INTERATOMIC INTERACTIONS ON THE SURFACES OF METAL-POLYMER TRIBOCOUPLING

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ABSTRACT

Tribology, which originated as the science of processes in macroscopic objects, thanks to advances in quantum chemistry and the development of experimental physics of X-ray photoelectron and Auger electron spectroscopy (XPS and AES), should now extend studies to micro- and nanolevels. It is necessary to examine in more detail interatomic interactions on the friction surfaces of both anti-friction and friction couplings.

The objective of the article is to present the results of studies of segregation phenomena of alloying and impurity elements in the tribosystem «wheel-brake shoes», based on finite-element method, X-ray photoelectron and Auger spectroscopy, modelling, mathematical computations and simulation.

Considering regularities of the impact of temperature and thermal gradient on tribomechanical, triboelectric and tribochemical processes within the contact area of «polymer – metal», generalized recommendations on the selection of filling and strengthening elements became available.

For anti-friction composite polymeric materials the main criterion of minimizing the coefficient of friction and high wear resistance is the ability to spontaneously form on the friction surface a bilayer film that combines lubricating properties and high adhesion due to bipolar tribocharging of its composites.

For friction materials the main criterion to avoid increased wear and transfer of metal on the conjugate plastic surface is the reduction of the degree of hydrogenation of the metal counterface by establishing the optimum temperature gradient and positive tribocharging.

The solution of related non-stationary thermoelastic problem of brake disc-pad showed that the maximum temperature within all the thickness of the disk is located not on the surface but at depth. It was established experimentally that the maximum concentration of hydrogen in the disc coincides with the maximum temperature.

The binding energy of atoms of different elements to the surface of the grain is a periodic function of the atomic numbers of the elements. This may serve as a theoretical basis for predicting the strength properties of steel with a different composition of alloying and impurity elements.

The obtained results indicate the promising application of XPS, AES and quantum chemistry in solving tribological tasks.

<u>Keywords</u>: *railway, system wheel-brake shoe, tribological coupling, metal-polymers, interatomic interaction, film, diffusion, contact thermoelastic problem, temperature, segregation, electrification.*

Background. *Tribology, which originated as the science of processes in macroscopic objects, today, thanks to advances in quantum chemistry and the development of experimental physics of X-ray photoelectron and Auger electron spectroscopy (XPS and AES) should extend studies to the micro- and nanolevels. Speaking objectively, it is necessary to study in more detail the interatomic interactions on the friction surfaces of both anti-friction and friction couplings.*

Objective. *The objective of the author is to present the results of studies of segregation phenomena of alloying and impurity elements in tribosystem «wheel – brake shoes».*

Methods. *The author uses analysis, scientific description, finite-element method, X-ray photoelectron and Auger spectroscopy, modeling, mathematical calculations.*

Results.

Antifriction tribocoupling

Composite based on non-woven fibers of polytetrafluoroethylene (PTFE), where phenol formaldehyde is used as a binding substance, was one of the very first objects studied by the method of XPS. [1–3].

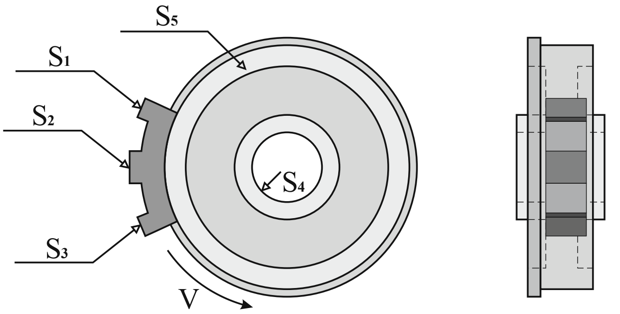
The result is a range of dependences of intensity of different X-ray lines of elements found in the friction transfer film, on time and load of frictional interaction. The analysis of these dependences allowed to adequately represent the process of friction where fluoroplastic is engaged, as well as three stages of formation of transfer film within the test time.

