

Phenomenological description of structural changes of the surface layers in a metal-polymer friction pair

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Abstract. The synergetic approach is suggested to use to describe physical and chemical processes conveying frictional interaction in a metal-polymer friction pair. The kinetic theory of the first-order phase transformations, based on the fluctuation depiction of the phase nucleation and the subsequent growth of its emissions, was applied to build a mathematical model of structural changes occurring in the surface layer. The model is brought to the system of Lorentz equations, where the temperature plays the role of the controlling parameter responsible for the process of the system structural rearrangement, the order parameter ε represents the shear strain component, and the conjugate field σ is the corresponding component of the elastic stress tensor. The representation of the thermodynamic potential in the form of expansion into a series of a variable h (the distribution density of the crystalline phase) is employed to make a qualitative analysis of the phase transition. The use of the expansion for the thermodynamic potential allows the nucleation of dispersed particles of the «new» phase in the old one.

1 Introduction

One of the ways to improve the working capacity of heavy loaded tribological conjunctions is the exploiting special polymer composites and coatings based on them in friction units. These materials due to the set of their physical and mechanical properties successfully compete with traditional construction materials. A distinctive feature of the frictional interaction in a metal-polymer friction pair is the occurrence of physical and chemical processes in the dynamic contact zone. The abovementioned processes lead to the composite destruction and the formation of the so-called «third body» whose properties differ from those of the contacting bodies [1]. In the progress of friction a mechanical load in the form of contact pressure p and sliding velocity V exert influence on the composite material that cause plastoelastic deformation of the surface layer co-occurred with a stress field formation. Being influenced by the state of stress and strain, the surface layer

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experiences certain changes in the polymer supermolecular structure (crosslinking, destruction, alterations in the molecules orientation, etc.), processes of structural and phase transformations characterized by a change in the crystallinity degree. In friction precisely these general structural and thermodynamic transformations underlie the self-organization process, the manifestation of which is the formation of a frictionally transferred film.

Frictional interaction is accompanied by an increase in temperature and heat accumulation, which, together with deformation following structural changes, activate the formation of a layered supermolecular structure and amorphization of the polymer material. The structure of the appeared third body is characterized by the fact that along with the amorphous phase there are clusters, which preserve the crystalline phase.

All of the facts mentioned above indicate that the description of the structural changes in friction in a metal-polymer friction pair is unachievable without involving the representations of a highly nonequilibrium condensed medium, based on the statistical ensemble nonergodicity, the appearance of hierarchical structures, structural relaxation, the mutual influence of the subsystem experiencing a phase transition and the environment, etc. The latter is possible on the basis of a synergetic approach that takes into account the characteristics of the collective behaviour of highly nonequilibrium statistical ensembles.

2 Purpose of the work

Building-up a mathematical model of structural changes occurring in the surface layers of a metal-polymer friction unit based on the kinetic theory of phase transformations.

3 Model of structural changes in the surface layer

The process of friction is characterized by a mass transfer between the boundary layer and its sublayer due to a change in the contact pressure and the structure of the boundary layer. In this case the formation of the transferred film is determined by loosening the material and transferring it to the counterbody's surface. As it is noted in [2], a steady state is achievable in the processes of formation and destruction of dissipative structures that occur during friction. The latter testifies to the existence of the feedback in the system: the destruction of dissipative tribostructures is recompensed by the kinetics of their formation. Therefore, a stable and minimal friction in the system is a manifestation of the Le Chatelier-Braun principle.

To build up a mathematical model of structural changes occurring in the surface layer of a polymer composite, it is necessary to apply the kinetic theory of first-order phase transformations, grounded on the fluctuation depiction of the phase nucleation and the subsequent growth of its distribution [3]. As indicated in [2], an increase in the temperature in the friction area to the phase transition temperature (327 °C) causes the transition of the PTFE crystalline phase to amorphous, and the subsequent formation of a more ordered layered tribostructure. Therefore, it is the temperature that functions as the controlling parameter. Now let us take the simplest expression for the temperature rate of change in the interaction zone

$$\frac{dT}{dt} = \frac{1}{\beta} [(T_e - T) - B\varepsilon\sigma], \quad (1)$$

where T – temperature, bracketed expression – function, determining the dissipative processes intensity and is dependent on temperature, shear strain component ε and elastic

stresses σ . β – the parameter determined by the temperature relaxation time, T_e – the typical scale of the temperature change, B – the positive coupling constant.

In its turn, the equation for the shear component rate of change is reduced to the Maxwell equation for a viscous-elastic medium [4]:

$$\frac{d\varepsilon}{dt} = -\frac{\varepsilon}{\tau} + \frac{\sigma}{\eta}, \quad (2)$$

where the first term corresponds to strain relaxation with time τ , the second term describes the medium under the stress σ . η – shear viscosity. In the steady state $\dot{\varepsilon} = 0$, equation (2) is reduced to Hooke law $\sigma = \mu\varepsilon$, where the shear modulus μ specifies the relaxation time τ according to the generally known relation $\tau = \frac{\eta}{\mu}$. Respectively, the equation for the elastic stresses rate of change is recorded in the following form

$$\frac{d\sigma}{dt} = -\frac{\sigma}{\tau_\sigma} + A_\sigma \varepsilon T \quad (3)$$

where τ_σ, A_σ – the positive constants, the first of which indicates the process of stress relaxation, the second one determines their growth due to the structural rearrangement.

