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IMPROVING CONTACT DURABILITY OF POLYCRYSTALLINE SYSTEMS BY CONTROLLING THE PARAMETERS OF LARGE-ANGLE GRAIN BOUNDARIES

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Досліджено полікристалічні металеві системи зразків сталі 40Х з різною морфологією і параметрами розподілу великокутових границь зерен за енергіями. Встановлено вплив структурно-енергетичного стану границь зерен на експлуатаційну надійність сталі 40Х після покращення. На основі ієрархічного моделювання будови полікристалів запропоновані нові підходи і створено алгоритми для визначення взаємозв'язків між структурою, яка формується при технологічних обробках матеріалів, і етапами життєвого циклу деталей. Виявлено, що в якості цифрового двійника структури полікристалічних сплавів, який описує їх поведінку в умовах контактних навантажень, доцільно використовувати матричне подання системної моделі з її наповненням кількісними характеристиками зерен. З використанням розроблених методик визначено шляхи технологічного управління енергетичним станом меж поділу зерен структурних складових для підвищення довговічності деталей, що працюють при контактних навантаженнях. Розроблено розрахунково-експериментальний метод для оцінки впливу кількісних характеристик структури на параметри міцності границь зерен і їх здатність до утворення межзеренних пошкоджень при зовнішніх навантаженнях. Рівень енергії границь зерен і потрійних стиків між групами зерен малого і великого розміру є вищим, ніж між зернами одного розміру. Поверхні розділу з високим рівнем енергії є місцями утворення пошкоджень при технологічних обробках і зовнішніх навантаженнях конструкційних матеріалів. Це вказує на вирішальну роль великокутових границь, розміщених між потрійними стиками з високим градієнтом енергії в процесах утворення мікроструктурно коротких тріщин і межзеренного руйнування полікристалічних систем. Використання методів ієрархічного моделювання і числового матеріалознавства дозволяє підвищувати експлуатаційну надійність виробів вибором оптимальних параметрів внутрішніх граничних поверхонь. Менша вартість життєвого циклу деталей досягається режимами термічної обробки, які змінюють кількісні характеристики структури сталей

Ключові слова: системне моделювання, ієрархічні моделі, розрахункове матеріалознавство, полікристали, енергія границь зерен, зносотривкість

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1. Introduction

The most important task of modern machine building is to construct articles with the predefined life cycle based on the computerization of all stages of their design, production, and operation. Solving this task necessitates improving the properties of traditional, as well as the use of new, materials with an elevated set of physical-mechanical and operational properties, and computer methods of their design.

The durability and reliability of sophisticated technical products depend on a set of factors related to the properties of materials, the geometric parameters of structures, and their manufacturing technologies. The lack of methods for transferring the data that characterize the properties of materials to their performance within structures is replaced in the practice of their calculations with insufficiently reasonable margins of strength. The development of informational support to engineering, construction of methods for computerized modeling of the structure and properties of materials make it possible to obtain highly technological products using flexible technologies at minimal cost.

Such an approach is based on the use of multifunctional computer systems, which coherently perform the volumetric design of an article, estimate the justification of its reliability and performance, prepare technological processes for the fabrication and control over an engineering project.

Software for computerized engineering analysis of reliability and performance make it possible, based on estimated substantiation, to state new approaches to the choice of materials and their processing technologies in order to improve the operational durability of articles. The use of the software is limited due to the lack of interconnections between the structure of parts and the stages of their life cycle. In this regard, research into this field is relevant.

Modern data on the physical and mechanical properties of materials make it possible to ensure sufficient strength of machine parts with a high resistance to destruction. However, the most common reason for the failure of parts is the wear and damage to their working surfaces. Wear management is one of the most important approaches to ensuring the reliability and safety of machines. However, its development requires studying patterns in the destruction of materials under conditions of contact interaction and establishing its connection with their structure, which in most cases refers to heterogeneous polycrystalline systems. The task on examining and modeling the behavior of such systems in order to ensure their maximum reliability under conditions of the assigned contact loads is important for modern machine building.

Prolonged frictional interaction between bodies is accompanied by processes of the loss of their strength, which negatively affects the functioning of machines and mechanisms. The development of new technological methods to improve the durability of parts, which are associated with the formation of heterogeneous surface structures, is constrained by limited scientific approaches and procedures for calculating the characteristics of structure in the polycrystalline metal systems based on the criteria of contact durability under the predefined operational modes. The construction of new models of mechanics and the development of calculation procedures to determine the parameters of structure of polycrystalline alloys in order to improve the durability of structures are of considerable interest.

2. Literature review and problem statement

Development of new approaches to mathematical modeling of heterogeneous metal polycrystals under conditions of contact loads, construction of algorithms for analytical-numerical analysis of the effect of quantitative characteristics of structure on contact durability parameters are necessary for the development of informational support to digital machine building.

The complexity of solving the task is predetermined by a large number of technological factors that affect the reliability of articles [1]. In many cases, there is no link among these factors and informational support to project stages at the level of mathematical and computer models, which necessitates the creation of appropriate databases [2].

