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Theoretical justification of the influence of change of dilaton and compression bonds of atoms of materials of machine parts on their tribological effect

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Abstract

The course of friction and wear processes in the surface layers of conjugations of machine parts is clarified on the basis of the idea of dilaton and compression bonds of atoms in the materials of parts. Dilaton-compression connections are random in nature, and therefore in this work the theory of destruction of parts by S.M. Zhurkov, thermodynamic and quantum physical approaches. The entropy at the macro-, meso- and microscopic levels and the local regions of the materials of conjugation of the parts subject to friction loading are considered. In the diagram of the state of atomic-molecular bonds the dependence curve $F_i(r_i)$ or $T_i(r_i)$ is considered and the analysis of transformations of bonds according to the specified diagram is carried out. From the point of view of solid state physics and tribophysics, the manifestation, evolution and consequences of the influence on the characteristics and properties of the friction zone of dilaton and compression bonds of material atoms are considered. Composite materials (composite coatings) are substantiated in more detail. This takes into account the assessment of the concept of material stresses in the friction zone, the ability to relax it, as well as the presence of the SD effect. The fracture process is associated with the modulus of elasticity of the components of the composite material and the bulk content of the filler. An appropriate condition is proposed, which determines the tribological efficiency of composite materials and coatings.

Key words: dilaton and compression connections, state diagram, entropy, fracture, composite material (coating), SD-effect, stress concentration.

Introduction

Increasing the intensity of load application to the materials of conjugations of parts, assemblies and units of machines determines the speed of their deformation, increasing the stress state and changing the tensile strength [1]. Under such conditions, the behavior, characteristics and properties of parts, local areas of their materials and work surfaces differ significantly. The nature of the processes of friction and lubrication that occur in the surface layer of parts is multifactorial. The micro-impact load in the process of collision of abrasive particles and wear particles with the working surfaces of parts, friction, as well as the destruction of the material is determined by its impact strength and strength [2, 3]. The behavior of the material of parts in such conditions is primarily determined by the following factors: the structure and properties of the material of parts; composition, properties and wear capacity of the working environment; the magnitude and nature of the load of external forces; their distribution, etc. [4, 5, 6].

The destruction of the materials of tribocouples of parts during operation has a thermofluctuation nature [7, 8]. For crystalline materials, an active specific change in the state of their surface layers under load has been established: from nanostructuring to amorphization, intensive dislocation processes to the formation of cracks, and so on.

Literature review

The kinetics of friction and wear of materials in tribophysics is considered at the atomic-molecular level, taking into account the state of the electronic subsystem of materials under load. Mechanical loading of the surface of materials leads to perturbations in the electronic subsystem, and the rupture of interatomic bonds means a sharp excitation of electronic states. In the kinetics of wear, the interlevel transition of processes is important. The results of detailed studies of the properties of the surface layers of materials indicate a close connection between mechanical processes and electronic ones. The nature and characteristics of the phenomena of wear of surface layers can be substantiated by tribophysical methods on the basis of the proposed methodology [9].

The operational wear resistance of most parts and working bodies depends on their working condition and the complex of physical-mechanical and operational properties of the working surfaces of the parts [9, 10, 11, 12, 19]. Their failure is primarily due to the size and nature of wear, as well as fatigue of the material.

Purpose

The purpose of this work is to clarify the possibility of using the theory of destruction of materials of parts S.M. Zhurkov and ideas about local areas of compression and dilaton connections, to explain the state and behavior of the material in the friction zone of the conjugation of parts, components and units of machines.

Results

During operation, the transition of materials of tribocouples of parts in the contact zone from nonequilibrium to equilibrium, the formation of micro-, meso- and macroformation in it depends on the formation of electromagnetic dipoles of local areas of dilaton or compression connections between them and their mutual transition. According to the theory of S.M. Zhurkov, from the point of view of thermodynamics [13, 14, 15, 16], the state of the *i*-th local region of the material of the part can be described by the equation:

$$P_i dV_i = T_i dS_i \,, \tag{1}$$

where P_i – is the load in the *i*-th local region with a volume of dV_i, which causes the formation of residual stresses;

dS_i – change in entropy associated with the development of defects in the structure of materials (internal entropy);

T_i – thermodynamic temperature;

$i = \overline{1, n}$.