The first phase covers the interval from 10 to 60 sec, in which the surface layer of the film is formed mainly by products of the binder transfer friction. The second stage has an interval from 1 minute to 0,5 hours: the content of products of friction transfer of PTFE products on the counterface surface increases while the content of binder transfer products reduces. The third stage lasts from 0,5 to 1 hour. The intensity of X-ray photoelectron lines $F1_s$ and $C1_s$, characterizing the amount of products of frictional transfer of PTFE in the film, reduces and the amount of lines $C1_s$ and $O1_s$ belonging to the binder elements increases.

In the course of friction transfer the composition of the surface layer of the film during the study interval changes three times, and a larger time span is required for each subsequent change. The process of film formation, during which non-monotonic change in its composition occurs, lasts no more than two hours and depends on the mode of friction.

To reveal the mechanism of formation of friction transfer film further studies were carried out. They were devoted to triboelectrification of metal-polymer contact based on the concept of surface states (hereinafter- SS), which are the energy levels on the surface and are centers of localization of free charge carriers. The study of composite based on nonwoven fibers of polytetrafluoroethylene and binding phenol formaldehyde showed that the component, when the friction proceeds with the steel, has positive tribocharging, and the binder has a negative one.

This means that during friction, first of all, wear products of the binder, having positive tri-



Pic. 1. Schematic representation of the system under study.

$$\begin{aligned}&(\lambda^{(i)}+2\mu^{(i)})\nabla\nabla\cdot\mathbf{u}^{(i)}-(\lambda^{(i)}+\mu^{(i)})\nabla\times\nabla\times\mathbf{u}^{(i)}-\gamma^{(i)}\nabla\theta^{(i)}-\rho^{(i)}\ddot{\mathbf{u}}^{(i)}=0,\\&\Lambda^{(i)}\nabla\cdot\nabla\theta^{(i)}-C_{\varepsilon}^{(i)}\dot{\theta}^{(i)}-T_0\gamma^{(i)}\frac{\partial}{\partial t}\nabla\cdot\mathbf{u}^{(i)}=0, i=1,2;\end{aligned}\qquad (1)$$

$$\begin{cases}u_R^{(1)}=u_Z^{(1)}=0, \mathbf{x}\in S_4,\\u_Y^{(2)}=u_Z^{(2)}=0, \mathbf{x}\in S_1\cup S_2\cup S_3,\\\dfrac{1}{\|S_1\|+\|S_2\|+\|S_3\|}\displaystyle\int_{S_1\cup S_2\cup S_3}\sigma_{RR}^{(2)}\,dS=P.\end{cases}\quad\begin{cases}\tau_{R\phi}=k\cdot\sigma_{RR}, \mathbf{x}\in S_{cont},\\q^{(2)}=a(\theta_{envir}-\theta^{(1)}), \mathbf{x}\in S_5,\\q_{cont}=k_{cont}(\theta^{(1)}-\theta^{(2)}), \mathbf{x}\in S_{cont},\\q_{cont}^{(1)\text{ген}}=k_{en}k_dE_{fr}, \mathbf{x}\in S_{cont},\\q_{cont}^{(2)\text{ген}}=k_{en}(1-k_d)E_{fr}, \mathbf{x}\in S_{cont},\\\theta^{(1)}=\theta^{(2)}=0, t=0,\\\dot{u}_{\phi}^{(1)}=V(t), t\in[0,T].\end{cases}\qquad (2)$$

bocharging, are formed and held firmly enough on the surface of the metal counterface. After the formation of the so-called first layer of the binder PTFE wear products due to their different polarities with binder are stored on the surface by means of electrical forces. Then a thin high-oriented transfer film is formed, which provides a low coefficient of friction. With increasing sliding speed tribocontact is heated and tribo-EMF accordingly decreases. At the same time the electrostatic forces holding the PTFE wear products on the binder decrease, and the intensive wear occurs.

