Investigation of Hydrogen Wear in Heavy Loaded Metal Friction Elements of Brakes

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Annotation

In the materials of the article, the following issues are considered: design, operation and energy loading of friction pairs of brake devices; the difference between internal and external friction of a metallic friction element; boundary conditions in the interaction of external and internal layers of material pairs. It has been established for what reason the subsurface layer of the metal friction element has a high surface-bulk temperature. This effect is associated with the action of pulsed specific loads during electrothermomechanical friction, which "tamp" the atoms of the crystal lattices in the layer and between the layers. As a result, the layers have high electrothermal resistance, which contributes to the accumulation of thermal energy. The thickness of the electrothermal layer of the metal friction element was determined by calculation.

Keywords: braking devices, friction pairs, metal friction element, crystal lattice, atoms, surface and bulk temperatures, subsurface layers.

DOI: 10.52171/2076-0515_2021_13_04_34_46

For citation:
Janahmadov A.Kh., Skrypnyk V.S., Volchenko N.A., Yahyayeva A.N., Zhuravlev D.Y., Yevchenko A.S.
[Investigation of hydrogen wear in heavy loaded metal friction elements of brakes]
Herald of the Azerbaijan Engineering Academy, 2021, vol. 13, no. 4, pp. 34-46 *(in English)*

Əyləclərin ağır yüklənmiş metal friksion elementlərinin hidrogen yeyilməsinin tədqiqi

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Xülasə

Məqalədə əyləc qurğularının sürtünmə cütlərinin konstruksiyası, işi və enerji yükü; metal friksion elementin daxili və xarici sürtünməsi arasındakı fərq; xarici və daxili təbəqələrin qarşılıqlı əlaqəsində sərhəd şəraiti kimi məsələlərə baxılıb. Metal friksion elementin səthaltı təbəqəsinin hansı səbəbdən böyük səthi-həcmi temperatura malik olması müəyyən edilib. Bu elektrotermomexaniki sürtünmə zamanı impuls nisbi yüklərin təsiri ilə əlaqədardır. Bunun nəticəsində təbəqələr böyük elektrotermik müqavimətə malik olurlar ki, bu da istilik enerjisinin toplanmasına təkan verir. Hesablama yolu ilə metal friksion elementinin elektrotermik qatının qalınlığı müəyyən edilib.

Açar sözlər: əyləc qurğuları, sürtünmə cütü, metal friksion element, kristal tor, atom, səthi və həcmi temperatur, səthaltı təbəqələr.

DOI: 10.52171/2076-0515_2021_13_04_34_46

УДК 625.08

Исследование водородного износа тяжелонагруженных металлических фрикционных элементов тормозов

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Аннотация

В статье рассмотрены вопросы: конструкция, работа и энергонагруженность пар трения тормозных устройств; различие между внутренним и внешним трением металлического фрикционного элемента; граничные условия при взаимодействии внешних и внутренних слоев пар материалов. Установлено, по какой причине подповерхностный слой металлического фрикционного элемента имеет большую поверхностно-объемную температуру. Этот эффект связан с действием импульсных удельных нагрузок при электротермомеханическом трении, которые «утрамбовывают» атомы кристаллических решеток в слое и между слоями. В результате этого слои имеют большое электротермическое сопротивление, которое и способствует накоплению тепловой энергии. Расчетным путем определена толщина электротермического слоя металлического фрикционного элемента.

Ключевые слова: тормозные устройства, пары трения, металлический фрикционный элемент, кристаллическая решетка, атомы, поверхностные и объемные температуры, подповерхностные слои.

Introduction

One of the most acute problems in the creation of high-performance equipment and machines with improved technical characteristics is the intensive wear of their mating surfaces of parts. Most road construction machines, vehicles and material handling equipment fail not because of breakdown, but due to premature wear and damage to the surfaces of parts.

Increased wear of parts leads to a decrease in engine power, traction qualities of road construction machines, braking efficiency of vehicles and material handling equipment, safety of goods, safety of service personnel and transported passengers. The above listed machines and equipment with braking devices are operated in a water-containing environment, which contributes to hydrogen wear of the working surfaces of the metal friction elements of the brakes.