The model is reduced to the system of Lorentz equations [5], where the temperature plays the role of the controlling parameter responsible for the process of the system structural rearrangement, the order parameter ε represents the shear strain component, and the conjugate field σ is the corresponding component of the elastic stress tensor.

Plastic strain involving rotational modes can be considered as the vortex motion of a turbulent system with a large Reyn-olds number and the deformed material as a two-phase structured system of dispersed particles where infinitesimal crystals as disperse phases are statistically uniformly distributed in the amorphous phase, which is a kind of cementing interlayer between the dispersed phase – small crystals.

Remaining within the framework of this model, an important point for a qualitative analysis of the phase transition is the representation of the thermodynamic potential in the form of an expansion in a series of independent variables, as suggested in [6]:

$$u = u_0 + \varphi_0 h - \frac{1}{2} \varphi_1 h^2 + \frac{1}{3} \varphi_2 h^3 - \frac{1}{4} \varphi_3 h^4, \quad (4)$$

where

$$\begin{aligned} u_0 &= \frac{1}{2} \lambda (\varepsilon_{ii}^e)^2 + \mu (\varepsilon_{ij}^e)^2 \\ \varphi_0 &= \varphi_0^* + g \varepsilon_{ii}^e + \frac{1}{2} \bar{\lambda} (\varepsilon_{ii}^e)^2 + \bar{\mu} (\varepsilon_{ij}^e)^2 \\ \varphi_1 &= \varphi_1^* + 2e \varepsilon_{ii}^e. \end{aligned}$$

Here λ, μ – the composite's elastic constants in the unperturbed state, $\varphi_0^*, \varphi_1^*, \varphi_2, \varphi_3$ – the expansion constants, $g, \bar{\lambda}, \bar{\mu}, e$ – the constants considering the dependence on the elastic strain, ε_{ij}^e, h – the distribution density of the crystalline phase.

The alternation of signs in the expansion (4) is selected in accordance with the Le Chatelier principle, i.e. each deeper thermodynamic process (at a higher degree of h) is directed towards compensation of the previous level process.

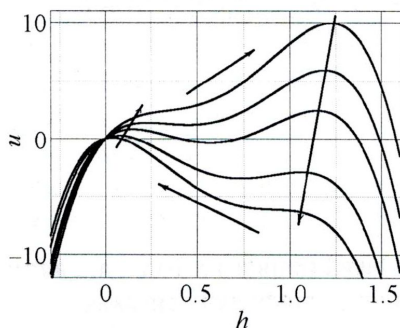


Fig. 1. Graphs of the thermodynamic potential at constant values of the controlling parameter.

The formation of a layered supermolecular structure can be considered as a transition from one steady state of the system (the left maximum) to another steady state corresponding to the origination of a liquid crystal mesophase (the right maximum), provided that the controlling parameter reaches a critical value at which the potential barrier between steady states disappears. Figure 1 demonstrates the specified position (various curves correspond to diverse values of elastic strain, which functions as a controlling parameter).

The basis of structural changes occurring in the friction area is the thermodynamic processes of mechanical energy dissipation caused by heat and a temperature gradient. The structural changes in the surface layer are influenced by both by the properties and structure of the materials involved in friction, and the structure and properties formed in the process of frictional interaction [7].

Using the representation of the thermodynamic potential in the above specified form (4) allows taking into account the presence of two phases in the surface layer simultaneously: amorphous one with crystalline elements impregnations. The latter proves the fact that the minimum of the thermodynamic potential at the point of the structural-phase transition is not achieved at the origin of coordinates, but is shifted.

High internal stresses in microcontacts have a determining impact on phase and structural transformations. The formed transferred film is a complex heterophase structure. In this case the stress field is conditioned with the intrinsic deformation emerged in the first-order phase transit, and the internal stresses are related by the new and old phase-conjugate condition. The absence of internal stresses leads to the nonoccurrence of the changes in the new phase fraction during the phase transition [8].

The classical theory of the first-order phase transition considers a change in the boundary between the «old» and the «new» phases as the movement of this very boundary related to the change in the internal stresses energy. The transition is conditioned by the tendency of free energy to reach the extreme state. It corresponds to the evolution of the heterophase system to equilibrium. In the proposed approach, the expression (4) for the thermodynamic potential allows the nucleation of dispersed particles of the «new» phase in the old one. In this case, the achievement of the extremum by the thermodynamic potential is related to the dependence φ on h .

The description of the first-order phase transition by means of the proposed model, supplemented by the representation of the thermodynamic potential in the form of expansion in a series of independent variables, allows taking into account the stresses

relaxation with time and their growth due to structural rearrangement. Applying the adiabatic approximation makes it possible to obtain the time dependence of the order parameter

4 Conclusions

The proposed phenomenological approach for describing structural changes in a metal-polymer friction pair in friction allows explaining some experimental results of the given process. It clears the kinetics of the formation of a frictionally transferred film, the constancy of the conjugation wear rate in the running-in state, the connection between the wear rate and the pressure in the contact zone, and the independence of the system properties in the running-in state from the initial parameters. In addition, it makes obvious that the «pure» reproduction of repeated experiments is impossible.

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