Similar results were obtained for composites using polyethylene (PE) and polycaproamide (PCA), PCA + PTFE, PCD + PE, where the decline in the coefficient of friction and increase of wear resistance at high loads are conditioned by formation on the metal surface of the first layer of PCA, and then of a high-oriented thin film of PE and PTFE with low shear resistance.

On the basis of research results it is stated that the binder is called not only to unite the composite together and to provide the ability to perceive the external load, but also to actively participate in the formation of a frictional transfer film.

Thus, for anti-friction composite polymeric materials the possibility of forming a double layer of the transfer film on the friction surface should be considered the main criterion of obtaining the minimum coefficient of friction and high wear resistance.

Modeling of disc brake system

When considering frictional units of friction, such as wheels and composite shoe of the brake system of the rolling stock, a huge role is played by diffusion and segregation processes with regard to their functional dependence on temperature.

It is known that the specific of polymeric materials is that their operation in tribosystems is accompanied by large heating and degradation processes with formation of chemically active products, including hydrogen, followed by diffusion into the metal counterface.

First, we define the temperature value by solving the thermoelastic problem concerning the system of wheel–brake shoes. Schematic representation of the system under study is shown in Pic. 1.

The wheel rotates counterclockwise with a velocity V on the time interval $t \in [0,T]$, the brake shoe is pressed against the wheel with force P. On the free surface of the wheel S_5 the condition of convective heat exchange with the environment is set with the coefficient a. In the area of contact friction is assumed to have the coefficient k.

In addition to the Cartesian coordinate system with the origin at the center of the brake disc we will refer to a cylindrical system (R, ϕ, Z) relative to the same center (Z-axis is perpendicular to the plane of the wheel).

The description of the motion is carried out by similar equations of coupled thermoelasticity (1) and boundary conditions (2). The superscript (1) corresponds to a wheel, superscript (2) refers to a shoe (1, 2).

We will show in more detail each of the boundary conditions (2). On the surface S_4 a limit is set on the movement of the railway wheel in the directions R and z, which allows to wheel to make only rotational movements. Similarly, on the surfaces S_1, S_2, S_3 there is a restriction to move in the directions Y and Z, which allows only horizontal movement of the brake sole. Power conditions in terms of the task are reduced to establishing

$$\begin{bmatrix} [M] & [0] \\ & [0] \end{bmatrix} \begin{Bmatrix} \{\ddot{u}\} \\ \{\ddot{T}\} \end{Bmatrix} + \begin{bmatrix} [C] & [0] \\ & [C^t] \end{bmatrix} \begin{Bmatrix} \{\dot{u}\} \\ \{\dot{T}\} \end{Bmatrix} + \begin{bmatrix} [K] & [K^{ut}] \\ & [K^t] \end{bmatrix} \begin{Bmatrix} \{u\} \\ \{T\} \end{Bmatrix} = \begin{Bmatrix} \{F\} \\ \{Q\} \end{Bmatrix} \quad (3),$$

distributed load on the surfaces S_1, S_2, S_3, which demonstrates pressing force of the brake system of value P. In the area of contact tangent stresses $\tau_{R\phi}$ are proportional to the normal σ_{RR} with friction coefficient k.

An important factor in the description of the temperature dependence of brake systems is the convective heat transfer to the environment, due to the air blow-off of the structure. The convection condition in the shown problem appears as the proportion of the heat flux value $q^{(2)}$ on the outer surface of the wheel S_5 and temperature difference of the wheel $\theta^{(1)}$ and the environment θ_{envir} with the coefficient a.