The issue of determining the causes of destruction of surface layers of contacting bodies under conditions of frictional interaction has a series of features. One of them is the locality and heterogeneity in the transmission of force, thermal and other types of loading [3]. In the process of making and operating machine parts their surfaces demonstrate the irregularities that form the topography of surfaces – macro deviations, undulations, roughness, subroughness, and nanoroughess. As a result, the contact interaction between bodies occurs not over the entire surface, but only in local areas (contact spots). In this case, there are nominal, A_a, contour, A_c, and actual areas of the contact surface, A_r. The total magnitude of a contour area A_c is 5...15 % of the magnitude of the rated area, and the magnitude of the actual area A_r is 1... 10 % of A_a.

The average diameter of a single contact spot for steels is 10 to 20 µm. The size of contact spots depends little on loading; the actual contact area varies mainly due to a change in the number of contact spots, which is directly proportional to the load applied [4, 5].

For polycrystalline alloys with the size of grains of 10...50 µm, there is a high probability that contact spots may include grains, boundaries, and triple grain joints. Friction of metal materials is accompanied by processes of deformation, formation and destruction of metal bonds on certain areas of contact surfaces. For alloys with a large grain, it is unlikely that a whole grain enters the contact spot, but it is always the case that the boundaries, as well as the joints of grains and subgrains, enter the actual contact area. The influence of the internal interfaces on the processes of deformation and destruction relates to their structural and energy state. However, processing technologies, which are based on changing the state of atoms at the boundaries of grains to improve the contact durability of articles, are used limitedly.

Contact interaction is characterized by the local nature of defects and cracks formation. The multi-stage process of alloy destruction includes the following stages [6, 7]:

1) accumulation of damage and disruption of a material's density in the field of stresses and deformations;

2) the development of microfractures in an environment with defects;

3) the growth of cracks and the separation of a material under the loads and movements assigned at the boundaries of a workpiece.

As a result of plastic deformation, two types of micro-damage develop – along a body and along the boundaries of grains [8, 9]. Since the mechanisms and the rate of accumulation of micro-damage in these areas are different, two internal variables of scalar nature are introduced, which determine the processes of damage accumulation – the energy of damage along a grain body W_p and the energy of damage along the boundaries of grains W_n:

$$W = W_p + W_n. \tag{1}$$

Damage W depends on the history of viscoplastic material deformation. The damage along the body and along grains boundaries is characterized by the relative parameters of damage W_p and W_n and their values are equal to, respectively:

$$0 \le W_p \le 1, \tag{2}$$

$$0 \le W_n \le 1. \tag{3}$$

Total damage W of a material:

$$0 \le W \le 1. \tag{4}$$

Damage increment:

$$\Delta W = dW_p + dW_n, \tag{5}$$

where

$$dW_n = dW_n\left(T, W_n, W_p\right), \ \ dW_p = dW_p\left(T, W_n, W_p\right). \tag{6}$$

Total damage increment:

$$\Delta W = \Delta W_n + \Delta W_p, \tag{7}$$

$$\Delta W_n = \Delta W_{nR} + \Delta W_{n\delta}, \tag{8}$$

$$\Delta W_p = \Delta W_{pR} + \Delta W_{p\delta}. \tag{9}$$

Here W_{nR}, $\Delta W_{n\delta}$ are the increments in grain-border damage, respectively, due to the viscoplastic deformation and as a result of changes in its conditions. ΔW_{pR}, $\Delta W_{p\delta}$ are the increments in the intragrain damage, respectively, due to deformation and as a result of change in the type of the stressed state and temperature.

Theoretical analysis reveals the low energy of propagation of intercrystalline cracks in materials, and the significant role of grain-border structure in the processes of their intragrain destruction [10, 11]. The large-angle boundaries are crucial for these processes while the special and low-angle boundaries exert a less impact. For the case of fragile inter-grain destruction, in the absence of deformation near the boundary, the energy of destruction is determined from ratio [12]:

$$\gamma = 2\gamma_s - \gamma_B, \tag{10}$$

where $2\gamma_s$ is the surface energy, γ_B is the free energy of a grain boundary, which depends on the grain-border structure.

The effect of the boundaries of grains of different types on the processes of deformation and destruction of polycrystals has not been fully studied [11]. This is largely due to the fact that existing models of grain boundaries do not take into consideration the structure, energy, and structural-phase state of the grain boundary zones [13].

3. The aim and objectives of the study

The aim of this study is to devise an approach based on the systemic model of structure in polycrystalline alloys, which would make it possible to predictively diagnose their behavior under conditions of contact loads.

To accomplish the aim, the following tasks have been set:

– to develop and substantiate the principles for constructing hierarchical models that describe the impact of parameters of the structure of different levels of hierarchy on the contact durability of alloys;

– to build a model of polycrystalline systems with interchangeable parameters of the grain structure and the structural-energy state of the internal interfaces of different levels of hierarchy;

– to assess the role of quantitative characteristics of the grain structure in the wear processes of steel 40X to incorporate them into the model;

– to investigate, based on the constructed model, the basic trends and their corresponding patterns in the influence of the structural and energy state of grains boundaries on the properties of polycrystalline alloys.

4. Using systemic approaches for developing hierarchical models of the polycrystal structure taking into consideration the dimensional characteristics of grains and the energy parameters of their boundaries

Methods of computational materials science for selecting technologies aimed at improving the reliability of mass-produced alloys, as well as creating new, with a higher set of properties, are used in a limited fashion at present and thus require the development of new approaches. Such approaches should include a set of metals- science, technological, and production aspects, as well as the quantitation of interconnections – the chemical composition of alloys – processing technology – structure – service properties – reliability.

