

Improving the energy efficiency of operation of elements of the structures of the rolling stock by means of surface engineering.

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Abstract. The manufacture of rolling stock components with a given life cycle based on the computerization of all design and production stages is the most promising way to increase the energy efficiency of its operation. The implementation of this approach requires the expansion of the use of technologies that provide parts with a high level of mechanical and operational properties. The state of the surface layers is important in the formation of the reliability parameters of high-loaded parts. The principles of using system approaches for the physical justification of the choice of the optimal modes of engineering grain boundaries depending on the operating conditions of products are presented. New approaches and algorithms have been created that allow quantitative and qualitative studies of the effect of technological treatments and the chemical composition of polycrystals on the strength of grain boundaries and the processes of softening of the boundary zones. Using the developed techniques, the ways to control the energy state of the internal interfaces by doping, microalloying and heat treatment were determined to increase the resistance to brittle fracture and wear of the steels used in the manufacture and repair of rolling stock.

1. Introduction

The operation of rolling stock with a given life cycle can significantly reduce the energy consumption of railways during transportation. The creation of such vehicles is possible based on the use of multifunctional computer systems at all stages of design, production and operation, consistently perform volumetric product design, design justification for its reliability and efficiency, the preparation of technological processes of manufacturing and engineering project management.

Computer engineering analysis programs make it possible to formulate new approaches to the choice of materials and optimize their processing technologies to improve product durability on the basis of a design basis.

Preparation of technological processes for obtaining products should include information on the parameters of the properties and behavior of materials during treatments and operating loads, making the creation of databases of computer modeling of the structure and properties of materials important. Solving these problems allows using the methods of computational materials science in digital engineering for the simultaneous design of materials and products with high reliability parameters. It should be noted that the

development and use of such programs is limited by the lack of simultaneously established relationships between the damage resulting from technological processing, its development during the operation of products and the stages of the life cycle of parts and machines. Therefore, research in this direction are relevant.

The reliability indicators of the rolling stock largely depend on the nature of the contact of the mating parts or their interaction with liquid, gas and other media. The quality of the outer layers of parts significantly affects their weariness, strength, and corrosion resistance, which makes it necessary to form them with the given parameters of properties by the methods of surface engineering. When operating loads on the surfaces there are flows of defects that contribute to the development of damage.

Sources of defects are the boundaries and triple joints of the grains facing the surface of the parts [1, 2, 3]. With a further increase in voltage sources are activated away from the surface. Surface plastically deformed grains are stress concentrators that contribute to the deformation of neighboring grains [4, 5]. Near the boundaries and joints of the grains, a higher concentration of stresses occurs than for dislocations and their clusters [4].

A slight increase in local stresses in the zones near the grain boundaries contributes to the initiation of

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plastic shears due to the difference in the elastic moduli of the contacting grains. Landslides occur on the interfaces, where there are dangling interatomic bonds, which can spread deep into the material.

Strengthening a thin surface layer of the material by creating functional gradient structures by surface engineering methods delays the localization of the deformation and significantly improves the macromechanical characteristics of the parts. At the same time, durability growth is achieved due to changes in the stress-strain state in the local areas of parts, allows to effectively manage surface defects, the development of softening and destructive material processes, but requires an analysis of the role of grain boundary parameters and, in particular, their structural-energy state in the destruction processes.

In this regard, the use of new approaches to modeling and analyzing the mechanical behavior of internal boundary zones becomes important. The development of such approaches allows the scientific substantiation of technological solutions to increase the resistance to the formation of blight damages and cracks in parts of the rolling stock operating under conditions of intensive loads.

2. The object of study

The object of the study is the internal interface of the steel used in the manufacture of rolling stock, and their role in the formation of damage and intercrystalline destruction of alloys under the action of power loads, depending on the structural and energy state of the internal interfaces. The choice of the object of research is connected with the need to substantiate the methods of managing the structure to eliminate the intercrystallite destruction of low energy intensity of structural steels.

When exposed to alternating loads in the details of railway structures, scattering or non-localized damage is formed [6]. As a result of structural inhomogeneity of materials, plastic deformation zones are randomly distributed, in which microscopic cracks originate. In the case of the development of such cracks, one of them spreads faster, which leads to destruction. The formation and growth of the main fatigue crack is called the stage of localized fatigue damage.

Scattering damage significantly affect the rate of development of the main crack. In a material with a large number of microscopic cracks of the appropriate size, a trunk crack develops faster, absorbing small cracks during its development.

Conventionally, the stage of formation of damage when exposed to cyclic loads is divided into the formation of microstructure and physically short cracks and long cracks. Microstructures of short cracks are characterized by discontinuities, the dimensions of which are of the same order as the structural elements. For the transition from the microstructure of short cracks in physically short cracks take the transition from shear cracks to separation cracks. When a region of elastic-plastic deformations forms at the tip of a crack, a short crack transforms into a long crack [7, 8].

It should be noted that the structure of the material significantly affects the formation of scattered damage, but this relationship has not been fully detected, due to the complex multi-level structure of the alloys. To take into account the peculiarities of their behavior when exposed to external loads, the following hierarchical levels of material consideration are used:

1. Macro level. At this level, the material is considered as a continuous continual medium with properties whose parameters vary slightly in space. The typical size of a piece of material is commensurate with the entire product.

2. Meso level. The material is considered as a discrete-continuous medium. The level of consideration of this scale corresponds to the structural components and their boundaries.