A required moment is accounting of heat conduction in the contact zone. In the situation described above, this condition is mandatory in modeling heat transfer from one body to another, and is expressed in the proportionality of the heat flow in the contact pair q_{cont} to the temperature difference of contact surfaces of $\theta^{(1)}$, $\theta^{(2)}$ (the coefficient of contact thermal conductivity k_{cont} is taken into account). The process of heat generation due to friction is identical to the appearance of additional heat fluxes at the boundaries of the contacting bodies with intensities proportional to the coefficient k_{en} and the amount of energy E_{fr} transferred from friction into heat, as well as to weighting coefficient k_d, denoting the distribution of heat between two surfaces.

Since this problem is non-stationary, it is necessary to have appropriate initial conditions, which are associated with the initial temperature of the bodies $\theta^{(1)}$, $\theta^{(2)}$, which is zero in this case, and the initial velocity of rotation of the wheel $\dot{u}_{\varphi}^{(1)} = V(0)$.

As material for all components the steel was selected with the following parameters: Young's modulus $E=2{,}0e^{11}$ Pa; Poisson's ratio $\nu=0{,}3$; density $\rho = 7850$ kg/m^3; thermal conductivity coefficient $\Lambda=48$ W/ (m·K); specific heat $C_\varepsilon = 452$ J/ (kgK); thermal expansion coefficient $\gamma = 1{,}1e^{-5}$ 1/K.

The complexity of the geometry and thermoelastic behavior of the system do not permit to obtain a solution analytically. In such cases, an effective method of solutions as shown is the use of finite element package [4], in particular ABAQUS. To partition bodies to finite elements we used eight-unit element C3D8T, allowing forthe purpose of modeling to account for both elastic and temperature fields, finite element matrix equations of which have a form (3): where M is mass matrix; C is damping matrix; K is stiffness matrix; u is displacement vector; F is sum of nodal forces and pressures on the elements; C^t is specific heat; K^t is diffusion conductivity matrix; T is temperature vector; K^{ut} is thermoelastic stiffness matrix.

Finite element analysis for a proper convergence was divided into two phases. The first phase solved the static problem of indentation with a force P of brake lining into the disc. The next step solved – the dynamic transient problem, in which rotation speed of the brake disc was set. As a result, it was found that the maximum temperature within all the thickness of the disk in the sections distant from the contact area is not on the surface, but at depth. In reality, the depth of this effect is approximately 200–500 microns.

Diffusion and segregation processes

It is known that during the thermomechanical degradation of polymers by friction in metal contacting zone inherently different solid, liquid and gaseous products of wear are released, among which there is a large amount of hydrogen. It is actively absorbed by contacting metal surface.

The presence of hydrogen in iron and steel radically alters their properties, e.g. reduces the ductility and increases the brittleness, hardness, physical properties, and eventually leads to spreadability of the metal on the polymer.

To determine the effect of the temperature gradient on the concentration profile of hydrogen in the metal counterface a methodology was developed and an installation was manufactured, allowing changing the temperature field through the thickness of the metal body made in the form of a set of tightly adjacent plates.

The level of gas content of steel samples was determined during the evolution of gas from the metal when it was heated and by further chromatography, as well as by the method of anodic dissolution. It is clarified that the maximum hydrogen concentration coincides with the maximum temperature.

Modern tribology has accumulated a wealth of information about the nature of friction and mechanisms of materials' wear. However, it should be recognized that the role, played by impurity and alloying elements in polycrystalline materials, is still underestimated. It is primarily about the phenomenon of grain boundary segregation (GBS), when the atoms of these elements approach the grain boundaries, and the consequences of this phenomenon. With regard to rail transport similar problem has been previously only designated. Today there is no direct experimental evidence to assess the impact of segregation processes on wear and defect formation of working surfaces of wheel and rail as far as they are operated.

Auger electron spectroscopy (AES) is a technique that allows directly studying the characteristics of grain boundary segregation. AES helped [4, 5] to determine elemental composition at the grain boundaries of steel of the railway wheel decommissioned due to numerous typical defects of its working surface (chips were mainly observed on grain boundaries). Samples were cut from defect places of the surface, already separated fragments, wheel sections at different depths. The volumetric composition and lattice parameters of the material of wheels were investigated, metallographic examinations were carried out and the depth profiles of the microhardness were evaluated.

