керування КА, високу надійність польоту та допомагає заощадити доволі великі запаси рідкого пального упродовж тривалих орбітальних місій.

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THE STRUCTURE OF THE NEAR-BOUNDARY ZONES OF GRAINS AND INTERGRANULAR DESTRUCTION OF STEELS

З використанням моделі функціонально-градієтної будови зернограничного шару великокутових границь подано аналіз впливу параметрів структури міжзеренних поверхонь на інтеркристалітне руйнування сталей. Керівним параметром схильності полікристалічних систем до міжзеренного руйнування є їх здатність до утворення вакансій і пор на границях зерен. Визначення оптимальних параметрів структурно-енергетичного стану міжзеренних поверхонь дає змогу вибирати раціональні технологічні рішення з підвищення міцності границь зерен сплавів.

Using the model of functional gradient structure of the grain boundary layer of large angle of borders presents the analysis of the influence of structural parameters on the grain surfaces intercrystalline destruction steels. The governing parameter of polycrystalline tendency to intergranular fracture systems is their ability to form pores on vacancies and grain boundaries. Determination of the optimal parameters of the structural and energetic state of the grain surfaces makes it possible to choose rational technological solutions to improve the strength of the alloy grain boundaries.

Statement of the problem. The current state of energy and transportation systems, metal stock aging require new scientific evidence-based recommendations for the possibility of safe operation of individual parts that went through their expected lifetime and have been through restoring repair.

Production processes of repair in most cases are carried out to restore the geometric dimensions of components without structural changes that significantly affect their performance properties and residual lifetime. The problem of reducing of machinery parts and components resource, which after the repair can be found in the boundary condition, prolongation of their work beyond the design parameters put a number of additional problems which solution has not been found yet. In this regard, it is important to create new approaches to determine the actual properties of materials, establishment of objective laws that describe change of their operation conditions.

Analysis of recent research and publications. In many cases, the destruction of parts is due to the appearance of cracks in places of local changes in mechanical properties of the products – embrittlement. Thus the problem of product efficiency of is closely linked to changes in the structural composition of the steel during the operation process and appearance for this reason of various types of defects [1] in the details material. Currently, there is a discrepancy between scientific advancements in the calculation of normalized strength and residual life assessment of equipment. Mechanical properties of steels used in the calculations are treated as constants and do not account for changes in the strength of the local inhomogenuity of the chemical composition and the stress-strain state of the material. In this regard, it is important to identify the impact of structural factors in the materials, changes in the mechanical characteristics in local zones.

The following levels of the steels structure evolution are distinguished at steels deformation [2]: mechanical, corresponding to elastic behaviour of the material; formation of defects of translational type; local discontinuity; global discontinuity, which form the main cracks. The appearance of lesions and development of cracks in places of local changes in mechanical properties in many cases is due to the redistribution of impurity atoms in the body of the grain boundaries during operation or regenerative repair of products. Traditional methods of calculating the strength of parts do not take into account the mechanical behaviour of the material in grain boundary segregations, which may be different from the behaviour of the material as a whole. Knowledge of material behaviour in local zones where the chemical composition of the steel is significantly different from the mean one because of impurity atoms segregation is essential for assessing the potential loss of bearing capacity and destruction of structural element [3].

During the steels exploitation each structure element gives its contribution to energy dissipation. Grain boundaries are the elements of the structure of polycrystalline systems that are constantly changing due to the accumulation of defects and their reconstruction. This comes as a second level phase transitions [4]. Activation barrier of such transitions is overcome during loading on the material in the operation process. Kinetics of such transitions from one state to another determines the properties of boundaries and of the material as a whole. Long-term maintenance of equipment parts and especially technological processes used in the regenerative repair of parts (welding, metal building) leads to disinhibition of diffusion processes. As a result, role of grain boundary segregations in formation of the mechanical properties of materials can become critically important [5, 6].

Intercrystalline internal adsorption of impurities at the grain boundaries can occur when heating of steels in the austenitic region as well as in the temperature range 450–550 °C followed by slow cooling. As a result, at grain boundaries there take place the processes that lead to decrease of intergranular adhesion as well as of mechanical strength of the whole system and make this phenomenon necessary to be taken into account when assessing the strength and residual life of details.

Statement of purpose of the study. Development of a model that would describe the change of the structure of grains near-boundary zones in terms of external loads and the effect of grain boundaries state on the basic mechanism of intergranular destruction.