Problem state

The paper [1] analyzes the features of hydrogen wear of parts of road-building machines. The general laws of hydrogen wear are considered as a specific type of surface destruction. The ways of hydrogenation of surfaces of parts of road-building machines have been established. The mechanism of hydrogen wear is discussed. Based on the study of the regularities of hydrogen destruction of machine parts and equipment, methods of protection against tribohydrogenation are formulated.

In works [2-5] the interaction of hydrogen with metals and non-metallic elements is considered. The influence of hydrogen on various properties of metals and alloys and on the occurrence of specific defects in them is illustrated. The information on hydrogen embrittlement and the effect of hydrogen on the mechanical characteristics in the "hydrogen - metal" pair in the groups of the periodic system of D. Mendeleev has been expanded.

The work [6] is devoted to the wear of the sub-roughness of friction surfaces in an aqueous medium. In the latter, hydrogen is pumped into the subsurface layer of the metal body and interacts with its crystal lattice. It is noted that the driving force in the processes of hydrogen wear is temperature, pressure, deformation, structure and crystal lattice defects.

In works [7, 8] investigated the physical and mechanical processes on the friction surface of hydrogen wear of machine parts and equipment. The reasons for the release of hydrogen, hydrogenation of rubbing surfaces and their destruction have been established. A complex picture of the behavior of hydrogen in the surface layers in the process of friction under the influence of various factors is shown, and the influence of "biographical" hydrogen on the wear of parts is determined. The reasons for the transfer of a harder material to a softer material during friction are stated: steel on bronze, cast iron on plastic.

Practical recommendations are given for suppression of hydrogen wear and increasing the durability and reliability of friction units of machines and equipment.

In this case, the following was not considered: the effect of external hydrogen on the surface layer of the metal friction element and its entry into the subsurface layer by injection; the phenomenon of adhesion and the types of contacts of friction pairs during their frictional interaction was not taken into account, as well as the combination of adsorption - diffusion phenomena observed in the surface and subsurface layers of friction pairs. And the most important thing is that the external and internal hydrogen and their role in tribological reactions were not isolated.

In works [1, 4] it was established that under severe friction conditions the maximum temperature is formed at a certain depth from the friction surfaces.

This creates conditions under which hydrogen, if it is adsorbed on the surface of the part, diffuses into the depth of the surface under the action of a temperature gradient, concentrates there, causes embrittlement of the surface layers and increases wear.

However, it was not specified what happens in the subsurface layer of a metal element with its crystal lattice structures.

Formulation of the problem

The main questions of the article: design, operation and energy loading of friction pairs of brake devices; the difference between internal and external friction of a metallic friction element; boundary conditions in the interaction of external and internal layers of material pairs.

Purpose of work - to investigate the factors affecting the energy loading of the subsurface layer of a metal friction element and to establish the relationship between internal and external friction in its structure.

Design, operation and energy loading of friction pairs of braking devices

The design of the metal friction element and its metal consumption significantly affect the intensity of hydrogen wear of the working surface.

In fig. 1 *a*, *b* shows the friction pairs of a disc-shoe brake.

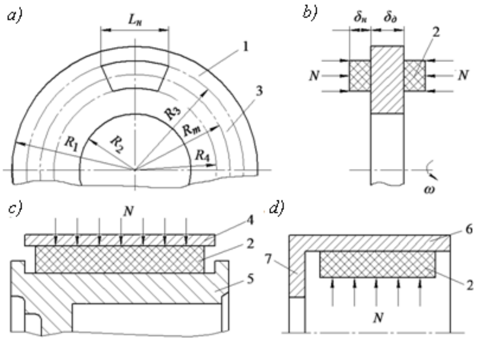

Figure 1 *a*, *b*, *c*, *d* – Diagrams of different types of friction units of braking devices: *a*, *b* - disc-shoe (longitudinal and transverse sections); *c* - tape-shoe (cross-section); *d* - drum-shoe (cross section)

They consist of 2 friction linings, which are located in the fixed brake pads. With the frictional interaction of the working surfaces of the linings *2* with the rotating brake disc *1* under the action of the normal pressing force *N*, a friction treadmill *3* is formed.