It was found that on the surfaces of defect sites and chips the atoms of following elements are present: Fe (matrix), alloying elements (C, Cu, Mn, Cr, Si), impurities (P, S), as well as Ba, Zn, Ca, K. The reasons for their appearance on the wheel tread are different. Barium and zinc atoms are contained in the fillers of the polymer composite brake shoe, which is based on hydrocarbon binder. Potassium and calcium atoms are elements of the environment. Silicon is included in the material of the wheel and is present in the environment.

The most important result of the measurement is that at the grain boundaries located on chips we observe segregation of atoms of alloying and impurity elements. The concentration of elements in the studied layers exceeds their volume content by dozens of times. On the surfaces of chips the excess is substantially larger (e. g., for S –up to 120 times). Given this experimental fact, and the fact that the impurities P and S and atoms Cu, Zn, Sr, Ca, K, while at the grain boundaries in the matrix of iron, soften the connection between the grains [6], there is reason to believe that the segregation of elements has contributed to the destruction of the working surface of the wheel. Carbon content in all studied cases is large and insignificantly varies from sample to sample. Such a segregation can be caused by contact with the polymer material of the brake shoe and be the result of contamination of the surface, because they are real, not model samples. The same applies to the oxygen concentration.

It is worth noting that manganese, nickel and silicon at the grain boundaries are not observed. At the same time, Mn and Si in significant volume are observed on the chips of mass transfer plate (product of catastrophic wear of the wheel), consisting mainly of a hard material of the wheel, «spreaded» during the contact of the wheel with the shoe on the surface of its relatively soft polymer.

Excess (compared to the volume) of copper content in the grain boundaries and the fracture surfaces may have its origin not only in the volume of the wheel, but in the material of the shoe (brass). Therefore, the analyzed data witnessed the intensity of exchange diffusion processes involving atoms of steel of the wheels, the brake shoe material and the environment. That is tribosystem during operation is not closed as for its atomic composition.

Methods of quantum chemistry

It is known that the atoms of phosphorus P and sulfur S embrittle metals. In [7] by simple estimates it is shown that the atoms of embrittling elements can weaken the bond between the grains. But it referred only to on the enthalpy of sublimation and the size of atoms of substances. In view of the assumptions, underlying theoretical calculations, the conclusions of [7] need experimental confirmation and (or) further study.

Appeared during last two decades, methods of quantum-chemical calculations, close to the density functional theory (DFT), allow for a more precise than in [7], analysis of interactions that affect the destruction of metals. These methods make it possible to study the transient metal compounds, including hundreds of atoms. They relate to events with varying measure of the chemical interaction: the adsorption of molecules on solid surfaces, homogeneous and heterogeneous catalysis, biochemistry and others. However, works in which the methods of quantum chemistry would be closer to the problem of destruction and wear resistance of metals are still rare, and they consider single specific questions.

In our calculations [8] relating to the issue of segregation, the software package ADF [9] was used. It seems to be adapted to the functional density theory. Initially polyhydric cluster size was as by its means of which the effects under study can be reproduced at qualitative and possibly semiquantitative levels. Model cluster should obviously contain a quantity of matrix atoms (of adjacent layers of two adjacent grains) and segregated atoms located at the boundary. On the basis of calculations by which the optimal geometry of the cluster and the binding energy per atom were determined, it was found that the cluster with the number of atoms $n \approx 18$ can be classified as a minimum, allowing to explore the phenomena accompanying changes in the chemical composition of the steel.