The development of digital machine building, the improvement of reliability of articles require computerized simulation of the structure and properties of materials. To this end, the finite-element and quantum-chemical modeling are applied. A finite element method makes it possible to assess the behavior of materials using approaches from continuum mechanics. The quantum-chemical modeling considers interactions between atoms [14]. To establish a link between the macroscopic behavior of materials and changes in its inner structure, new approaches (hierarchical modelling) must be used that have not been fully developed up to now [15].

To quantify the impact of elements in the structure of different levels of hierarchy on the intragrain destruction of polycrystals, the work applied the toolkit from the theory of hypercomplex dynamic systems [16].

Systemic study of alloys was carried out in the following sequence:

– we built a model that adequately reflected the systemic properties of the alloy structure;

– based on an analysis of the system's common patterns, the system model's individual properties were established;

– we established empirical connections between the systemic properties that are characterized by the matrix definer, and the physical-mechanical properties of the alloy;

– we defined the value for a matrix parameter, which allows achieving the optimal physical-mechanical properties of the alloy;

– we defined the limits of change in the systemic properties of the alloy, which ensure obtaining the optimal matrix parameter.

In the general form, the operations that are carried out correspond to the following algorithmic chain:

$$(VD)_o \rightarrow S_o \rightarrow S \rightarrow P(S) \rightarrow Res \rightarrow V(D)_R. \tag{11}$$

In expression (11), the initial data for analyzing the microstructure of alloys are indicated as $(VD)_o$, and their conversion to the system-forming environment – S_o. The hyper-complex dynamic system S, processed by $P(S)$ methods, provides an opportunity to obtain a result Res, which is translated into the subject language of mechanics and materials science $V(D)_R$.

Incorporating specific characteristics for the parameters of the alloy microstructure into systemic invariants has made it possible to develop the invariant models of microstructures, which include their varied parameters.

To construct the invariant models, we used quantitative parameters of the grain structure [16]: histograms of grain distribution by size, the angles between grain boundaries that form triple joints, the areas of boundaries around grains of certain sizes.

The following order was used to build a hypercomplex matrix:

1. Based on the source grain distribution data on size, the alloys were assessed in terms of difference in their size; that was used to form the elements of the system.
2. We arranged and numbered a sequence of levels of hierarchy in the original system.
3. A square matrix was built in the form of a table whose size was determined by the number of groups of grains that characterize the steels' grain differences.
4. Information about the system was incorporated in the matrix.

Along the main diagonal of the matrix, we indicated the characteristic of grain in a group of grains of a certain size. To the left and right of the main diagonal, we gave information about the interaction between individual groups of grains. Such information is the area of boundaries between grains of different sizes and the distance between unbalanced joints, which was determined from studying the structures [16]. In a general case, the matrix that describes the state of the system was denoted through Y.

The representation of the systemic model of the polycrystal structure in the form of a matrix is shown in Fig. 1.

$$Y = \begin{vmatrix} A_1 & Y_{12} \\ Y_{21} & A_2 \end{vmatrix}$$

Fig. 1. Matrix representation of the systemic model of a material's structure

"A" letter with the corresponding indices indicates the following elements: A_1, A_2 – areas of boundaries around the grains corresponding to the first and second groups of size. Interactions between the elements include the following characteristics: Y_{12} – area of boundaries between the grains of the first and second groups of size; Y_{21} – area of grains boundaries between unbalanced triple joints.

5. Methods for studying the structural-energy state of grains boundaries in terms of contact durability of steel 40X

We studied steel 40X after improvement to determine the impact of the structural-energy state of the internal interface boundaries in the processes of destruction at contact interaction. Steel of this brand is widely used in the manufacture of parts that operate under conditions of contact interaction (gears, shafts of transmissions, toothings).

A change in the state of grains boundaries was induced by thermal treatment – hardening at different temperatures. The samples were made from rolled steel; after annealing, they were hardened at temperatures in the range of 860 °C...1,050 °C and tempered at 600 °C.

Studying the boundaries of grains was conducted following the ion-plasma etching [17]. The structural-energy state of the grain interface boundaries was assessed according to procedure from [18]. When determining relative energy of the boundaries at the triple joints of grains, we used Herring-Young analytical dependence.

Analysis of the structural-energy state of grain boundaries in steels λ was carried out by a metal-graphic method based on determining a ratio between angles at triple joints of grains using the following analytical dependence:

$$\frac{\lambda_1}{\sin\alpha_1} = \frac{\lambda_2}{\sin\alpha_2} = \frac{\lambda_3}{\sin\alpha_3}. \qquad (12)$$

A quantitative assessment of the effect of different-in-quality parameters of the steel 40X microstructure on contact durability was carried out using the developed methodology of hierarchical modeling [16].

The effect of the state of grain boundaries on the accumulation of damage at contact interaction was studied during testing for wear using a disk-pad scheme under a dry sliding friction mode. The speed of sample sliding along a counter-body is V=0.5 m/s, the load on samples is P=300 N, material of the counter-body is steel 45, hardness of the counter-body is 42...44 HRC. Following the alignment, each sample was worn for 10 hours. The mass intensity of wear I_m was assessed based on the results from testing six samples.