In fig. 1 *c* depicts the friction assembly of the drawworks band-shoe brake. When tightening the brake band *4* under the normal clamping force *N*, the working surface of the friction lining *2* interacts with the friction track of the pulley rim *5*. The latter is connected to the drum flange by means of the fastening protrusion *8*.

The frictional unit of the drum-shoe brake of the vehicle is shown in fig. 1 *d*. It contains a brake drum rim *6* with a flange *7*, as well as friction linings *2* located on the brake pads. When the latter are expanded, the working surfaces of the linings *2* frictionally interact with the inner (working) surface of the rim of the brake drum *6*.

The quality and reliability of the created structures of the frictional units of the braking devices depend on the processes, phenomena and effects occurring during the frictional interaction of the microprotrusions of their friction pairs. The contact of microprotrusions is discrete and is estimated by the dynamic coefficient of mutual overlap of friction pairs, and its value is up to 0.25 (for disk-shoe brakes) and up to 0.75 (for drum and band-shoe brakes).

According to the molecular-mechanical model of electrothermomechanical friction, the interaction of microroughnesses of the surfaces of rubbing bodies can be represented in the form of viscous sliding of the actual contact areas (adhesive component). This is accompanied by deformation of irregularities (deformation component) causing them to be stressed. Therefore, the heat release during friction is due, on the one hand, to the destruction of adhesive bonds in the actual contact zones, and, on the other hand, to the stress-strain state of microroughnesses.

The stress-strain state of microprotrusions of friction pairs with different types of contacts (ohmic, neutral, blocking) leads to volumetric heat release in the surface and subsurface layers of frictionally interacting materials. In this case, the friction power of the latter is a significant part of the total (taking into account the adhesive component) heat release power.

In braking devices of the tape-and drum-shoe type, the rim of the pulley and the drum in section can be represented as a horizontal plate (Fig. 2 *a*), and a solid disc - in the form of a vertical plate (Fig. 2 *b*). At the same time, in a band-shoe brake, the upper surface of the pulley rim is polished, and the lower surface is matte. In a drum-shoe brake, the opposite is true. In the considered brakes, a one-way supply of heat is carried out to the polished surfaces of the pulley rim. A solid disc or a left half disc of a self-ventilated brake disc with spikes has a design feature that a polished annular friction belt is surrounded by matt surfaces on the side of the maximum and minimum radii of the friction belt. In addition, in a disc-shoe brake, a two-way supply of heat is carried out to the friction belts.

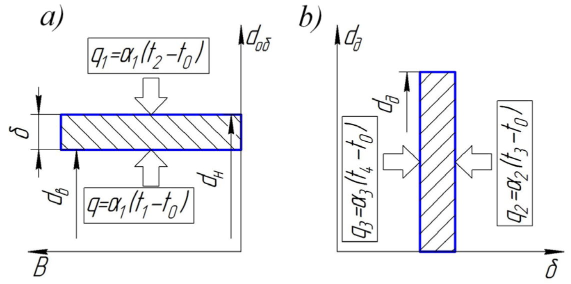

Figure 2 *a*, *b* – Design parameters of metal friction elements: *a* - working surfaces of the pulley rim and drum; *b* - surfaces of a solid disk and heat fluxes generated on their working surfaces

In fig. 2 *a*, *b* the following symbols are used: $d_в$, $d_н$, $d_д$ - diameters: inner drum; outer pulley; solid disc; *B*, δ - width and thickness of elements; q_i - heat fluxes; t_i - surface temperatures; t_0 is - the ambient temperature.

Heat transfer *K* through the rims, which are structural elements (thickness: lateral surfaces of the brake disc, pulley rim and drum) of metal friction elements, is determined by the dependence of the type

$$K = \frac{1}{\frac{1}{\alpha_1} + \frac{\delta}{\lambda} + \frac{1}{\alpha_2}}, \qquad (1)$$

where $1/\alpha_1$, $1/\alpha_2$ - thermal resistance of heat transfer; δ/λ - thermal resistance to thermal conductivity; λ - coefficient of thermal conductivity; δ - the thickness of the metal friction elements.