3. Micro level. The level of consideration of lattice defects inside the crystallite.

4. Nano level. Consideration of the material corresponds to individual atoms (or their groups). At this level, a discrete model description is predominantly used.

Simultaneous model and computational consideration of all levels of material is a complex scientific problem, and therefore is currently used mainly in the theoretical direction [9].

In applied research, only one of the hierarchical levels is considered using the results obtained from analyzing the behavior of the material at other large-scale levels.

Of great importance is the need to determine the relative contribution of individual levels of the structural hierarchy in models of material behavior under external load [10, 11]. Such an analysis becomes possible on the basis of computer models of calculations, to ensure their reliability, they are supplemented by experimental data [12].

Computer simulation of materials and technologies for their processing includes the following steps: formulation of a physical model, mathematical modeling (development of a system of equations), generation of a computational grid, selection of programming algorithms, numerical solution, presentation of computational results.

At the present stage of development of computational materials science for computer modeling, the methods of molecular dynamics, finite element and hierarchical modeling are used. Molecular dynamics models the interaction of particles and examines phenomena at the nano level. The method of finite element modeling refers to the macro level and evaluates the behavior of the material by the methods of continuum mechanics. Between these scale levels there should be methods that have to bind nano-and macroscale models of material behavior. These are hierarchical models that are currently only at the beginning of their development [13]. To predict changes in properties in local volumes of materials, depending on the technological characteristics of their production, methods for parametric modeling of the microstructure begin to develop.

It should be noted that there are currently no databases on the properties of materials that determine their reliability with regard to technological processing processes, which is an unsolved problem in computer science.

3. The purpose and objectives of the study

The aim of the work is to create models and methods for controlling the reliability parameters of the steels used in the manufacture of rolling stock, by optimizing the structural-energy state of the interfaces between the grains of the structural components.

To achieve this goal, the following tasks were formulated:

1. To conduct a study of the influence of the structural-energy state of the interfaces between the grains of the structural components on the reliability parameters of the grinding steel.

2. To build a multilevel model of polycrystalline systems with variable parameters of the grain structure and the structural-energy state of the interfaces between the grains of the structural components and their influence on the performance properties of the alloys.

3. On the basis of the obtained experimental results and the constructed model, explore the main trends and the corresponding laws of the influence of the structural and energy state of internal interfaces on the properties of structural steels, conduct a scientific substantiation of technological solutions for the formation of a microstructure that provides for the output of polycrystalline systems from the area of operational instability.

4. Research existing solutions to the problem

In the materials of parts during the operation of railway structures in the conditions of the action of power loads there is an accumulation of damage. To assess the residual life of parts, it is important to establish the patterns of their formation, as well as the conditions for the transition from scattered to localized damage. In particular, the size of structurally and physically short cracks, as well as exploitation to the formation of a main crack.

The study of the formation of localized damage is carried out by methods of fracture mechanics. The structure of the material of the products has a significant impact on the stages of the formation of scattered damages. In this connection, for their research, they use the approaches of physical materials science, locally gradient mechanics of a deformable solid body, and also linear and nonlinear fracture mechanics. The multi-level structure of metals and alloys and the complexity of the processes influencing the formation of scattered damage require the use of new approaches associated with the development of computer materials science.

Structural features of metals and alloys have a significant impact on the value of their endurance limit. It is determined by the shape, size of the structural components, the presence of defects, and factors determining the intensity of this effect. Criteria for fracture mechanics allow describing the effect of defects on the fatigue fracture resistance of alloys, but they require determining their priority and size.

The use of fracture mechanics criteria is effective for those alloys for which the fundamental laws of the structure bonds and fracture resistance characteristics are established.

The heterogeneity of the structure of the alloys, the size, shape of the structural components, the difference in the modules of their elasticity, the particular stress state of the local metal volumes specify the conditions for the initiation of microscopic cracks and the transition from diffuse to localized damage at stresses exceeding the fatigue limits. Microscopically short cracks during the action of alternating loads arising at stresses lower than the fatigue limit, that is, the possibility of their formation under the operational loads of the railway structure.

Studies aimed at establishing the structural units that are responsible for the formation of scattered steel damages in similar chemical composition to those used in the manufacture of rolling stock, showed the correspondence of the sizes of microstructural short cracks to ferritic and perlite grains [7]. It is shown that the size of the cracks in the transition from scattered to localized damage with bagatocycle fatigue is 0.01..0.02 mm. The influence of the material state of the boundary zones of the grains, the possibility of formation of damages and defects in them depending on the endurance limit on the grain size has been revealed [8]. At the same time, the correspondence of the size of such cracks in alloys to the size of the elements of their structure has not been unequivocally established.

The principles of determining structural parameters for various alloys that are responsible for the formation of short cracks are not fully substantiated.

5. Research methods

Modern methods of controlling the properties of polycrystalline alloys with minimal resources include technology based on the concepts of grain boundary engineering and the principle of grain-boundary structure design. Its main provisions include the selection of such technological modes of processing materials, ensuring the formation in them of the maximum proportion of grain boundaries (special boundaries), characterized by the minimum value of grain boundary energy [14]. Such boundaries are characterized by high fracture resistance due to the easy transfer of slip from one grain to another.

The widespread use of such approaches is hampered by the insufficient knowledge of the influence of the energy characteristics of grain boundaries of different levels of the hierarchy on the behavior of alloys under the influence of force loads. In this connection, the study of the structure of grain boundaries in alloys of various

doping systems and the determination of the influence of their energy characteristics on the formation of grain-boundary damage and on the secondary grains of polycrystals becomes important.