6. Results of studying the effect of parameters of grain structure on the contact durability of steel 40X

The microstructure of steel 40X is shown in Fig. 2; parameters of the distribution of the microstructure based on grain size are shown on Fig. 3.

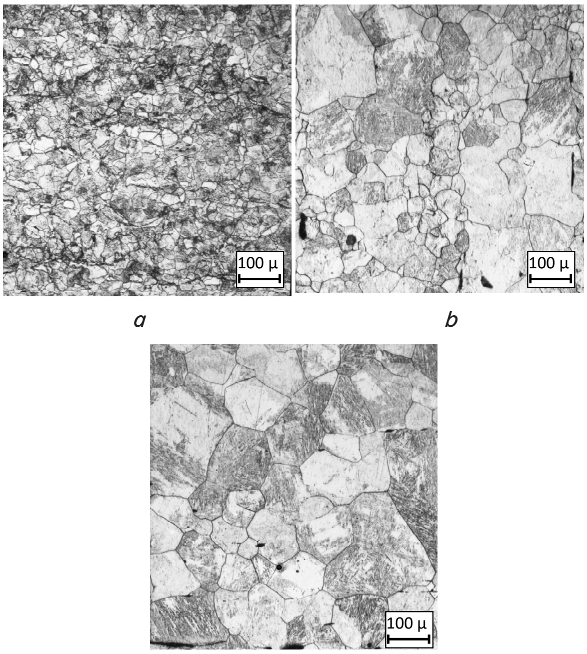

Fig. 2. Microstructure of steel 40X after hardening at temperatures: *a* – 860 °C; *b* – 950 °C; *c* –1,050 °C (exposure to hardening – 30 minutes)

After heating up to 860 °C, 30 minutes of aging, and rapid cooling of steel 40X, we observed grains the size of 21.5 μm (Fig. 3). Heating up to 950 °C results in the emergence of grains with dimensions between 20 μm and 210 μm. The average diameter of the grains is 52.4 μm; the standard deviation is 36.5 μm. After aging at 1,050 °C, grains the size of 35...270 μm form in the steel. Their mean diameter is 102.0 μm; and the standard deviation is 50.5 μm. The quantitative estimate of grain size difference by $\left(D_{\max}/\bar{D}\right)$ indicator revealed its value after heating to 860 °C – 2.79; 950 °C – 3.81; 1,050 °C – 2.94; indicating the structure's grain size difference after tempering at 950 °C.

Results from determining angles at the triple joints of grains in steel 40X after hardening at temperatures of 860 °C, 950 °C, and 1,050 °C are shown in Fig. 4.

The assessment of boundaries' energy at the triple joints of grains showed its growth at the boundaries located opposite sharp angles and the decrease at the boundaries, which are located opposite the blunt angles. At each junction, the ratio between boundary energies changes, which affects their behavior when external loads are applied.

The greatest relative energy value is observed at the boundaries, which are placed at triple joints opposite the angles of 80...100°. It was established that after hardening at 860 °C the number of such boundaries is 10.0 %, at 950 °C – 12.12 %, and after 1,050 °C – 9.09 %. The grain size difference that forms when heated to 950 °C increases the proportion of grains with a greater energy magnitude (Table 1).

Our study of microstructure after tempering at 600 °C has shown that the size of the former austenite grain did not change significantly, but the boundaries of grains are detected worse after etching (Fig. 5).

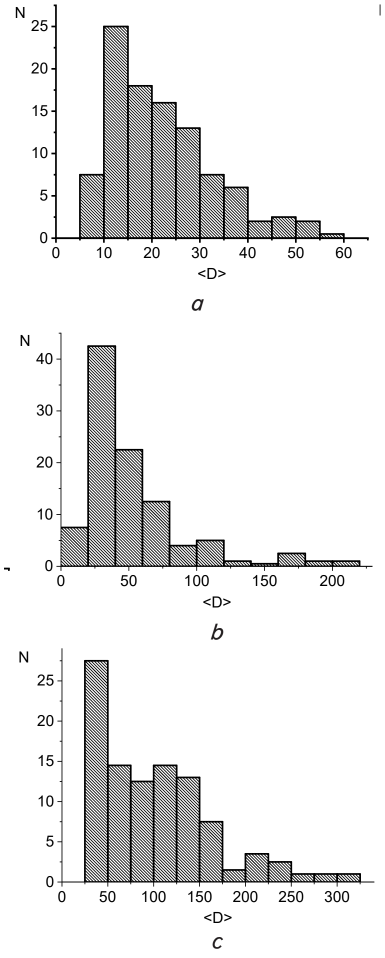

Fig. 3. The distribution, based on size of mean diameters (<*D*>, μm), of grains of former austenite in steel 40X after hardening at temperatures: *a* – 860 °C; *b* – 950 °C; *c* – 1,050 °C (exposure to hardening –30 min)