To simulate the conditions in which the segregation occurs, we used the fact that at the narrowest part of the boundary between the grains in a polycrystal (the point of contact of grains), its width is approximately equal to the lattice constant [10]. This makes it possible to take into account a simple model of a boundary: in a 18-atom cluster of iron $Fe_2Fe_6X_2Fe_2Fe_6$, consisting of five layers, the atoms of the middle layer are replaced with segregated, denoted by the symbol X. Moreover, two upper and two lower layers imitate corresponding grains of the polycrystal, and the middle layer is a boundary between the grains.

We have calculated the energy of binding of the clusters that contain adsorbed and segregated atoms of chemical elements of the first four periods of the periodic table of D. I. Mendeleev, with numbers from 1 to 36 (from hydrogen to krypton). On the basis of the obtained data the energy value E_{bb} is calculated, which is required to break the clusters with formation of two parts, imitating grains in the model.

The calculations imply that the atoms of boron, carbon, manganese firmly «sew» grains of iron, because the energy required to break the clusters containing these atoms is greater than the corresponding energy for the same size of the cluster of pure iron. Conversely, atoms of lithium, silicon, phosphorus, sulfur, copper and nickel, though enter into a chemical bond with the iron, weaken the bond between the grains, since the energy to break the clusters of these elements is less than in the presence of a cluster of pure iron. It is obvious: the weakening of the bond between the grains in the surface layer reduces the wear resistance of steel.

If the calculated results are used into practice (for example, to solve the problem of increasing the wear resistance of steel by introducing atoms of strengthening elements into its surface layers), it is necessary to take into account the solubility properties of the elements. In the bulk phase of iron (i. e. grains) that part of them which remains on the surface of the grains may be too small and insufficient to create the effect of hardening. From this viewpoint, the most efficient way is the introduction of boron in the steel which, although has less value of E_{bb} as compared to carbon, is much less soluble in the metal surface layer.

Once boron is introduced in the steel in an amount to fill intercrystalline boundaries (in fact it is one hundredth of a percent of the total sample), and we can expect a significant increase *in wear resistance of steel. If the amount of boron is increased further, a part of its atoms will penetrate the iron grains and inside them chemical compounds of boron with iron, carbon and other metals (borides and carbides) will appear. Such compounds come significantly short of strength as compared with iron, and steel properties will deteriorate. Thus, to improve the strength and wear resistance of steel it is necessary to use only a small concentration of boron.*

CONCLUSIONS

1. With account for established patterns of influence of temperature and temperature gradient on tribomechanical, triboelectric and tribochemical processes in polymer-metal contact zone, generalized recommendations are formulated on the choice of fillers and reinforcing materials:

– For anti-friction composite polymeric materials the ability to spontaneously form on the friction surface a bilayer film that combines lubricating properties and high adhesion due to bipolar tribocharging of its composites should be considered the main criterion of minimizing the coefficient of friction and high wear resistance;

– For friction materials the main criterion for exclusion of increased wear and transfer of metal on the conjugate plastic surface is the reduction of the degree of hydrogenation of the metal counterface by establishing on it the optimum temperature gradient and positive tribocharging.

2. The solution of related non-stationary thermoelastic problem of brake disc-pad showed that the maximum temperature within the thickness of the disk is not on the surface but at depth. It was established experimentally that the maximum concentration of hydrogen in the disc coincides with the maximum temperature.

3. The obtained results indicate the promising application of XPS, AES and quantum chemistry in solving tribological tasks. The studied exchange-diffusion processes between the wheel and the brake shoe and segregation processes inside the metal of the wheel should be taken into account for the development of measures to improve the wear resistance of the system of wheel – rail – brake shoe.

4. The binding energy of atoms of different elements to the surface of the grain is a periodic function of the atomic numbers of the elements, which corresponds to the periodic law of Mendeleev. This may serve as a theoretical basis for predicting the strength properties of steel of a different composition of alloying and impurity elements.