It should be noted that thermoelectric power. etc. with. is only one (first) component of the total integral emf, which also includes: caused by the entrainment of carriers of electric charges by waves of mechanical and temperature stresses (the so-called acousto-electric effect), the interaction of metals of the friction pair in the presence of an electrically conductive electrolytic liquid (e. etc., arising from the interaction of a friction pair in an electromagnetic field or when at least one of its elements is in a magnetized state. The magnitude and direction of the integral e. etc. with. depends on the physical and mechanical properties of the metals of the friction pair, on the speed and load modes of friction, on the state of rubbing surfaces and many other factors,

Moreover, pulsed high-frequency mechanical vibrations in the friction zone are inseparable from thermoelectric relaxation processes, and both of these factors always jointly affect the scatter of the experimental values of wear resistance of parts of friction pairs of brakes. The effect of thermal current on the wear resistance of parts is associated with the peculiarities of relaxation, oxidation, diffusion and other processes affecting each other.

Suffice it to note that oxide films on the surface of contacting metals have semiconducting properties and high resistivity and are capable of playing the role of amplifiers of thermoelectric effects, which can cause the appearance of rather significant eddy currents at the points of closest contact of the contact points and, due to the low thermal conductivity of oxides, contribute to localized heat release.

Contact conductivity also depends on the combination of materials of the friction pair (for example, copper-copper, steel-copper, etc.) and the state of the rubbing surfaces. When studying the conductivity of the contact, its hysteresis is noted: if with an increase in specific loads, the electrical conductivity of the contact increases relatively quickly, then with a smooth load shedding it decreases much more slowly and does not coincide with the initial values.

In addition, when unloading pairs of contaminated surfaces that have boundary layers of products of cracking processes occurring in the surface layers of the polymer lining, the conductivity hysteresis curves show not a monotonic decrease in the contact conductivity, but a paradoxical "swelling" of the curves, the reason for which remains unclear.

It has been established that the transfer of heat during electrothermomechanical friction during its accumulation in the surface layer of the metal friction element occurs along the normal from places with a higher temperature to places with a lower temperature. In this case, a surface temperature gradient arises. The largest deep temperature drop occurs in the direction normal to the area of the contact spot of the microprotrusion.

In fig. 3 shows the interaction of two surfaces and the direction of the unit vectors coinciding with the direction of the normal to the unit contact area.

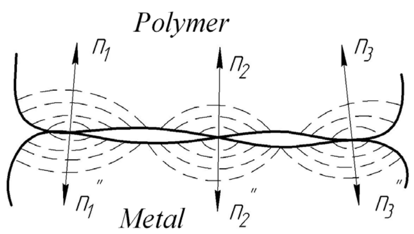

Figure 3 – Contacting two rough surfaces

Obviously, in the general case, the direction of the common normal n to the contact does not coincide with the unit vectors. The temperature field, propagating deep into the material, leads to a change in its mechanical properties in a thin surface layer.

The magnitude of the heat flux depends on the work of friction and the size of the area on which it accumulates consider the nonstationary temperature problem of friction according to *V.A.Kudinov.*

Imagine a metal bar of rectangular cross-section pressed by the specific load *p* to the surface of a rotating disk (fig. 4).

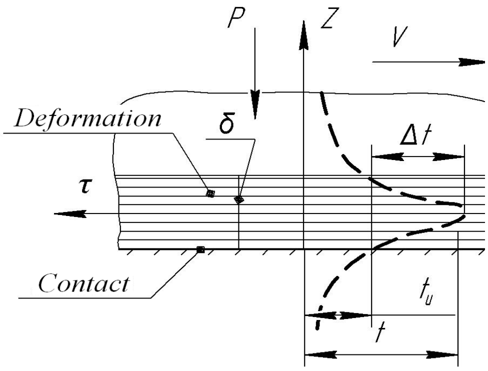

Figure 4 – Change in temperature t along the normal z to the friction surface (in the surface deformable layer) of the metal friction element

Legend in fig. 4 are the following: temperatures: layer (t); initial ($t_н$); increments (Δt); environment (t_o); shear stresses (τ); surface layer (δ); sliding speed (V); z - the origin of the coordinate axis is located on the middle surface of the layer.