Statement of main results. Decisive role in formation of damages and processes of intergranular destruction of constructional steels is played by big-angle grain boundaries, which are formed in two-phase zone and solid state. During the steel crystallization and cooling processes there are formed cast (primary) grains with an internal cellulous or dendritic structure [7]. In low-carbon steels there are also formed secondary crystallites. Their boundaries are, in general, randomly oriented with respect to the marginal zones of the primary crystallites. Moreover, the formation of new boundaries takes place in the temperature range that is 30–40 °C below the real solidus when the surface ingot is solid conglomerate of fused primary crystallites.

Plastic deformation with stages that allow to make a cast structure leads to the formation of internal surfaces of section that result from the processes of grain structure crystallization and transformation. When heating the deformed metal there are formed grain boundaries of large, equiaxial austenite grain that during slow cooling is transformed into pearlite, and during an accelerated cooling – into martensite.

The influence of boundaries of the various origins on the processes of deformation and destruction of steels is not studied. To a large extent this is due to the fact that in the existing models of grain boundaries the structure and structure-phase state of near-boundary zones grains are not taken into account. On these results and other studies [4, 8] basis the following model of big-angle grain boundaries structure is proposed.

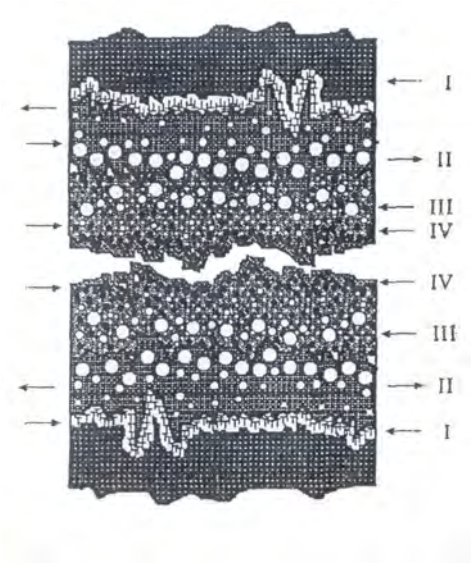

Fig. 1. Scheme of the transition layer structure at the boundary of two grains in the metal

The internal structure of grain-boundary layer is complex, involves several zones and a layer on the grain boundary (Fig. 1).

The arrows show the zones that are under compressive (arrows aimed at each other) and tensile (arrows directed in opposite directions) stresses.

The structure of the grain boundary and near-boundary layer should be considered as a functionally gradient one. At transition from a homogeneous distribution of properties in the bulk part of the crystalline body a mass dislocation takes place and the first zone (I) with high density of linear defects is formed. In this zone the compressive stresses retain their shape and properties of the grain middle volumes. Moreover, in the first zone the heterogeneity of geometric and energetic properties are founded, which are exerted in the following zones of near-boundary layer, depending on the stage of dislocation subsystem evolution (chaotic distribution of dislocations, tangles, cells, fragments). The dislocation structure of zone I can be considered as a result of dissipation of elastic energy, which leads to self-organization of non-equilibrium structures, ensuring the stability of grains system.

The next zone (II) (Fig. 1) has a loose, porous structure associated with breakage of dislocations in the first zone. Tensile stresses are present in it. In the porous part of the near-boundary layer the tensile stresses increase grid periods, so that the energy of this zone is more important than the energy of the bulk part of crystallic grid.

Vacancy supersaturation of transitional surface layer leads to the formation of structural and concentration inhomogeneities in the system. The result of chemical interaction of vacancies-saturated crystal grid with the phases is the formation of zone (III) of nonstoichiometric transition layer, in which the compounds are formed the chemical composition of which may vary. This zone of

nonstoichiometry is the zone of range of solid solutions or adhesive-fixing layer, where there are phases of nonstoichiometric composition and phases characteristic for the internal volumes of grain. In this layer there is no stable coordination number to accommodate the atoms , which is present in crystallically-ordered central part of the grain. The result is the chemical instability of the layer, as the coordination number of the material can be changed as the result of reaction to external conditions such as temperature and mechanical loads. The IV zone is the middle part of the transition between adjacent crystallites.

Under the action of external loads in the porous structure there occur the internal transformations to the local structure [9] that is the most energetically favourable for load perception. Due to the fact that during creation and use of material the defects in the crystal structure occur as a result of energy dissipation that is introduced into the material, the boundaries are the local volumes in which there is an accumulation of defects and restructuring similar to the second order phase transitions. The energy barrier of phase transitions activation is overcome with a load of material during exploitation.