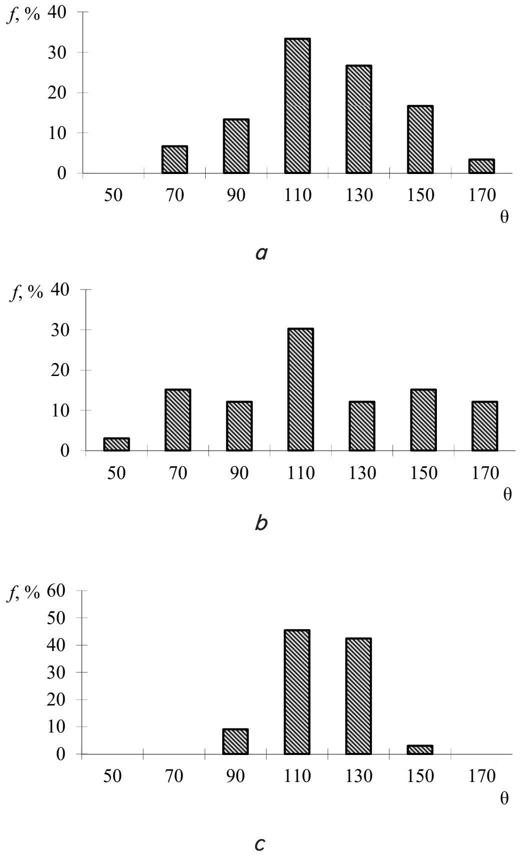

Fig. 4. The histograms of distribution of flat angles between boundaries of the former austenite grains at triple joints of steel 40X after hardening at temperatures: *a* – 860 °C; *b* – 950 °C, *c* – 1,050 °C (exposure to hardening – 30 min)

Results from studying angles between the boundaries at the triple joints of grains in steel 40X after hardening at temperatures of 860 °C, 900 °C, 950 °C, 1,050 °C and tempering at 600 °C are shown in Fig. 6.

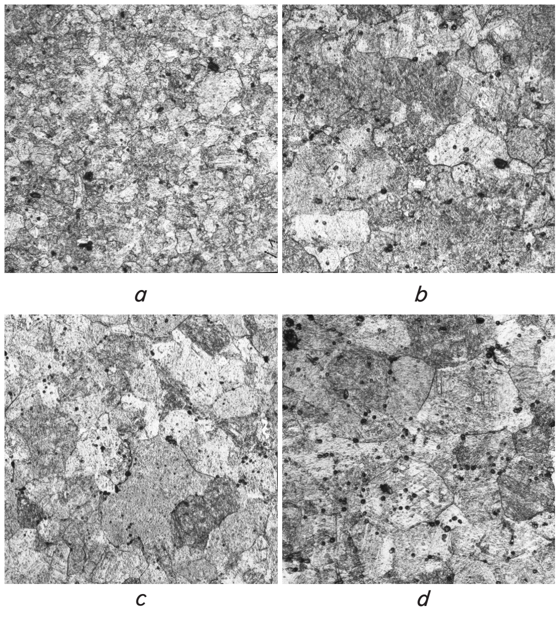

Fig. 5. The microstructure of steel 40X, tempered at 600 °C, hardened at temperatures: *a* – 860 °C; *b* – 900 °C, *c* – 950 °C, *d* – 1,050 °C (exposure to hardening – 30 min), x200

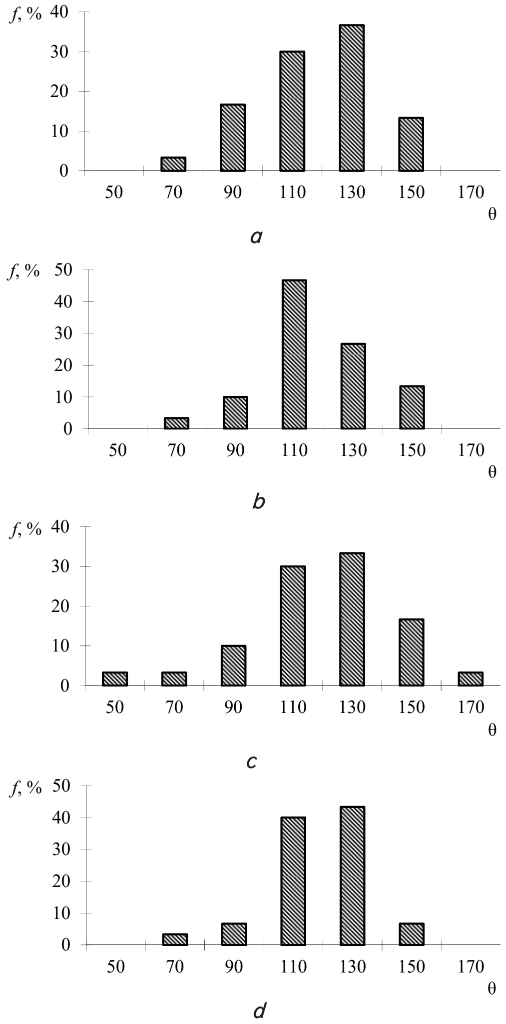

Fig. 6. The histograms of distribution of flat angles between boundaries of the former austenite grains at triple joints of steel 40X, hardened at temperatures: *a* – 860 °C, *b* – 900 °C, *c* – 950 °C, *d* – 1,050 °C (exposure to hardening – 30 min)

After heating up to 860 °C for hardening, the share of boundaries with the greatest amount of energy, located opposite angles of 80°...100°, is 16.67 %; 900 °C – 10.00 %; 950 °C – 10.00 %; 1,050 °C – 6.67 % (Table 2). The share of boundaries that are located opposite angles of 161°...180° and characterized by a minimum energy value equals, after hardening at 860 °C, 0 %; 900 °C – 0 %; 950 °C – 3.33 %; 1,050 °C – 0 %. The microstructure's grain size difference, which is detected at heating up to 950°C, contributes to the formation of boundaries that differ significantly in terms of energy.