In this case, it was assumed that the disc material has a higher strength, and plastic deformations occur in the surface layer of the rod, which are the same in thickness, therefore, the temperatures of the planes bounding the surface layer are equal to each other.

Provided that there is no polymorphism, ie, there is no change in the type of crystal lattice (face-centered cubic [FCC], body-centered cubic [BCC] and hexagonally close-packed [HCP]) depending on specific loads and surface-volume temperature.

The latter act on the under- and subsurface layer of the metal friction element of the brake device. If we adhere to the model of solid layers, then in the first case, the layers remain close-packed (PU), but moved away from each other, and in the second, the atoms of neighboring layers touch each other, but a gap appears between the atoms in the layer itself, and therefore all real hcp are structures are not truly PU-mi.

In reality, however, the difference *c/a* (where *c* and *a* are the height and width of the ribs) is variable *c/a* <1,633; *c/a* =1,633; and *c/a* >1,633; (1,633 is an ideal value) means that the atoms in hcp metals are not spheres, but ellipsoids (compressed spheres of atoms with the ratio in the planes

$1{,}633 < \frac{c_г}{a_в} > 1{,}633$) [9].

Thus, under the action of pulsed specific loads in the friction pairs "metal - polymer" of brakes, the atoms in the layers, as well as the layers themselves, are compacted, which contributes to the accumulation of energy in them due to the high electrothermal resistance, and, as a consequence, an increase in the surface-bulk temperature. In [10], a method is proposed for determining the electrothermal layers of a treadmill of materials "SCh-15 - FK-24A" of a disc-shoe brake with their maximum energy load. The calculation results are shown in table 1.

Table 1 – Results of calculations of electrothermal layers of a treadmill of friction pair "SCh15 - FK-24A" of a disc-shoe brake

Thickness electrothermal layers, mm:		Time of pulsed electric and heat currents, $\tau \cdot 10^4$, s							
		one	3	five	7	nine	eleven	13	fifteen
overlays	δ_1	0.025	0.043	0.055	0.066	0.074	0.082	0.089	0.096
disk	δ_2	0.094	0.163	0.211	0.249	0.283	0.313	0.34	0.365
	δ_{2*}	0.013	0.023	0.026	0.031	0.033	0.035	0.034	0.037

*Note: δ_2 * - refers to the steel disc.

Based on the data obtained in table. 1, it seems possible to draw the following conclusions:- with an increase in the time of action of pulsed electric and thermal currents, the thickness of the electrothermal layers also increases; due to the lower thermal conductivity of the lining material than the disc material, the thickness of the thermal layer in the lining is on average 26% less; when comparing the electrical and thermal layers, it can be seen that the thickness of the thermal layer is an order of magnitude higher than the thickness of the electrical one.

The difference between internal and external friction of a metal friction element

The distinction between external and internal friction is quantitative and qualitative. This is an important question, since in the first case, the patterns of internal friction could be extended to external friction, in the second, other patterns should be expected.

Studies of the mechanism of external friction show that it is fundamentally different from internal friction. The only similarity between them is that they are dissipative processes. What is their main difference?

First, in the geometry of the interaction of rubbing surfaces with external friction of contact of two solids occurring at separate points of their microprotrusions, the contact is discrete due to impulse application of the load. With internal friction, the contact surfaces of the layers of the body are continuous.

Secondly, internal friction is characterized by the parallel movement of the material in the direction of the relative velocity vector, and in external friction - perpendicular to the relative velocity vector.

Third, with external friction, the formation and destruction of bonds is localized in a thin surface layer; with internal friction, the deformation zone covers the entire volume of the layers. A necessary condition for external friction is the presence of a positive gradient of the mechanical properties of each of the rubbing bodies in depth, for internal friction - the presence of a negative gradient in the thickness of the layers of the body. A positive gradient is achieved by reducing the strength of the surface layer under the influence of a temperature gradient in the friction zone, which affects the gradient of the mechanical properties of the body material. Molecular seizure of two solids is inevitable; therefore, localization of destruction in a thin surface layer will take place only with a positive gradient of mechanical properties.