In the details of railway transport, made from pre-steel grades, the grain size of austenite can vary widely, and in many cases grain is formed. The presence of crystals with different characteristics leads to the formation of grain boundaries that differ in structural and energetic state.

Studies were conducted on steel 40XHM (C – 0.40%, Si – 0.24%, Mn – 0.61%, Cr – 0.58%, Ni – 0.99%, Mo – 0.18%; international analog 8640 according to ASTM-SAE) industrial smelting. Billets were made of rolled products, which were annealed at a temperature of 840°C...870°C and subjected to quenching after heating in a salt bath from temperatures of 870°C... 1180°C. Then, tempering was done at a temperature of 600°C.

To study the state of grain boundaries with minimal changes in the structure, ion-plasma etching was used at the VUP-4 vacuum post [15]. During digestion, grooves were formed on the surface of the samples, which define the boundaries of the grains and phases. The depth and angle at the top of the digestive streams were determined experimentally using a Linnik interferometer (MII-4).

The analysis of the structural-energy state of the grain boundaries was performed using the metallographic estimation technique proposed in [16, 17]. To identify the relative change in the energy of the grain boundaries, the property of triple junctions was used, which consists in the formation of an equilibrium configuration of the boundaries at the place of their meeting. That is, the ratio of the surface energy of the tension of the grain boundaries λ and the angles α opposite to them is described by the analytical dependence of Hering – Young relationship [17].

6. Research results.

Analysis of the microstructure of steel 40XHM showed the formation of austenite grains when heated to a temperature of 860°C with an exposure time of 30 minutes, whose dimensions are in the range from 2 μm to 70 μm . The average grain diameter is 11.4 microns (Fig. 1, Fig. 2).

Heating to a temperature of 950°C leads to an increase in the average grain diameter of austenite, which is equal to 77.2 microns. The grain size is in the range from 20 μm to 220 μm , and the standard deviation is 44.2 μm (Fig. 1, Fig. 2).

After quenching from a temperature of 1050°C, the size of the former austenitic grains is in the range from 20 μm to 270 μm . Their average diameter is 98.7 microns, and the quadratic deviation is 52.0 microns (Fig. 1, Fig. 2).

When heated to a temperature of 1180 °C, austenite grains with an average diameter of 328 μm are formed, and grains 800 μm in size also appear (Fig. 1, Fig. 2).

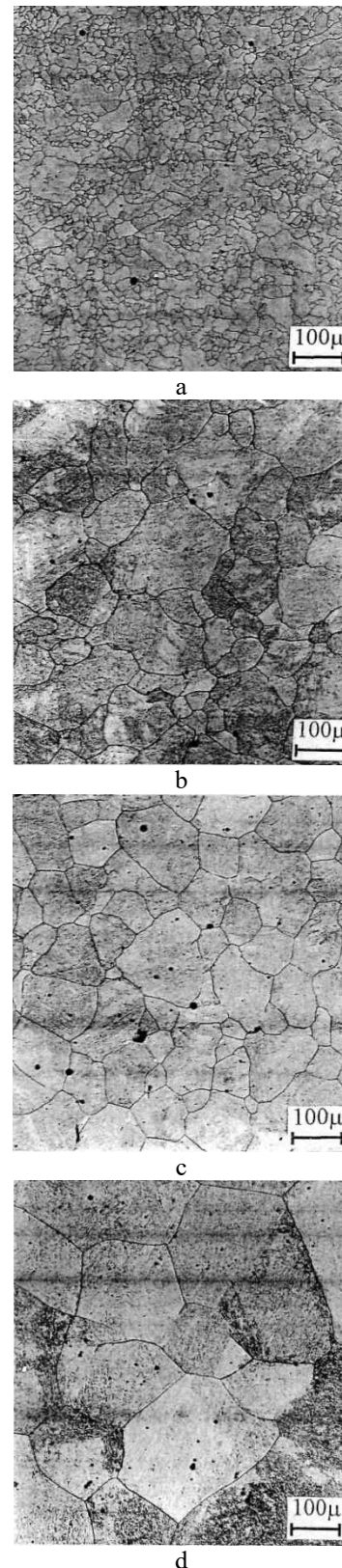


Fig. 1. Microstructures of steel 40XHM after quenching from temperatures of 860°C (a), 950°C (b), 1050°C (c) and 1180°C (d), quenching for 30 minutes.

The analysis of the grain roughness of steel after quenching from various temperatures showed that the quantitative indicator of grain roughness (D_{max} / D) after quenching from 860°C is equal to 4.72, 950°C - 2.91,

1050°C - 2.78, 1180°C - 4.57. That is, the grain-graininess is characteristic of steel after quenching from temperatures of 860°C and 1180°C.