One of major factors that determines the properties of the boundaries is their hollow-rough porous structure. Depending on free or excess volume (porosity) and grain-boundary defects the same boundary has different properties. A measure of the allocation limit deviation from equilibrium is the value of free volume, which is determined by the specific number of voids per area unit of the boundary surface:

$$\nu_f = \frac{V_f}{S}, \tag{1}$$

where V_f – the absolute volume of interparticle voids in the structural element material within the boundary layer; S – the boundary area of the structural element. As the voids there may be pores, non-integrities, vacancies, vacancy clusters of micro and nano sizes. There is a critical free volume ν_f^k in which the boundary is transformed into two non-interacting surfaces. The dependence of the grain boundaries energy on the size of free volume is shown in Fig. 2.

Attainment of critical free volume value υ_f^k at the section boundary of structural elements is dangerous, because in this case pores and cracks are formed that lead to the alloy destruction. At the certain value of free volume υ_f^0 the boundary energy corresponds to the equilibrium υ_{gb}. In the free volume interval within the range from υ_f^0 to υ_f^k there may exist not one but several possible non-equilibrium boundaries.

During the process of intergranular destruction of the material new surfaces are formed. In case of brittle intergranular destruction at the absence of plastic deformation near the boundary the destruction energy is defined by the following formula:

$$\gamma^* = 2\gamma_S - \gamma_B, \tag{2}$$

where γ_S – the surface energy; γ_B - the free energy of grain boundaries. Due to the fact that the grain

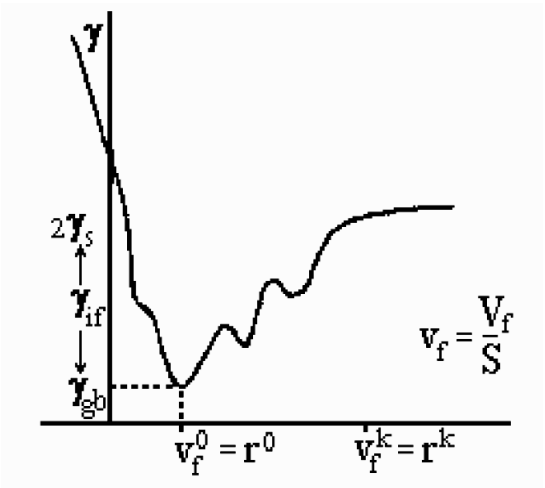

Fig. 2 Dependence of the polycrystalline alloys boundaries energy on the size of free volume [4]: $2\gamma_s$ – the energy of two noninteracting surfaces of destruction nucleus; γ_{gb} – the energy of equilibrium grain boundaries; γ_{if} – the interval of possible values of boundaries energy

boundary energy γ_B depends on grain-boundary structure, the intergranular destruction energy γ^* also depends on the structure. When plastic deformation accompanies the intergranular destruction, its energy γ^* is higher than in case of its absence, and the impact of grain-boundary structure is stronger. The intergrain alloys destruction occurs as a result of stress concentration, which is due to the development of grain boundary sliding on various irregularities of random boundaries – ledges, separations, triple junctions [8].The slip degree depends on the structure of alloys. The small-angle and special boundaries have lower threshold energy values γ_b than the random boundaries. Therefore, they are more resistant to intergranular destruction, that does not occur at boundaries of these types. A crack that originates at a random boundary moves along the boundary surfaces, choosing this type of boundaries in each triple junction. Factors that reduce the cohesive strength of random boundaries increase the probability of cracks passing through them.

The effect of structure on the intergranular destruction is determined not only by irregularities of grain boundaries, but also by the presence of topological defects [9] in the alloys structure. It should be noted that the role of these defects in the processes of intergranular destruction remains unexplored. The presence of boundary curvature in the structure of grains, which vary by the number of sides and the radius, will increase the concentration of vacancies in the grains with inbent boundaries and thus affect the distribution of impurities in the near-boundary zones. It has been experimentally shown that there are different amounts of Sb impurities of facets of intergranular fracture and preferential P placement at the fracture faces where packing is more loose [10]. The received experimental data are well described by the model of functionally graded structure of grains near-boundary zone.

The processes of plastic deformation and destruction from the perspective of energy approach are similar to melting. They are described as a violation of materials crystallic grid. The violation of atomic bonds during melting and destruction of the crystallic grid under the influence of mechanical stress are similar. There are a number of mathematical relationships obtained by different authors, linking energy required to fracture of metal unit volume under applied load of specific energy, which is consumed for melting [4].

For the local destruction of the metal it is necessary to bring its volume to the state close to melting. At that the leading role in the local destruction belongs to vacancies. Their diffusion and coagulation under the influence of temperature and stress leads to the formation of melt nucleuses in the zone of nonstoichiometric grain structure boundaries that are submicroscopic cracks.