Entropy is a general characteristic of irreversible thermodynamic changes observed in the material and have a macro-, meso- and microscopic nature. Macroscopic changes in entropy determine the formation of cracks, dents, streaks, porosity, scratches, various transitions from geometric shape, and others. Mesoscopic changes in entropy are due to the ability of the structure of the structural material of the parts to phase transitions. Microscopic changes in entropy are an indicator of the degree of perfection of the material structure of machine parts. They need to take into account both the number of atomic-molecular bonds and their energy evaluation.

According to quantum solid state physics (SSP), based on Debye's theory, there is a directly proportional relationship between microscopic entropy and the number of atomic-molecular bonds and their relative energy:

$$S_i = k_B N_{i\,bon} \delta_i \,; \tag{2}$$

$$\delta_i = -\frac{9}{8}\frac{\theta_i}{T_i} + 1 - 3\ln\frac{\theta_i}{T_i} + \frac{\pi^4}{5}\left(\frac{T_i}{\theta_i}\right)^3 , \tag{3}$$

where k_B – became Bora;

$N_{i\,bon}$, δ_i – respectively, the number and coefficient of relative energy of atomic-molecular bonds;

T_i, θ_i – respectively thermodynamic and characteristic temperatures in the i-th region.

The state of interatomic or molecular bonds is determined by the local temperature T_i and the free energy F_i in this region. The condition of the material of the part is significantly affected by the processes occurring at the microscopic level. Because the critical change in the material is the formation of microcracks in it, which are associated with the destruction of the crystal lattice.

The diagram of the state of atomic-molecular bonds of local regions of the material is graphically represented by the curve dependence $F_i(r_i)$ and $T_i(r_i)$ (fig. 1), which consists of a depression (acceleration pit) and a ridge (brake barrier).

The ratio of these thermodynamic temperatures is as follows:

$$T_b > T_f > T_d . \tag{4}$$

Let us analyze the state diagram of atomic-molecular bonds in the local region of the friction zone, in the surface layer of conjugation details (fig. 1).

In the local region of the acceleration cavity (brake hole), state diagrams $(r_1,\ r_2)$ form dilaton types of bonds in the material, and in the local region of the brake barrier $(r_2,\ r_3)$ – compression types. From the point of view of SSP, the type of bond is characterized by the directions of spins of atoms (molecules) in the nodes of the crystal lattice of the material [26, 28]: for dilatons spins are parallel, which causes electrostatic repulsion of atoms (molecules) and back, which leads to the appearance of forces of attraction and the creation of local areas of compression deformation.

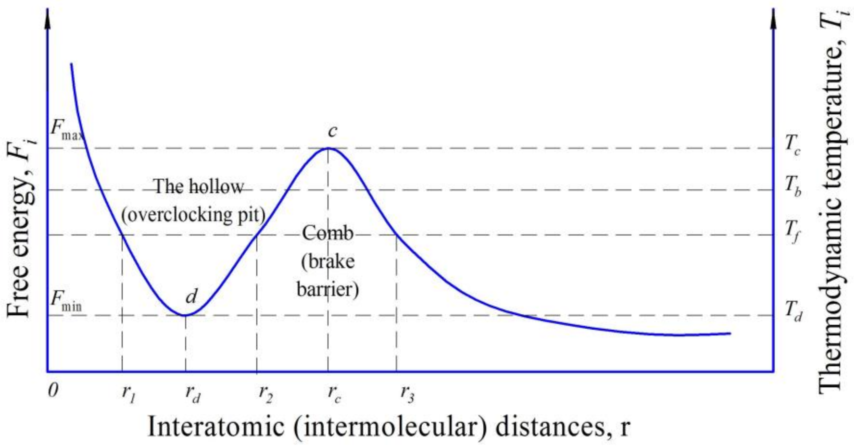

Fig. 1. Diagram of the state of atomic-molecular bonds of local regions of the material as a function of free energy and thermodynamic temperature from the interatomic (intermolecular) distance:
T_d – the minimum thermodynamic temperature in the depressions, which is characteristic of the dilatonic type of bonds of atoms or molecules;
T_b – thermodynamic equilibrium temperature;
T_f – phase transition;
T_c – the maximum thermodynamic temperature in the ridge is characteristic of the compression type of connections

From the diagram of the state of atomic-molecular bonds it can also be seen that dilaton bonds are formed in the low-temperature region with a minimum of free energy, and compression – in the high-temperature region with a maximum of free energy. When phonons are emitted by compresses, the local temperature of the material decreases and it passes into the dilaton region, while the dilaton region cannot pass into the compresson region. Under the influence of friction loading in the dilaton regions of the materials of conjugations of parts there is a fragile deformation and destruction, and in the compression, during their transition to the dilaton region - plastic. Of course, these processes are random. At their imposing the whole macroregions of brittle or plastic deformation, and also directions of development and distribution of microcracks in surface layers of material of details can be observed.