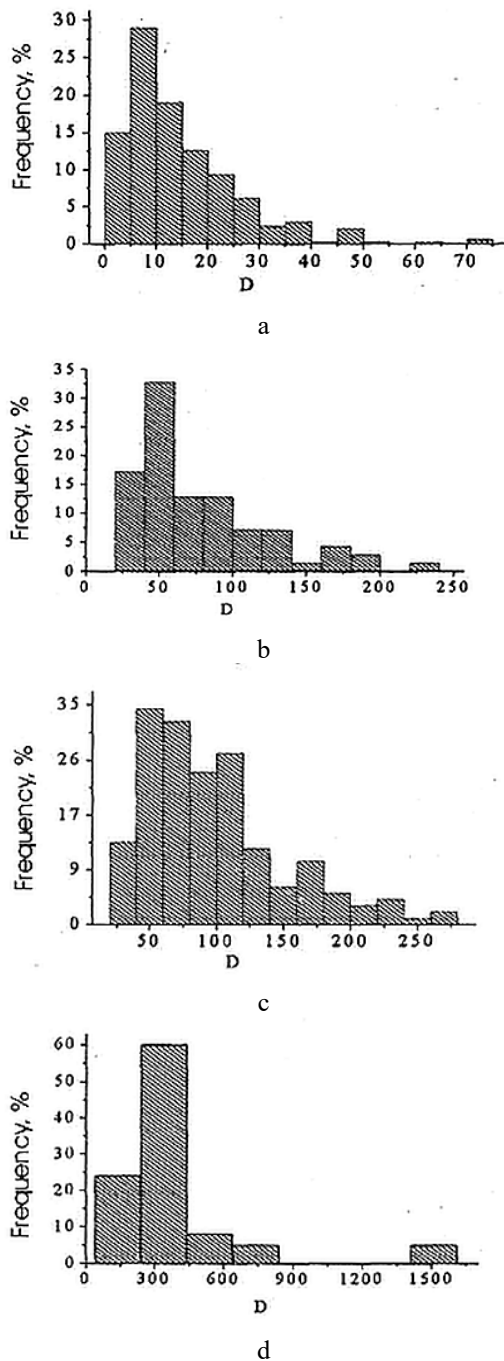


Fig. 2. The distribution of average diameters (D, μm) of austenite grains (a, b, c, d) in size in steel 40XHM after quenching from 860°C (a), 950°C (b), 1050°C (c), 1180°C (d), quench aging 30 min.

The results of determining the angles in the triple joints of the grains of steel 40XHM after quenching from 860°C, 950°C, 1050°C and 1180°C with an exposure time of 30 min are presented in Fig. 3.

An analysis of the relationship between the energy of the grain boundaries and the angles between them in the triple junctions showed their dependence on the grain size and grain size.

The proportion of grain boundaries, which are located opposite 80°...100° angles and are characterized by a higher relative energy value, is 10.0% for steel hardened from 860°C, 950°C - 16.67%, 1050°C - 10.0%, 1180°C - 16.67%. Most of the boundaries with a high value of grain-boundary energy after quenching from 860°C and 1180°C are in correlation with the results of a quantitative assessment of the roughness of steel.

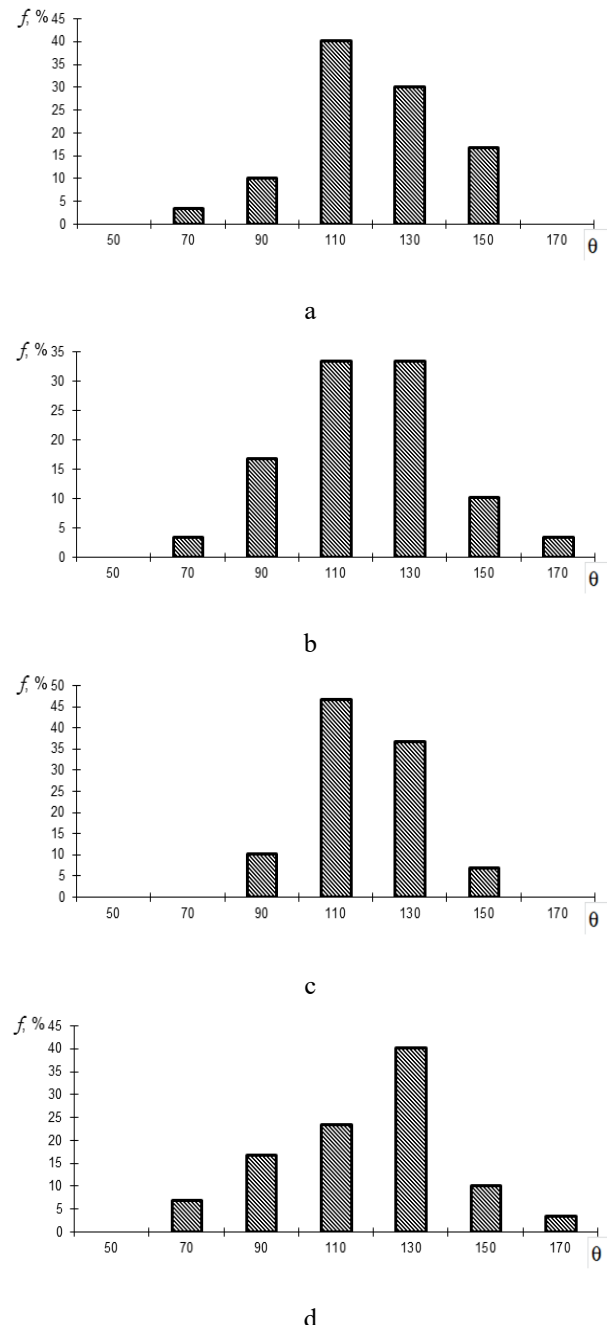


Fig. 3. Histograms of the distribution of flat angles between the boundaries of the former austenitic grains in steel 40XHM after quenching from temperatures of 860°C (a), 950°C (b), 1050°C (c), 1180°C (d), aging for hardening 30 min.