Results from studying the microstructure of steel 40X after improvement when exposed to hardening for 80 minutes are shown in Fig. 7.

When heated to 860 °C, separate groups of former austenite grains with an average diameter of 38...43 μm and 79...81 μm were identified in the steel. Heating above 900 °C leads to the formation of grains the size of 45...55 μm and 100...110 μm; hardening at 950 °C results in the formation of groups of grains the size of 80...100 μm and 130...150 μm. The diameter of individual grains exceeds 180 μm. An increase in the hardening temperature to 1,050 °C leads to the emergence of groups of grains with a diameter of 85...90 μm and 150...170 μm.

Results from studying the distribution of angles at triple joints between the boundaries of grains are shown in Fig. 8.

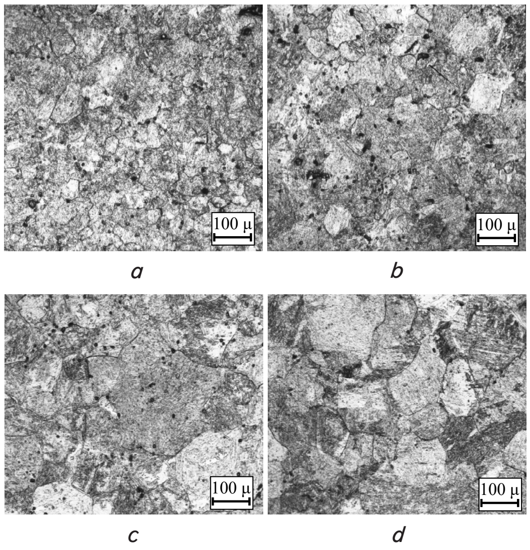

Fig. 7. The microstructures of steel 40X, tempered at 600 °C, hardened at temperatures: *a* – 860 °C, *b* – 900 °C, *c* – 950 °C, *d* – 1,050 °C (exposure to hardening – 80 min)

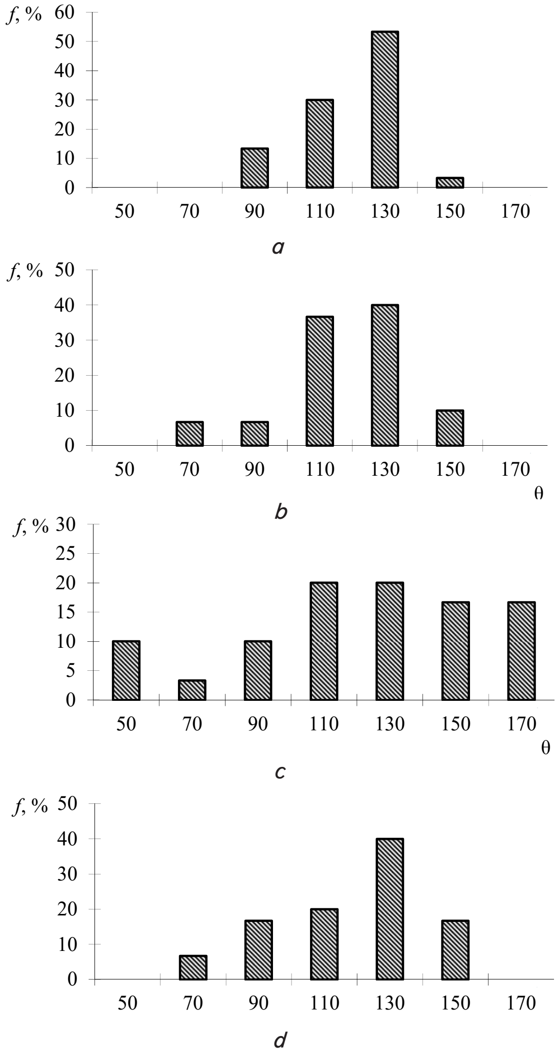

Fig. 8. The histograms of distribution of flat angles between boundaries of the former austenite grains at the triple joints of steel 40X, tempered at 600 °C, hardened at temperatures: *a* – 860 °C; *b* – 900 °C; *c* – 950 °C; *d* – 1,050 °C (exposure to hardening – 80 min)

Increasing the aging time during hardening at 860 °C to 80 minutes leads to the emergence of grains boundaries with a higher energy magnitude, to 13.33 %. After hardening at 900 °C, the share of such boundaries is 6.67 %; 950 °C – 10.0 %; 1,050 °C –16.67 % (Table 3). At the same time, the proportion of grain boundaries with a minimum amount of energy changes significantly; they are located opposite angles of 161°...180°. Thus, after hardening at 860 °C, it is 0 %; 900 °C – 0 %; 950 °C – 16.67 %; 1,050 °C – 0 %. Increasing the aging time at hardening to 80 minutes leads to an increase in the proportion of triple joints, which are formed by the boundaries of grains with a significant difference in the level of grain-border energy.

Results from studying wear are given in Table 4.

When exposed to hardening over 30 minutes with a temperature rise to 950 °C the wear intensity increases by 16 % and, after hardening at 1,050 °C, reduces by 20 %. Increasing the exposure to hardening to 80 minutes leads to an increase in the intensity of steel wear, and to a greater extent after hardening at 950 °C. It should be noted that in this case the wear is 46 % larger compared to samples hardened at 860 °C at exposure over 30 minutes.