Fourth, during tangential displacement, the embedded unevenness drives a hemispherical wave of deformed material in front of it. Behind the embedded unevenness, the material is strongly stretched. A point located on the crest of the wave in front of the irregularity, as it passes, being crushed by the indenter, is lowered. Therefore, each point on the surface vibrates in a plane perpendicular to the tangency plane.

With internal friction, the material shifts in the direction of movement in the plane of contact. This is the fundamental kinematic difference between external and internal friction.

Table 2 compares external and internal friction. The nature of internal friction is the same, it is associated with the transfer of momentum from one layer of the body material to another, but it is necessary to take into account: structural defects, phase transformations, electronic and ionic processes in the structure of the material.

The nature of external friction is twofold, since it depends on changes in the properties of surfaces caused by deformation, surface temperature and its gradients, stresses, and chemical action of the environment. All of these factors contribute to cyclic structural transformations in the surface layer of the material.

The effect of the gradient of mechanical properties on the transition from external friction to internal friction is illustrated by an experiment performed by *V.N. Kashcheev* and *I.A. Solomennym* different weight characteristics of the nickel disc rubbing its bottom against the surface (Fig. 5).

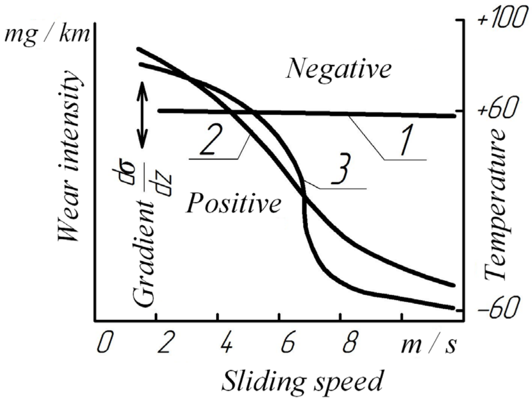

Figure 5 – Transition from external to internal friction depending on the gradient of mechanical properties

In this case, the triboelectric potential of the bronze sample was 4.2 eV, and that of the nickel disk was 4.5 eV. The difference between the triboelectric potentials of the materials was 0.3 eV.

During the experiment, the sliding speed and volumetric temperature of the glass were changed (curve 2) (Fig. 5).

Surface temperature ϑ_s, measured thermo-e. etc., was maintained constant, corresponding to 60 ºC (curve 1), due to the introduction of liquid air into the glass, placing a heating coil in it and changing the thickness of the circle and cylinder of the glass.

When passing from a negative to a positive gradient, the wear value (curve 3) decreases slightly due to the small value (only 0.3 eV) between the triboelectric potentials of the materials.

If we proceed from the fact that the cylinder of the glass is a storage of thermal energy, then in the processes of "heating - cooling" of the circle and the cylinder of the glass, due to the different rates of their flow, a negative gradient of the volume temperature arises.

Table 2 – Comparison of external and internal friction

Characteristic	Friction:	
	internal	external
Touching Offset direction. Displacement character Gradient of mechanical properties in depth Excitatory factors Processes, phenomena and effects in the dislocation-vacancy nature of the selective transfer of heat and wear products	Continuous By vector speed Layered (parallel) **Negative** Energy levels, atoms Diffusion, interstitial or substitutional atoms, dislocation (sliding and vibrations), transformation of materials from one to another, electrical and magnetic losses associated with backgrounds and electrons; Fermi, Brillouin, Bose, etc.	Discrete Perpendicular to the velocity vector Sinusoidal (wave) **Positive** Performance parameters Friction occurs in the following fields: - mechanical; - thermal; - electric; - chemical; - electromagnetic. Each field has certain processes, phenomena, and effects with their own energy levels

Of particular interest is the study and application of the theory of highly excited states in crystals of a metal friction element of plasticity and strength of its surface and nsurface layers. In this case, plastic deformation (stresses) should be considered in compliance with the laws of behavior of inhomogeneous, strongly nonequilibrium systems undergoing local structural transformations and following to equilibrium by the movement of the constituent new structures along the crystal under the action of gradient stresses. Whenthis a deformable crystal is capable of carrying out plastic flow in local volumes, which proceeds as a dissipative process, due to a relay-race rearrangement between two adjacent structures.