The results of the study of steel after quenching and tempering at 600 °C are shown in fig. 4.

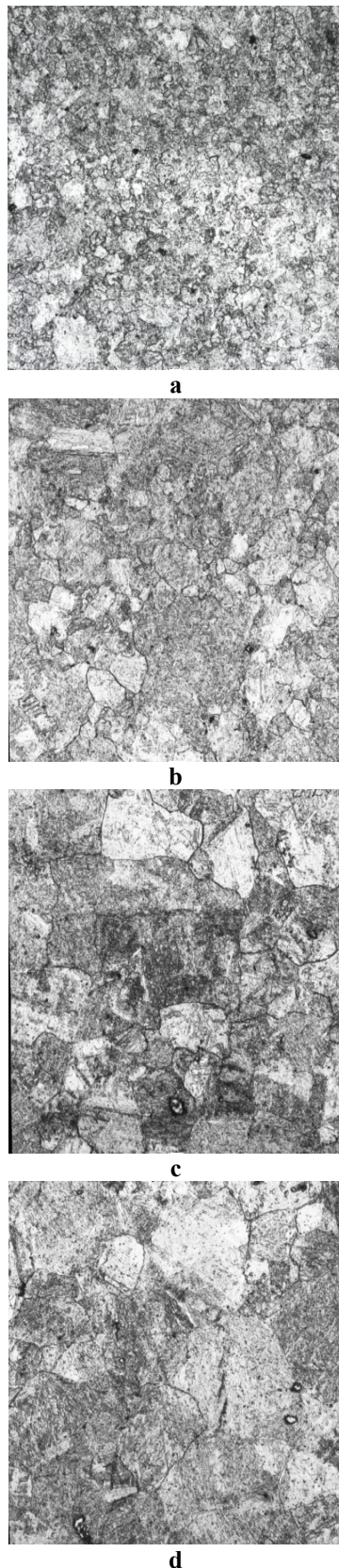


Fig. 4. Microstructure of steel 40XHM after quenching at temperatures of 860°C (a), 900°C (b), 950°C (c), 1050°C (d) and release at 600°C, shutter speed at tempering 30 min, x200.

The proportion of grain boundaries located opposite the corners $81^\circ \dots 100^\circ$, characterized by a high energy level of steel after quenching from 860°C is 13.33%,

950°C - 16.67%, 1050°C - 13.33%. The change in the number of grain boundaries with a higher energy level indicates the passage of the processes of their movement and the heterogeneity of phase precipitation during steel tempering (Tables 1, 2).

It should be noted that after quenching, most of the grains form boundaries, the angle between which is within $101^\circ \dots 20^\circ$. After the holidays, the proportion of borders increases significantly, forming an angle of $121^\circ \dots 140^\circ$.

The presence of grain size after quenching from 950°C and 1180°C increases the proportion of triple grain joints, in which there are angles that are within $161^\circ \dots 180^\circ$, both after quenching and after improvement (Fig. 5).

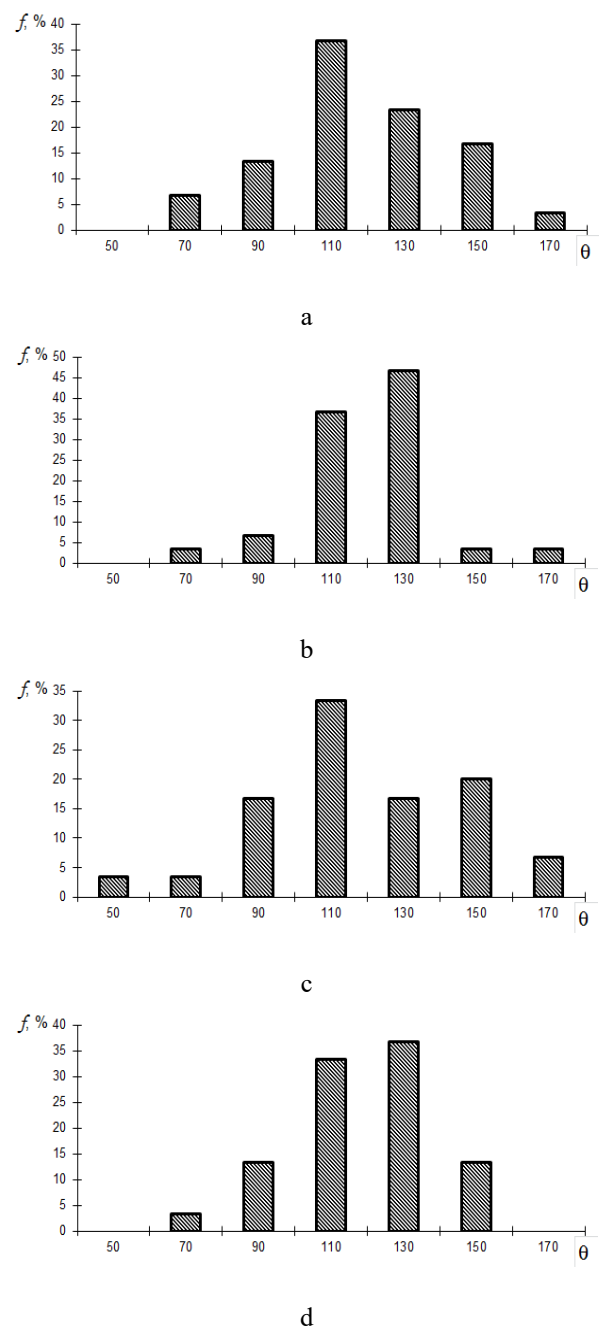


Fig. 5. Histogram distribution of flat angles between the boundaries of the remaining austenitic grains in 40XHM steel after quenching at temperatures of 860°C (a), 900°C (b), 950°C (c), 1050°C (d) and release at 600°C.