It was found that metals and alloys capable of phase transformations (PT) [5, 17, 18] have mainly atomic bonds of the compression type, while abrasive materials and solid fillers in composite materials have mainly dilaton bonds. type. Based on the SSP, compresses and dilatons have an electromagnetic nature and are electromagnetic dipoles. The flow of AF in the materials of parts indicates their role as energy characteristics of the crystal lattice nodes, which in the process of friction and wear of the material go into nonequilibrium, and in the transition to steady state dipoles emit a stream of electromagnetic wave energy [20]. Under the action of an external load or the influence $\vec{A}_{PT}$ of a physical field, the state of dipoles changes with intensity. Dipoles perpendicular to the direction of the external field $\vec{A}_{PT}$ emit phonons and the temperature of the local region approaches Td, and in the planes in which the dipoles are located along the field, the bonds absorb phonons at

$T \Rightarrow T_c$, increasing the size of the local regions of the material.

The nonequilibrium state in the local region of the material of the part during friction is described by the equation:

$$p_i V_i \left(dV_i / V_i + dp_i / p_i \right) = k N_{i\,bon} T_i \delta_i \left(dN_{i\,bon} / N_{i\,bon} + dT_i / T_i + d\delta_i / \delta_i \right), \tag{5}$$

in which the deviation from equilibrium is due to deformation dV_i / V_i and changes in load resistance dp_i / p_i and is accompanied by a decrease in the number of connections $dN_{i\,bon} / N_{i\,bon}$, thermal radiation dT_i / T_i and disruption of energy connections $d\delta_i / \delta_i$. The nature of the friction processes is determined primarily by the strength of the flux of atomic-molecular bonds in the local regions of the material.

Static and dynamic tension in this case causes a reduction in the cross-sectional area of the material near the fracture site, because $N_{T_c} > N_{T_d}$. Note that with tired wear $N_{T_c} \approx N_{T_d}$. The fracture surface usually has two zones: the actual fatigue fracture, which is formed due to the decay of the dilaton type of bonds at temperature T_d, and the final fracture at temperature T_c of the compressor type of bonds. The duration of stable existence of atomic-molecular bonds of local regions of the material is determined by the range of thermodynamic temperatures (T_c, T_d), which does not exceed 15 … 20 % of the full temperature range [16]. At critical temperatures T_c or T_d, the bonds are destroyed and energy is emitted in the form of a pulse:

$$q_1 = k_B \delta; \quad q_2 = (k_{\hat{A}} / h_P)\, \Delta r m \delta^2, \tag{6}$$

where h_P – is the Planck constant (h_P = 6,62·10^{-34} J·s);

m – is the mass of interacting atoms.

If the difference in thermal deformation of the inhomogeneous material or matrix and filler in the composite material when the temperature changes by ΔT is $\delta_{\text{т}}$, then in the local areas of significant inhomogeneity or matrix with a shear modulus G_m around each filler particle there are stresses, the maximum values of which reach $2G_m \delta_{\text{ò}}$ and can cause plastic deformation.

When the macrodeformation corresponding to the yield strength of the composite material $\sigma_{\text{т}}$, shear stresses are concentrated due to flat clusters of dislocations of local regions of inhomogeneity either in the composite material and the coating around or in front of the filler particles [21, 27]. This leads to a decrease in reverse stress and an increase in stresses in the main clusters of dislocations. In this regard, new flows of dislocations are generated, and existing dislocations pass along the plane of sliding at a distance much greater than L_n. The value of the yield strength is:

$$\sigma_{\text{т}} = \sigma_{\text{тм}} + \sqrt{G_m G_n \vec{b}_B / 2 L_n \xi_n}, \tag{7}$$

where G_m, G_n – shear modules of the matrix material and filler particles;

ξ_n – numerical coefficient, $\xi_n \approx 30$ [21, 26];

$\sigma_{\text{тм}}$ – yield strength of the matrix material. This is true for dispersed materials, when the maximum level of hardening of parts is achieved provided: $d_n = 2G_m b_B / \sigma_{\text{тм}}$. If $d_n \le 2G_m b_B / \sigma_{\text{тм}}$, then the radius of curvature of the dislocation $r_0 = 4b_B$ can not be neglected [27] and the yield strength of the composite material is equal to:

$$\sigma_{\text{т}} = \sigma_{\text{тм}} + G_n c_n^{\frac{1}{3}} \Big/ 4c_n \left(0{,}82 - c_n^{\frac{1}{3}} \right), \tag{8}$$

where c_n – is the volumetric content of the filler.