The generation of entropy in the considered zone of the crystal is a local kinetic structural transition that promotes the initiation of plastic shear.

The noted structural transformation differs from the thermodynamic structural transition and should correspond to nonequilibrium thermodynamics, which is a component of nonequilibrium tribology in the frictional interaction of friction pairs of braking devices. In this case, at each point of the deformable spots of contacts of microprotrusions at a given time, only one system of slip planes occurs, in which there is a loss of shear stability.

Shear information, which is anisotropic in nature, is always accompanied by material rotation inside the structural element of deformation (block grains, cells of the dislocation structure, etc.). In this case, the material rotation, in contrast to the crystallographic one, does not affect the spatial orientation of the crystal lattice [9, 10]. This, in turn, on the side of the surrounding material at the boundary of the structural element of the deformation causes a turning moment. Rotational modes (one of the numerical characteristics of the probability distribution of a random variable, estimated by their density) of deformation sets in motion the entire hierarchical structure of the levels of deformable spots of contacts of microprotrusions. Structural elements begin to move as a whole, experiencing translation (transmission) and crystallographic rotation.

The relationship between shears and rotations shows that the elementary act of plastic deformation is not shear, but a translational-rotational vortex. The latter, in terms of its scale, can be at the meso, micro and macro levels. The vortex hierarchy arises behindscore the formed hierarchy of various structural levels deformations. Trafficthe whole hierarchy of structural levels deformations and causes her vortex character, spowith this occurrence new channels energy dissipation, more efficient, than from movement of individual dislocations.

Rotary mods strain on various scale levels differ from each other. Their evolutionat increasing degree deformation is naturally reflected in the change in the fractal dimension in the places where the mechanicaliCal stresses on the surface of the metal friction element.

Boundary conditions for the interaction of external and internal layers of material pairs

When assessing the energy loading of friction pairs of brake devices, you need to know: geometric parameters of friction pairs and their shape; thermophysical characteristics of materials; initial and boundary conditions;-the maximum energy load of metal friction elements and their heat exchange capacity, which consists in the combined action of conductive heat exchange with radiation and conductive heat exchange from their surfaces, as well as the permissible temperature for polymer lining materials.

These four conditions are called uniqueness conditions, and the set of initial and boundary conditions are called boundary conditions (Table 3).

The energy load of the working surfaces of the pulley rim and drum, as well as the friction treadmill of the disks (solid and self-ventilated) depends on their metal consumption.

The smaller the latter, the faster this or that metal friction element will warm up. In addition, the ratio of the areas of matt and polished surfaces of metal elements affects the efficiency of convective and radiative heat transfer. In this case, these types of heat transfer must interact with the conductive type of heat transfer.

Table 3 – Classic list of boundary conditions

Kind of boundary condition	Dependencies	
	1st	The body surface temperature (t_p) is known
	II	The intensity of the heat flux from the outside into the body is given (q_v) $$-\lambda \frac{\partial t_n}{\partial x}\Big|_{x=+0} = q_v. \quad (2)$$
	III	The heat flux coming from the washing medium is directly proportional to the temperature difference between the medium and the body surface $$-\lambda \frac{\partial t_n}{\partial x}\Big|_{x=+0} = \alpha\left(\vartheta - t_{x=+0}\right). \quad (3)$$
	IV	The body is in contact with another body that has different thermophysical characteristics $$t_{n1}\Big|_{x=+0} = t_{n2}\Big|_{x=-0}. \quad (4)$$

Legend: λ, α - coefficients: thermal conductivity, heat transfer; q_v - specific heat flux; indices x = + 0 and x = -0 - external and internal surfaces; $\partial t_n/\partial x$ - the temperature gradient over the thickness of the body; ϑ - heating temperature.

The metal friction elements of the brakes fall into the zones of the steady state and thermal stabilization state.

In the first case, the amount of heat generated by the friction pair is removed to the environment. In the second case, the temperature gradient across the thickness of the metal friction element becomes minimal.