Table 1. The fraction of the angles between the boundaries in the triple joints of 40XHM steel grains after quenching

Endurance for 30 minutes							
Tempe- ring tempe- rature	Share in the total number of measured angles, %						
	40	61	81	101	121	141	161
	60	80	100	120	140	160	180
860°C	-	3,3	10,0	40,0	30,0	16,7	0,0
950°C	-	3,3	16,7	33,3	33,3	10,0	3,3
1050°C	-	-	10,0	46,7	36,7	6,7	-
1180°C	-	6,7	16,7	23,3	40,0	10,0	3,3

Table 2. The fraction of the angles between the boundaries in triple stacks of 40XHM steel grains after improvement (30-minute hardening)

Quenching, tempering 600°C							
Tempe- ring tempera- ture	Share in the total number of measured angles, %						
	40	61	81	101	121	141	161
	60	80	100	120	140	160	180
860°C	-	6,7	13,3	36,7	23,3	16,7	3,3
900°C	-	3,3	6,7	36,7	46,7	3,3	3,3
950°C	3,3	3,3	16,7	33,3	16,7	20,0	6,7
1050°C	-	3,3	13,3	33,3	36,7	13,3	-

The analysis of the influence of the structural and energy state of the grain boundaries on the processes of accumulation of damage and destruction was carried out on the basis of the results of the study of contact durability of steel under friction conditions. Testing for wear was carried out according to the scheme of "disk block" in the mode of dry sliding friction. The velocity of slipping the samples on the counterface $v = 0.5$ m / s, the load on the samples $P = 300$ N, the counterpart material - steel 45 (C - 0.45%; international analog 1045 according to ASTM-SAE), the hardness of the countertile - 42 ... 44 HRC [18]. After spin, each sample was worn for 10 hours. The values of mass intensity of wear were evaluated by the results of tests of six samples. The results of the studies are presented in table 3.

Table 3. The dependence of the mass intensity of wear on the tempering temperature of 40XHM steel after release at 600 °C (excerpt hardening under 30 minutes)

Tempering temperature $t, ^\circ\text{C}$	$I_m, 10^{-8}$	I_m/I_{mc}
860	2,599	100
900	2,698	104
950	3,228	124
1050	2,451	94
1180	2,821	109

As can be seen with the increase of the tempering temperature to 950°C, the wear resistance of the steel decreases. Standing from 1050°C increases its wear resistance. After quenching from 1180°C, the intensity of wear of steel increases.

Such a change in thickness is due to the significant influence of the structure on the accumulation of damage in terms of contact interaction. Reduced wear resistance

after quenching from 950°C, 1180°C of improved steel is due to the growth of a fraction of triple grain boundary joints, in which the edges form corners $161^\circ \dots 180^\circ$.

According to modern notions, triple grains are one of the types of linear defects along which three grain boundary surfaces are contacted. In this regard, this type of joints is characterized by a more "loose" structure and increased specific energy parameters. Moreover, the contribution of such structural units in the processes of weakening and fracture of parts of structural elements is greater than the usual boundaries of grains of polycrystals.

We note that at the moment the issue of the structure on the nanowire area of the triple junction remains open.

At the energy level, the structure of this area of polycrystalline materials is taken into account with the aid of the Herring-Young ratios, which indicate the relative energy of grain boundaries, and its distribution, depending on the angles between them:

$$\left(\sum_{i=1}^3 \sigma_i \vec{b}_i + \left(\frac{\partial \sigma_i}{\partial \varphi_i} \right) \vec{n}_i \right) = 0, \quad (1)$$

$$\frac{\sigma_1}{\sin \lambda_1} = \frac{\sigma_2}{\sin \lambda_2} = \frac{\sigma_3}{\sin \lambda_3}, \quad (2)$$

where σ_i - energy of i boundary, \vec{n}_i - unit vector which is normal to i boundary, \vec{b}_i - unit vector along the junction of i boundary, φ_i - angle, that defines orientation of i boundary, λ_i - the angle opposite to i boundary ($i = 1, 2, 3$).

As can be seen from equation (2), the energy equilibrium and the strongest is the junction in which $\lambda_1 = \lambda_2 = \lambda_3 = 120^\circ$. In the case of angle differences λ_i from 120° , it is possible energy inequalities of the boundaries σ_i , which leads to the appearance of a gradient of properties in the zone of "direct" triple junction, which is often the source of the destruction.

Its evaluation will be based on the ratio:

$$\Delta = |\sigma_1 - \sigma_2| = \left| \sigma_1 - \sigma_1 \cdot \frac{\sin \lambda_2}{\sin \lambda_1} \right|, \quad (3)$$

where $|\dots|$ - module, Δ - increase in the energy of grain boundaries in the triple junction area.