In parts reinforced with composite materials and coatings, the SD-effect can be observed [21], which consists in the appearance of micropores in the vicinity of the filler particles during tensile deformation and their absence during compression deformation. If the connection between the components of the material and the coating is strong, the dislocations are repelled from the boundary of their separation. If a micropore is present, the dislocation is attracted to the interface between the filler particle and the matrix. When the matrix is strengthened by solid particles of spherical filler [22, 23, 24], the maximum concentration of tensile stresses is on the surfaces of these particles. At uniaxial tension ($\sigma_{Np} > 0$), we have:

$$\sigma_{Np}/\sigma_p = 2/(1+\mu_{cm(cc)}) + 1/(4-5\mu_{cm(cc)}), \tag{9}$$

where σ_{Np} – is the tensile stress on the surface of the filler particle at points with coordinates ϑ = 0 and ϑ = 180°;

σ_p – applied tensile stress;

$\mu_{cm(cc)}$ – Poisson constant of the composite material, and at a compressive stress of $\sigma_{Np} < 0$, we obtain:

$$\sigma_{Nc}/\sigma_c = (1-\mu_{cm(cc)})/(1+\mu_{cm(cc)}) - (5-5\mu_{cm(cc)})/(8-10\mu_{cm(cc)}) . \tag{10}$$

If the interfacial boundary does not have sufficient strength, then the concentration of tensile stresses can cause its local destruction. This determines the presence of SD-effect, the manifestation of which is influenced by: the ratio of the modulus of elasticity of the matrix and the filler; chemical interaction at the interface of material components; correspondence of their crystal lattices; volume content of filler; test speed and temperature. When compressing stresses, such a concentration is not observed and the interface is not destroyed. Increasing the temperature increases the ability of the material to relax internal stresses and at some value the stress concentration will be lower than the strength of the interface of the material components, in which case there will be no breaks and SD-effect at the filler-matrix boundary.

V.I. Trefilov and V.F. Moiseev [25] identified two main factors influencing the nature of the destruction of disperse-strengthened materials: the strength of the interfacial boundary and the plasticity of the matrix. In this case, a qualitative characteristic of the strength of the interfacial boundary in the material may be the presence or absence of SD-effect: if SD = 0, the interfacial boundary is strong and does not collapse to σ_{T} , and if SD > 0, the interphase boundary collapses even in the elastic local region.

To assess the plasticity of the matrix of the composite material in the friction zone and the ability to relax the stress concentration, you can use parameter K_p [21]:

$$K_p = (G_n - G_m)/(G_n + G_m) . \tag{11}$$

Studies show that the smaller the value of $K_{пл}$, the lower the level of stress concentration in the region of dislocation clusters, and for the interface between brittle and plastic local regions of materials – K_p = 0,3 [25].

Given the value of K_p and the presence or absence of SD-effect, we have the following groups of materials reinforced with composite materials and coatings:

– fragile matrix and weak interfacial boundary (K_p < 0,3, SD > 0);

– plastic matrix and weak interfacial boundary (K_p > 0,3, SD > 0);

– brittle matrix and strong interfacial boundary (K_p < 0,3, SD = 0);

– plastic matrix and strong interfacial boundary (K_p > 0,3, SD = 0).

In each of these groups of materials, the filler particles (strengthening phase) play a different role in inhibiting the movement of cracks [8, 9]. Cracks can form both inside the filler particles and on the interface. The test results [10, 23] show that the cracks tend to be located perpendicular to the direction of maximum tensile deformation. J. Gerland [29, 30] proposed two theoretical models of the destruction of filler particles: the mechanisms of loading and accumulation of dislocations. According to the first model, the increase in stresses in the filler particles is associated with the shape or coefficient of their shape. The modulus of elasticity of the material $E_{cm(cc)}$ is within:

$$E_m E_n / [(1-c_n)E_n + c_n E_m] \le E_{cm(cc)} \le (1-c_n)E_m + c_n E_n . \tag{12}$$