Table 1

The proportion of angles between boundaries at the triple joints of grains in steel 40X after hardening

Exposure to hardening – 30 minutes							
Hardening temperature, °C	Share in the total number of measured angles, %						
	40...60°	61...80°	81...100°	101...120°	121...140°	141...160°	161...180°
860°	0.00	6.67	10.00	33.33	33.33	13.33	3.33
950°	3.03	15.15	12.12	30.30	12.12	15.15	12.12
1,050°	0.00	0.00	9.09	45.45	42.42	3.03	0.00

Table 2

The proportion of angles between boundaries at the triple joints of grains in steel 40X after hardening and tempering at 600 °C

Exposure to hardening – 30 minutes							
Hardening temperature, °C	Share in the total number of measured angles, %						
	40...60°	61...80°	81...100°	101...120°	121...140°	141...160°	161...180°
860°	0.00	3.33	16.67	30.00	36.67	13.33	0.00
900°	0.00	3.33	10.00	46.67	26.67	13.33	0.00
950°	3.33	3.33	10.00	30.00	33.33	16.67	3.33
1,050°	0.00	3.33	6.67	40.00	43.33	6.67	0.00

Table 3

The proportion of angles between boundaries at the triple joints of grains in steel 40X after hardening and tempering at 600 °C

Exposure to hardening – 80 minutes							
Hardening temperature, °C	Share in the total number of measured angles, %						
	40...60°	61...80°	81...100°	101...120°	121...140°	141...160°	161...180°
860°	0.00	0.00	13.33	30.00	53.33	3.33	0.00
900°	0.00	6.67	6.67	36.67	40.00	10.00	0.00
950°	10.00	3.33	10.00	20.00	20.00	16.67	16.67
1,050°	0.00	6.67	16.67	20.00	40.00	16.67	0.00

Table 4

Dependence of mass wear intensity I_m on the temperature-time conditions for hardening the improved steel 40X

Hardening temperature t, °C	Exposure to hardening at t °C, min	$I_m \cdot 10^{-8}$	I_m/I_{mb}, %	$I_{m80\min}/I_{m30\min}$, %
860	30	3.719	100	121
	80	4.500	121	
900	30	3.905	105	127
	80	4.946	133	
950	30	4.314	116	126
	80	5.430	146	
1,050	30	3.012	80	122
	80	3,682	98	

Note: I_{mb} stands for the mass wear intensity of a sample hardened at 860 °C exposed to hardening for 30 minutes

The increase in a hardening temperature to 950 °C leads to an increase in the number of triple joints in the steel, which are formed by boundaries with significant differences in the magnitude of grain-border energy.

Thus, after hardening at 950 °C and exposure over 30 minutes the share of such joints is 3.33 %, and after heating for hardening for 80 minutes – 16.67 % (Table 2, 3). After hardening at 1,050 °C, the joints, formed by boundaries with large differences in energy, are absent both after aging when heated for 30 minutes (Table 2) and 80 minutes (Table 3). The increased steel durability after hardening at 1,050 °C is largely due to a decrease in the number of local volumes of structure with a high gradient of grain-border energy.

7. Assessing the impact of the structural-energy state of large-angle grain boundaries on the contact durability of steel 40X using the developed model

The stages of damage formation under the action of cyclical loads include the formation of microstructurally- and physically short cracks, as well as long cracks [20]. Under conditions of changing contact loads, these stages are implemented at frictional interactions. Intergrain damage under external loads would mainly occur in local areas whose energy is close to the surface energy. Such zones are the boundaries located between triple joints with the presence of sharp and blunt angles. Therefore, the area of such boundaries was introduced to the hierarchical models that describe the effect of the polycrystalline structure on the contact longevity of steel. Results from determining a matrix parameter for the structure of the improved steel 40X after hardening at different temperatures are given in Table 5 and shown in Fig. 9.

Table 5

Quantitative characteristics of the microstructure and the value for a matrix parameter of steel 40X after hardening at temperatures 860 °C...1,050 °C and tempering at 600 °C

Hardening temperature, °C	Exposure time to hardening at temperature	Area of grain boundaries, cm^{-1}	Share of triple grain joints with angles between boundaries of 161...180°, %	Value for matrix parameter Y, cm^{-2}
860	30	1,697.5	–	720,376
	80	926.2	–	214,452
900	30	795.2	–	158,096
	80	516.7	–	66,736
950	30	647.2	3.33	82,480
	80	371.4	16.67	27,851
1,050	30	347.6	–	30,206
	80	292.9	–	21,440

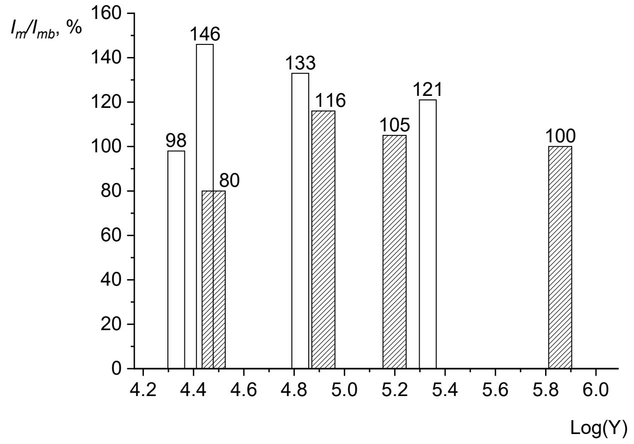

Fig. 9. Dependence of relative wear (I_m / I_{mb}) on the matrix parameter for structure (Y). I_m stands for the mass wear intensity after hardening at 860°, exposure – 30 minutes, and tempering at 600 °C: ▨ – exposure to hardening – 30 minutes; ☐ – exposure to hardening – 80 minutes