To simplify the calculations we will assume that there is a leading angle λ_1 , and λ_2, λ_3 have the condition:

$$\lambda_2 = \lambda_3 = \frac{1}{2}(360 - \lambda_1). \quad (4)$$

In this case, the expression (3) will look:

$$\Delta = |\sigma_1 - \sigma_2| = \left| \sigma_1 - \sigma_1 \cdot \frac{\sin(0.5\lambda_1)}{\sin \lambda_1} \right|. \quad (5)$$

In the dimensionless form (5) it transforms into the following equation:

$$\Delta = \left| 1 - \frac{\sin\left(\frac{\lambda_1}{2}\right)}{\sin \lambda_1} \right|. \quad (6)$$

The qualitative analysis of equation (6) shows that when the angle is changed λ_1 on the interval $(0;180^\circ)$ the Δ changes too. In this case, you can distinguish the characteristic three zones for the parameter Δ from λ_1 : zone of minor parameter change Δ , $\lambda_1 \in (0;80^\circ) \cup (130^\circ;140^\circ)$, the zone of small Δ - $\lambda_1 \in (80^\circ;130^\circ)$, and the zone of sharp ("catastrophic") growth Δ - at $\lambda_1 \in (140^\circ;180^\circ)$. When λ_1 is in the limits $(140^\circ;180^\circ)$ this indicates a lack of a thermodynamic equilibrium at the junction, which allows us to assert about the significant difference in the energy of the boundaries forming the given joint, and its ability to form microdefects under load conditions.

The graphic representation of the obtained dependence (6) is shown in Fig. 6.

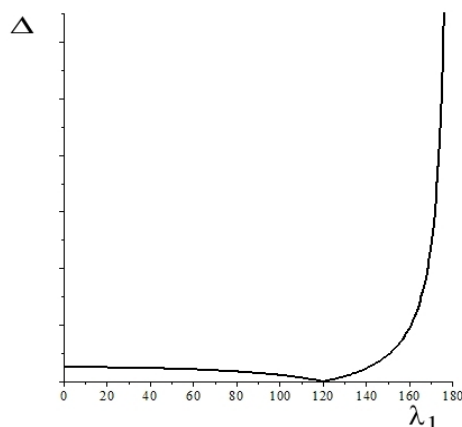


Fig. 6. Dependence of energy growth Δ of grain boundaries in the triple junction area in dimensionless form from angle λ_1 .

The results obtained in the work point to the need to manage the structural and energy characteristics of triple joints to increase the reliability parameters of structural steels.

The study of improved steels showed a tendency to intergranular damage and cracks in external loads with an increase in the structure of the grain boundary fraction with a high energy level. It was established that the decrease of the proportion of such boundaries in the grains joints, which reach the surface of the parts, by changing the temperature and time of exposure to quenching, as well as the modes of release, allows us to achieve a significant resistance to the destruction of alloys in conditions of shock and contact loads.

Analysis of the research results showed that in the steel after the quenching from 860°C , the average values

of the angles of triple grained joints are in the range from 70° to 150° . Gantry from 950° extends the range of angles. Appear angles ranging from 70° to 170° . After quenching from 1050°C , the range of angles decreases from 90° to 150° . The largest share in the total number is 110° and 130° . Their total number is more than 82%.

After quenching from 1180°C , the range extends from 70° to 170° . The proportion of angles in the range from 100° to 140° while decreasing to 63%. The improvement leads to some change in the ratio between the corners of triple joints of grains, which is due to recrystallization processes. So the release after quenching at a temperature of 950°C contributes to the increase in the number of joints in which the angles between the borders are within the limits of $161^\circ \dots 180^\circ$ (Table 2).

Determination of the average distance between the triple joints with high gradient energy showed that the distance between them along the boundaries of grains after quenching from 860° and release is up to 0.01 mm, and after quenching from 950° to 0.07 mm. The energy level of the grain boundaries between such joints is higher than other boundaries and approaches surface energy. Therefore, these boundaries are the places of origin of scattered damage (cracks).

The size of the cracks formed under the action of external loads in steel tempered from 950°C will be greater than after the quenching of 860°C . As a result, after the quenching from the higher temperature in the contact spots, the stage of development of localized damage and destruction is accelerated.

That is, multi-grain steel moves faster to the stage of formation of localized damage in the conditions of contact interaction, which leads to a decrease in its wear resistance. The established regularity is confirmed by tests of steel tempered from a temperature of 1180°C .

After quenching from 1050°C and improvement in steel, no triple joints with an elevated gradient of energy are observed. In addition to the formation of carbide heterogeneity, which corresponds to the mechanical friction pattern [20], this is one of the main factors in increasing the wear resistance of steel after the release.

Thus, the characteristics of the local volumes of grains significantly affect the stages of formation of scattered and localized damage in steels at contact loads. This ensures the possibility of introducing technologies for forming the structure of parts, which allows to significantly increase their reliability parameters - durability, resource, fault with minimum economic costs.

Conclusions

1. The structural and energetic state of the grain boundaries of the structural components significantly affects the shrinkage of steel 40XHM. Quenching from the temperatures at which the grain-graininess of steel is formed is accompanied by the formation of triple grain joints, the boundaries of which differ significantly in energy. The boundaries between the joints with a larger amount of energy correspond to the size of the scattered damage, which are formed when exposed to external loads.

2. The increase in wear resistance of steels being improved after quenching from 1050°C, besides the distribution of carbides, which corresponds to the mechanical scheme of friction, is associated with the formation of the great-cut boundaries of sorbitol grain separation with a more uniform value of grain boundary energy.
3. The propensity to increase energy in the field of triple joints with external loads depends on the proportion of boundaries that have a significant difference between the energies, and therefore reducing it helps to ensure the growth of resistance of the joints to the formation of microdefects due to the introduction of technologies for grain-boundary structure design to increase the parameters reliability of parts - durability, resource, reliability with minimal economic costs.