REFERENCES

1. Evdokimov, Yu.A., Kolesnikov, V.I., Kozakov, A.T., Kravchenko, V.N., Nikol'skiy, A. V. Investigation of friction transfer of polytetrafluoroethylene by X-ray photoelectron spectroscopy method [*Issledovanie friktsionnogo perenosa politetraftoretilena metodom rentgenoelektronnoy spektroskopii*]. *Vestnik mashinostroeniya*, 1985, Iss. 2, pp. 33–36.

2. Kravchenko, V.N., Kozakov, A.T., Kolesnikov, V.I., Migal', Yu.F., Nikol'skiy, A. V. The study of formation of friction transfer film of antifriction self-lubricating composite on the basis of polytetrafluoroethylene fibers [*Issledovanie obrazovaniya plenki friktsionnogo perenosa antifriktsionnogo samosmazyvayuschegosya kompozita na osnove volokon politetraftoretilena*]. In: Dynamics and Strength of Rolling Stock. Interuniversity subject collection of works *[Dinamika i prochnost' podvizhnogo sostava: Mezhvuz. temat. sbornik]. 1986,* Iss.185, pp. 75–80.

3. Nikol'skiy, A.V., Kozakov, A.T., Kravchenko, V. N. Dynamics of changes in the chemical state of the friction surfaces of metal-polymer interface during frictional interaction [*Dinamika izmeneniya himicheskogo sostoyaniya poverhnostey treniya metallopolimernogo sopryazheniya v protsesse friktsionnogo vzaimodeystviya*]. *Trenie i iznos,* 1988, Vol. 9, Iss.5, pp.860–869.

4. Chebakov, M.I., Lyapin, A.A., Kolesnikov, I. V. Calculation of temperature fields in the interaction of the brake shoe and the railway wheel on the basis of thermoelastic model [*Raschet temperaturnyh poley pri vzaimodeystvii tormoznoy kolodki i zheleznodorozhnogo kolesa na osnove termouprugoy modeli*]. *Vestnik RGUPS*, 2013, Iss.2, pp. 76–79.

5. Kolesnikov, V.I., Migal', Yu.F., Doron'kin, V.N., Novikov, E.S., Kolesnikov, I. V. The interaction of atoms of impurity and alloying elements with the surface of the grains in the steel [*Vzaimodeystvie atomov primesnyh i legiruyuschih elementov s poverhnost'yu zeren v stali*]. *Vestnik nauchnogo tsentra RAN*. 2012, Vol, 8, Iss.4, pp. 27–33.

6. Surface analysis by Auger and X-ray photoelectron spectroscopy techniques [Translated from English. Original title: Practical surface analysis by Auger and X-ray photoelectron spectroscopy. Russian title: *Analiz poverhnosti metodami ozhe- i rentgenoelektronnoy fotoelektronnoy spektroskopii*]. Ed. by. Briggs, D., Seah, M.P. Moscow, Mir publ., 1987, 600 p.

7. Seah, M. P. Adsorption-induced interface decohesion. Acta Metallurgica, 1980, V. 28, pp. 955–962.

8. Kolesnikov, V.I., Migal', Yu.F., Mizhiritskaya, S.N., Doron'kin, V. N. Quantum-chemical study of the influence of grain boundary segregation on the wear resistance of steel [*Kvantovo-himicheskoe issledovanie vliyaniya zernogranichnoy segregatsii na iznosostoykost» stali*]. *Trenie i iznos*. 2008, V. 29, Iss.2, pp. 134–143.

9. Te Velde, G., Bickelhaupt, F. M., van Gisbergen, S. J. A., Fonseca Guerra, C., Baerends, E. J., Snijders, J. G., Ziegler, T. Chemistry with ADF. Journal of Computational Chemistry, Vol. 22, No. 9, 931–967 (2001).

10. Orlov, A.N., Perevezentsev, V.N., Rybin, V. V. Grain boundaries in metals [*Granitsy zeren v metallah*]. Moscow, Metallurgiya publ., 1980, 156 p. ●

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