8. Discussion of results of improving the contact durability of polycrystalline systems

Analysis of the results obtained has shown that the quantitative characteristics of the structure, which are described by a matrix parameter, significantly affect the relative wear of steel. The increase in wear occurs after hardening at 950 °C in the presence of joints in the steel structure that are formed by boundaries whose energy is significantly different. Such joints, with a high gradient of grain-border energy, are formed by the boundaries of grains, the angles between which are in the range of 40°...60° to 161°...180° (Table 5), and their existence is due to the presence of grain size difference. With an increase in the size of the grain under exposure to hardening over 80 minutes the relative wear in the presence of grain size difference increases by 46 % due to the increase in the number of gradient joints and a larger area of boundaries, with an elevated energy level.

This points to the crucial role of the large-angle boundaries placed between triple joints with a high energy gradient in the process of forming the microstructurally-short cracks and the intergrain destruction of polycrystalline systems.

The structure of the large-angle boundary of a grain and the border zone is gradient and includes areas with the enhanced density of dislocations, pores, structural and concentration heterogeneities, as well as area of transition to the neighboring grain. The main factor that determines the behavior of a polycrystal is the excess volume or a void-rough structure of the boundaries.

When a critical value of free volume is reached at the interface, pores and microcracks form. Intragrain destruction occurs due to the concentration of stresses, which is caused by grain-border slippage on ledges, protrusions, and triple grain joints.

Triple joints are characterized by a "looser" structure and the increased specific energy parameters. Their contribution to the processes of unbuilding and destruction of materials is greater than that from the usual boundaries of polycrystals grains.

If, at joints, angles between the boundaries differ significantly from 120°, the boundaries vary in energy magnitude. As a result, a property gradient appears in the junction area, which could be a source of destruction.

Under contact loads, the scattered or non-localized damage emerges in steel, which give rise to microscopic cracks. When they develop, one crack propagates faster that leads to a localized fatigue damage.

Our study has shown that the average distance between triple joints with an increased gradient in steel after hardening at 860 °C and tempering is 0.01...0.02 mm and corresponds to the size of cracks in the transition from scattered to localized damage. The energy level of grains boundaries between such joints is higher than that for other boundaries and approached the surface energy. Therefore, such boundaries are the places where scattered damage is initiated.

The number of triple joints with a high energy gradient in the steel hardened at 950 °C will be greater than after hardening at 860 °C.

As a result, following the hardening at high temperature, there increases the number and size of cracks, which are formed under the influence of external loads, thereby accelerating the stage of development of localized damage.

After hardening at 1,050 °C and tempering, steel does not demonstrate the formation of triple joints with a high energy gradient, which is one of the factors to improve resistance to wear.

The developed approaches of hierarchical modeling make it possible to determine the physically justified parameters of change in the local properties at grain-border areas of alloys, to assess susceptibility to forming intragrain damage. Energy characteristics of the large-angle grains boundaries significantly affect the stages of formation of the scattered and localized damage to steel under contact loads. Control over energy parameters of grains boundaries makes it possible to use innovative technologies to form the structure of parts in order to improve their durability and resource while reducing the cost of their life cycle.

The main limiting factor, which has a significant impact on implementing the procedures, devised in this work, into engineering practice, is the laborious procedure for determining energy characteristics of the large-angle boundaries of grains. The use of hierarchical and computer simulations of polycrystalline systems, taking into consideration their structure, requires the development of appropriate software.

9. Conclusions

1. Based on systemic approaches, a hierarchical model of the structure of polycrystalline alloys has been developed, which describes their different qualitative characteristics – the presence of grains of different sizes, boundaries and triple joints of grains, whose energies are essentially different. The use of such models makes it possible to analyze the accumulation of intragrain damage, identify the structural units responsible for the destruction of a material, establish quantitative links between the energy state of local volumes of parts and the parameters of their life cycle.

2. An invariant model of polycrystalline systems with interchangeable parameters of grain structure and structural-energy state of internal interface boundaries has been built. It is shown that it is advisable to use, as a digital counterpart of the alloy structure, which describes their behavior under conditions of contact loads, a matrix representation of the systemic model incorporating it with the structure's quantitative characteristics.

3. It has been established that the life cycle of parts, made from steel 40X after hardening and high tempering, under conditions of contact loads is largely dependent on the energy state of boundaries of the structural components' grains. The presence of large-angle boundaries at triple joints, which differ significantly in terms of energy magnitude, reduces the life cycle duration.

4. It is shown that the increase in the life cycle of parts is achieved by reducing the amount of local volumes with an increased energy level in the alloy. Large-angle boundaries with a minimum gradient of grain-border energy are formed under conditions of optimal temperature-time thermal treatment regimes. The use of methods of hierarchical modeling and computational materials science makes it possible to implement technical solutions in order to improve the operational reliability of articles at a lower cost of their life cycle.

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