilibrium entropy; T_e —temperature of friction surfaces; κ —thermal conductivity; $x, y,$ and z —Cartesian coordinates; K —spring stiffness; M —mass of upper rubbing block; L —external load applied to friction surfaces; X —coordinate of upper rubbing block; ΔX —spring elongation; V_0 —velocity of movement of free spring end; t' —time; $V_{01}, V_{02}, V_{03},$ and V_{04} —fixed values of velocities; $n_1, n_2, n_3,$ and n_4 —fixed values of normal stresses; $T_{e1}, T_{e2}, T_{e3},$ and T_{e4} —fixed values of temperatures of friction surfaces.

REFERENCES

1. *Nanotribology and Nanomechanics*. Bhushan, B., Ed., Berlin: Springer Verlag, 2005.
2. Persson, B.N.J., *Sliding Friction. Physical Principles and Applications*, Berlin: Springer Verlag, 2000.
3. Boiko, V.I., Valyaev, A.N., and Pogrebnyak, A.D., "Metal Modification by High-Power Pulsed Particle Beams" *Phys.-Usp.* 1999, vol. 42, pp. 1139–1166.
4. Metlov, L.S., Khomenko, A.V., and Lyashenko, I.A., Multidimensional Thermodynamic Potential for Descriptions of Ultrathin Lubricant Film Melting between Two Atomically Smooth Surfaces, *Cond. Matt. Phys.*, 2011, vol. 14, p. 13001.
5. Popov, V.L., *Contact Mechanics and Friction: Physical Principles and Applications*, Berlin: Springer Verlag, 2010.
6. Pogrebnyak, A.D., Bratushka, S.N., Il'yashenko, M.V., et al., Tribological and Physical–Mechanical Properties of Protective Coatings from Ni–Cr–B–Si–Fe/WC–Co–Cr before and after Fission with a Plasma Jet, *J. Friction Wear*, 2011, vol. 32, pp. 84–90.
7. Yoshizawa, H. and Israelachvili, J., Fundamental Mechanisms of Interfacial Friction. 2. Stick-Slip Friction of Spherical and Chain Molecules, *J. Phys. Chem.*, 1993, vol. 97, pp. 11300–11313.