References

1. Shemiakin E. I. *Sinteticheskaia teoriia prochnosti Fizicheskaiia mezomekhanika* **т. 2. - № 6.** – с. 63-69 (1999) [in Russian]
2. Panin A. V. *Zarozhdenie i razvitie potokov defectov na poverkhnosti deformiruemogo tverdoho tela* Fizicheskaiia mezomekhanika. – **т.3. - № 1.** – с. 83-92 (2000). [in Russian]
3. Panin A. V. *Vliianiie sostoiianiia poverkhnostnogo sloia na mekhanizm plasticheskogo techeniia i soprotivlenie deformatsii malouhlerodistoi stali* Fizicheskaiia mezomekhanika **т.4. - № 4.** – с. 84-52. (2001) [in Russian]
4. Koneva N. A. *Istochniki polei napriazheniy v deformirovannykh polikristalakh* Fizicheskaiia mezomekhanika **т.9. - № 3.** – с. 93-101 (2006) [in Russian]
5. Kelli A. *Vysokoprochnyye materialy* – Moskov.: Mir., – 264 p (1976) [in Russian]
6. Troschenko V. T. *Ustalost metallov. Vliianiie sostoiianiia poverkhnosti i kontaktnogo vzaimodeistviia.* – K.: IPP NAN Ukrainy., 661 p. (2009) [in Russian]
7. Kobayashi H. *A stress criterion for fatigue crack propagation in metals* Proc. of the Inter. Conf. on Mechan. Behavior of Mater. Kyoto, Japan Aug. 15-20, – **Vol. 2.** – P. 199-208 (1971).
8. Kinio T. *The role of prio austenite grains in fatigue crack initiation and propagation in low carbon martensite/* T. Kinio, M. Shimizu, K. Ymada et all/ *Fatigue Fract. Eng. Mater. Struct.* – **2, № 3.** – p. 231-299 (1979)
9. Makarov P. V. *Ob ierarkhicheskoi prirode deformatsii i razrusheniia tvedykh tel* Fizicheskaiia mezomekhanika **т.7. - № 4.** – p. 25-34. (2004) [in Russian]
10. McDowell D.L. *Material design: a useful research focus for inelastic behavior of structural metals* Theoretical and Applied Fracture of mesomechanics in the 21th centure: current thinking on multiscale mechanics problems. – **v. 37.** – p. 245-259. (2001).
11. McDowell D.L. *A perspective on trends in multiscale plasticity* International Journal of Plasticity. – **v. 26.** – p. 1280-1309 (2010).
12. Curtarolo S. *The high through put highway to computational materials design.* Nature Materials. – **v. 12.** – p. 191-201 (2013).
13. Wargnier H. *Proposal for multi-material design procedure* Materials and Design. – **v. 56.** – p. 44-49 (2014).
14. Derhach T. A. *Nautchnoe obosnovanie vybora nizkolehrovannoi stali i tehnologii izhotovleniia neftegazoprovodnykh trub povyshennoi korroziinoi stoikosti* Sbornik nauchnykh trudov «Stroitelstvo, materialovedenie, mashinostroenie». «Starodubovskie tshteniia - 12». **64.** – p. 202 – 210 (2012) [in Russian]
15. Kuzin O. A. *Vykorysnnannia ionno-plazmovoho travlennia dlia analizu strukturno-enerhetychnoho stanu vnutrishnich poverkhon rozdilu.* Visnyk Derzhavnoho universytetu «Lvivska politehnika». Optymizaciia vyrobnychych procesiv i tekhnichnyi control u mashynobuduvanni i pryladobuduvanni. – **№ 359** – C. 73-76 (1999). [in Ukrainian]
16. Derhach T. A. *Analiz kachestvennykh kharakteristik korrozionno-stoikich aerito-austenitnykh staley s tseliu rasshirenia oblastey ich primeneniia.* Metaloznavstvo ta termichna obrobka metaliv. – **№ 3(66).** – с. 20 – 29 (2013) [in Russian]
17. Mak Lin D. *Granicy zeren v metalach* Moskov: GNTI. – 322 p. (1960) [in Russian]
18. Kuzin O. A. *Vplyv mikrostruktury na znoshuvannia stali 40Ch pislia polipshennia.* Visnyk Derzhavnoho universytetu «Lvivska politehnika». Optymizaciia vyrobnychych procesiv i tekhnichnyi control u mashynobuduvanni i pryladobuduvanni. **№ 371.** – P. 49-51 (1999). [in Ukrainian]
19. Kusyi Ya. M., Kuzin O. A., Kuzin M. O. *Vplyv tekhnolohichnoho marshrutu obroblennia na formuvannia miszzerennoi poshkoshennosti* Schidno-Evropeiskii zhurnal peredovykh tekhnolohiy. **№ 1/5 (79).** – C. 39-47 (2016). [in Ukrainian]
20. Kuzin O. A. *Struktura i protsesy znoshuvannia pokraschenykh staley 40X i 40XHM.* Visnyk NU «Lvivska politehnika». Optymizaciia vyrobnychych procesiv i tekhnichnyi control u mashynobuduvanni i pryladobuduvanni. **№ 422.** – P. 104-113 (2001). [in Ukrainian]