The left part of inequality (12) means that the filler and the matrix are equally stressed, and the right - that they are equally deformed. Note that the particle size of the filler does not affect the modulus of elasticity of the composite material (composite coating) $E_{cm(cc)}$, if the coefficient of thermal expansion (CTE) of the matrix and the filler are almost equal. At the same time, if the CTE are different, cracks may appear around the larger filler particles $E_{cm(cc)}$. The shape of the filler particles does not affect the value of $E_{cm(cc)}$, if the particles are not oriented in the composite material. When the filler content is $\tilde{n}_n$ > 0,3, especially if the filler is fine, pores may form in the composite material and the value of $E_{cm(cc)}$ will decrease [10, 11].

This indicates that the particles of the filler of the composite material depends on both strengthening and destructive effects. They can be the initiators of cracks that occur under load of friction, and large particles are more dangerous than fine ones. If cracks do not occur in the composite materials, then controlling the modulus of elasticity of the components E_n and E_m, you can influence the size and nature of the strengthening of the materials of the parts, in their tribological efficiency.

Conclusions

1. The use of the theory of S.M. Zhurkov for the description of tribophysical processes in local regions of conjugations of details of knots of systems and units of machines on the basis of the diagram of a condition of atomic and molecular communications of them with dilaton and compression thermodynamic temperatures.

2. It was found that dilaton bonds are formed in the low-temperature region with a minimum of free energy. If phonons are emitted during tribophysical processes, the compresses reduce the local temperature and the material passes into the dilaton region, while the dilaton regions cannot pass into the compression region. In the dilaton areas of the material there is a fragile deformation and destruction, and in the compression, in the transition to dilaton - plastic. It is revealed in which cases metals and alloys have dilaton and compression type of atomic-molecular bond of atoms.

3. Based on solid state physics, compresses and dilatons have an electromagnetic nature and are electromagnetic dipoles. Phase transformations in materials can be associated with the influence of external physical fields on the behavior of electromagnetic dipoles and changes in their state and orientation.

4. The material in the friction zone of the tribocouples of parts has a non-equilibrium state, the degree of non-equilibrium of which is determined by the relative values of deformation and load, change in the concentration of the number of bonds, relative intensity of thermal radiation and energy bonds.

5. For composite materials and coatings theoretically substantiated their behavior in the friction zone, the ability to relax the stress concentration K_p and the presence of SD-effect, using the theory of S.M. Zhurkov and the idea of electromagnetic dipoles. Taking into account the specified parameters the characteristic groups of the materials strengthened by composite materials and coverings are resulted, their characteristics concerning formation of cracks are given.

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Аулін В.В., Лисенко С.В., Гриньків А.В., Деркач О.Д., Макаренко Д.О., Жилова І.В. Nеоретичне обґрунтування впливу зміни ділатонних і компресонних зв’язків атомів матеріалів деталей машин на їх трибологічну ефективність.

З'ясовано протікання процесів тертя та зношування в поверхневих шарах спряжень деталей машин на основі уявлення про ділатонні і компресонні зв'язки атомів в матеріалах деталей. Ділатонно-компресонні зв'язки мають випадкову природу, а тому в даній роботі використано теорію руйнування деталей С.М. Журкова, термодинамічний та квантово-фізичний підходи. Розглянуто ентропію на макро-, мезо- і мікроскопічному рівнях та локальні області матеріалів спряження деталей, що підлягають навантаженню тертям. В діаграмі стану атомно-молекулярних зв'язків розглянуто криву залежності $F_i(r_i)$ або $T_i(r_i)$ та здійснено аналіз перетворень зв'язків згідно зазначеної діаграми. З точки зору фізики твердого тіла та трибофізики розглянуто прояв, еволюція та наслідки впливу на характеристики і властивості зони тертя ділатонних та компресонних зв'язків атомів матеріалу. Більш детально обґрунтовано композиційні матеріали (композиційні покриття). При цьому враховується оцінка концепції напружень матеріалу в зоні тертя, здатність релаксувати її, а також наявність SD-ефекту. Процес руйнування пов'язується з модулями пружності компонентів композиційного матеріалу та об'ємного вмісту наповнювача. Запропоновано відповідну умову, яка визначає трибологічну ефективність композиційних матеріалів та покриттів.

Ключові слова: ділатонні і компресонні зв'язки, діаграма стану, ентропія, руйнування, композиційний матеріал (покриття), SD-ефект, концентрація напружень.