8. Lyashenko, I.A., Tribological System in the Boundary Friction Mode under a Periodic External Action, *Tech. Phys.*, 2011, vol. 56, pp. 869–876.
9. Lyashenko, I.A., First-Order Phase Transition between the Liquidlike and Solidlike Structures of a Boundary Lubricant, *Tech. Phys.*, 2012, vol. 57, pp. 17–26.
10. Lee, R.-T., Yang, C.-R., and Chiou, Y.-C., A Procedure for Evaluating the Positioning Accuracy of Reciprocating Friction Drive Systems, *Tribol. Int.*, 1996, vol. 29, pp. 395–404.
11. Yang, C.-R., Lee, R.-T., and Chiou, Y.-C., Study on Dynamic Friction Characteristics in Reciprocating Friction Drive System, *Tribol. Int.*, 1997, vol. 30, pp. 719–731.
12. Lyashenko, I.A., Tribological Properties of Dry, Fluid, and Boundary Friction, *Tech. Phys.*, 2011, vol. 56, pp. 701–707.
13. Filippov, A.E., Klafter, J., and Urbakh, M., Friction through Dynamical Formation and Rupture of Molecular Bonds, *Phys. Rev. Lett.*, 2004, vol. 92, p. 135503.
14. Brener, E.A. and Marchenko, V.I., Frictional Shear Cracks, *JETP Lett.*, 2002, vol. 76, pp. 211–214.
15. Smith, E.D., Robbins, M.O., and Cieplak, M., Friction on Adsorbed Monolayers, *Phys. Rev. B: Condens. Matter*, 1996, vol. 54, pp. 8252–8260.
16. Khomenko, A.V. and Lyashenko, I.A., Melting of Ultrathin Lubricant Film Due to Dissipative Heating of Friction Surfaces, *Tech. Phys.*, 2007, vol. 52, pp. 1239–1243.
17. Khomenko, A.V. and Lyashenko, Ya.A., Periodic Intermittent Regime of a Boundary Flow, *Tech. Phys.*, 2010, vol. 55, pp. 26–32.
18. Khomenko, A.V., Lyashenko, I.A., and Borisyuk, V.N., Multifractal Analysis of Stress Time Series during Ultrathin Lubricant Film Melting, *Fluct. Noise Lett.*, 2010, vol. 9, pp. 19–35.
19. Khomenko, A.V. and Lyashenko, I.A., Stochastic Theory of Ultrathin Lubricant Film Melting in the Stick–Slip Regime, *Tech. Phys.*, 2005, vol. 50, pp. 1408–1416.
20. Khomenko, A.V. and Lyashenko, I.A., Hysteresis Phenomena during Melting of an Ultrathin Lubricant Film, *Phys. Solid State*, 2007, vol. 49, pp. 936–940.
21. Demirel, A.L. and Granick, S., Transition from Static to Kinetic Friction in a Model Lubricating System, *J. Chem. Phys.*, 1998, vol. 109, pp. 6889–6897.
22. Reiter, G., Demirel, A.L., Peanasky, J., et al., Stick to Slip Transition and Adhesion of Lubricated Surfaces in Moving Contact, *J. Chem. Phys.*, 1994, vol. 101, pp. 2606–2615.
23. Israelachvili, J., Adhesion Forces between Surfaces in Liquids and Condensable Vapors, *Surf. Sci. Rep.*, 1992, vol. 14, pp. 109–159.
24. Lyashenko, I.A., Khomenko, A.V., and Metlov, L.S., Thermodynamics and Kinetics of Boundary Friction, *Tribol. Int.*, 2011, vol. 44, pp. 476–482.
25. Lyashenko, I.A., Khomenko, A.V., and Metlov, L.S., Nonlinear Thermodynamic Model of Boundary Friction, *J. Friction Wear*, 2011, vol. 32, pp. 113–123.
26. Lyashenko, I.A., Khomenko, A.V., and Metlov, L.S., Phenomenological Theory for the Melting of a Thin Lubricant Film between Two Atomically Smooth Solid Surfaces, *Tech. Phys.*, 2010, vol. 55, pp. 1193–1199.
27. Lyashenko, I.A., Metlov, L.S., Khomenko, A.V., Non-Equilibrium Stationary Modes of Boundary Friction, *Zh. Nano- Elektr. Fiz.*, (J. Nano- Elektron. Phys.), 2011, vol. 3, pp. 59–69.
28. Landau, L.D. and Lifshits, E.M., *Theoretical Physics, Vol. 7. Theory of Elasticity*, Moscow: Nauka, 1987; Oxford: Pergamon, 1993.
29. Kachanov, L.M., *Foundations of the Theory of Plasticity*, Moscow: Nauka, 1969; Amsterdam: North-Holland Publ. Com., 1971.
30. Luengo, G., Israelachvili, J., and Granick, S., Generalized Effects in Confined Fluids: New Friction Map for Boundary Lubrication, *Wear*, 1996, vol. 200, pp. 328–335.
31. Metlov, L.S., Formation of Internal Structure of Solids under Severe Load, *Phys. Rev. E*, 2010, vol. 81, p. 051121.
32. Olemskoi, A.I., Axiomatic Theory of Self-Organizing System, *Physica A*, 2002, vol. 310, pp. 223–233.
33. Olemskoi, A.I., Khomenko, A.V., and Kharchenko, D.O., Self-Organized Criticality within Fractional Lorenz Scheme, *Physica A*, 2003, vol. 323, pp. 263–293.
34. Popov, V.L., Thermodynamics and Kinetics of Shear-Induced Melting of a Thin Layer of Lubricant Confined between Solids, *Tech. Phys.*, 2001, vol. 46, pp. 605–615.
35. Gee, M.L., McGuiggan, P.M., and Israelachvili, J.N., Liquid to Solidlike Transitions of Molecularly Thin Films under Shear, *J. Chem. Phys.*, 1990, vol. 93, pp. 1895–1906.