In addition, the surface layer of the polymer lining changes its state of aggregation.

Taking into account the above listed elements of the friction pair requires different initial conditions for the temperature zones, which leads to variable conditions of uniqueness.

The following initial conditions correspond to the classical list of boundary conditions

$$t\ (x, y, z, \theta) = f_3\ (x, y, z). \quad (5)$$

In the general case λ, c, ρ, p, q, α can be functions of coordinates, temperature, time. In each specific case, especially in problems with moving boundaries, where phase transformations occur, the writing of the boundary conditions may have a slightly different form, but in principle the boundary conditions of the I-IV kind cover all possible cases.

In recent years, works have appeared where the question of the formalism of boundary conditions of the I-IV kind, especially for non-stationary problems, has been raised. For example, in [11, 12] it is shown that non-stationary problems of heat transfer should, in the general case, be solved as conjugate, that is, it is necessary to simultaneously solve the equations of heat transfer for the medium washing the body. It was shown in [11, 12] that when solving heat transfer problems, the boundary conditionsThe second kind corresponds better to the physical picture of the phenomena than the conditions of the third kind. For non-stationary modes, the coefficients α_q, α_m are fictitious to a greater extent than for stationary ones, where both α_q and α_m are introduced formally. In principle, the problems of heat exchange of media with solids should be solved as conjugate problems, but in a number of cases the boundary conditions of the II and III kind are quite justified [11, 12].

The choice of boundary conditions depends on the problem being solved. Currently, in works [1 - 8], there are five types of boundary conditions:

- "free" when the near-boundary atoms form a free surface in contact with vacuum, and can move in the same way as atoms inside the volume of the calculated crystal lattice. This type of boundary conditions is sometimes used to study the deformation of a computational cell under the influence of thermal and dynamic factors, or in cases where there is no need for this boundary condition, for example, in studies related to large molecules (polymers, fullerenes, etc.);

- "hard" - when the coordinates of the boundary atoms are fixed. In this case, it is assumed that a sufficiently large number of mobile boundary atoms acts on the phenomenon under study. This type of boundary condition is attractive for its simplicity, but it requires a larger number of atoms in the computational block and does not allow solving problems associated with a significant change in the thermodynamic parameters of the computational block. In the molecular dynamics method, this type of boundary condition is mainly used in combination with other types.

- "flexible", or mobile, which are more natural than rigid. Boundary atoms in some periods of time and sometimes with certain restrictions are allowed to move during the operation of the model in accordance with their redistribution in the computational cell. This boundary condition requires fewer atoms in the computational block than the stringent condition and is a more adequate real condition. As a rule, this boundary condition is used in cases of a possible change in the volume of the computational block due to the influence of thermal and dynamic factors;

- "periodic" - when there is a periodicity in a certain direction, provided that a settlement cell is selected in this direction, equal to the identity period. This allows you to simulate an infinite crystal in the direction in question;

- "viscous" - when the absorption of elastic vibration energy is simulated at the boundaries of the computational cell due to the presence of a damping area around the computational block. When using a viscous boundary condition, one strives to ensure that the computational block is considered to be surrounded by an infinitely ideal crystal. These conditions are met when studying the structures of defects, but in problems related to thermal activation, it becomes necessary to comply with the law of conservation of energy.

When compiling a model describing the processes occurring inside the crystal at the atomic level, the following sequential steps are performed:

- the basis of the crystal structure is set, which extends in three directions along the coordinate axes, forming a computational cell, and the size of the computational block is determined, on the basis of which the initial packing of atoms in the material structure arises;

- the interaction potential is selected, which should be sufficiently simple and reliable, and then the potential is tested according to the most characteristic and known from experimental data properties of the material;

- determined "boundary conditions" imposed on the calculation block of the crystal;

- the method and the described mathematical apparatus for evaluating the motion of atoms (or particles) and external and internal hydrogen in the crystal structure of the metal lattice are determined.

Conclusion

The preliminary stage of research on hydrogen wear of heavy-loaded metal friction elements of brakes has been completed.

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Received: 23.12.2020
Revised: 11.12.2021
Accepted: 21.12.2021