Analysis of the role of Sb, Sn, P and As impurities in the intergranular destruction of improved steels showed that the degree of their influence on the strength of grain boundaries depends on the ability to form the grain-boundary phases with low melting temperature in accordance with the charts of iron impurities. The lower is the melting point of chemical compounds which are released at the grain boundaries, the more evident is intergranular destruction. The absorption of grid dislocations by the grain boundaries under the influence of external loads, the formation of nonequilibrium grain boundaries and increase of vacancies concentration in them resulting from the plastic deformation causes the transformation of isolated pores that are located near the phases with low melting temperature, into the pore space. Such transformation is due to compliance with energy expended on the deformation and destruction of local microscopic objects and energy of their melting. The governing parameter of polycrystalline susceptibility to intergranular destruction is the ability to form vacancies and pores at the grain boundaries under the action of external loads. The existence of two structural causes of influence on intergranular fragility segregation is related to this: segregation within the solid solution and the phase particles allocation [10].

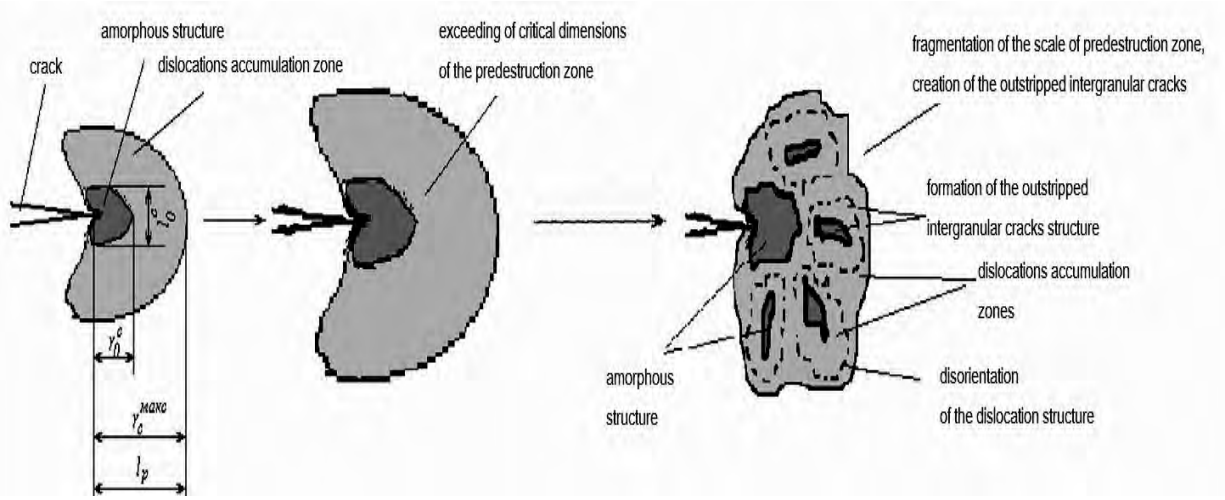

Fig. 3. Critical dimensions of zones with marginal density of deformation at the crack top at the micro-(r_0) and macro-(r_c^{max}) levels. Setting up of the system of outstrip intergranular cracks in the material load

Impurities that form solid penetration solutions (C, B, N) can heal pores and do not have an embrittling action and intergranular fragility occurs when penetration contaminants are part of the penetration of grain-boundaries phases particles. The lower tendency to intergranular destruction of simple carbon steels and higher – of alloyed steels is related to this.

Damage formed in steels at the grain boundaries under the action of external loads contain elements of surface transition layers and during the process of energy dissipation finish their structure building to the structure of the surface layer. Completion of the formation of a transition layer appears as the formation of new surface (crack). Local stresses in the zone of the transition layer formation are transformed into the surface energy of the crack.

At the top of the crack an amorphous zone is formed that corresponds to the II zone of the surface transition layer. There is a local temperature increase, which contributes to amorphization of the material at the crack top. During the crack extension the predestruction zone is formed (Fig. 3), which defines the length of the crack to the growth $I_p = r_c^{max}$ with stress coefficient K_{1c}. The K_{1c} value with the same concentration of impurities at the grain boundaries at the intergranular destruction depends on embrittling action and is associated with low work of creation of intergranular facets γ^*. This is due to the structural changes that accelerate achievement of the critical pores damage at the grain boundaries.

Conclusions. According to the material structure and defects the grain-boundary layer has a functionally gradient structure. It includes the porous zone dislocations accumulation placed closer to the adjacent grain, porous zone saturated with vacancies, and the zone of intergranular phases with nonstoichiometric composition which coordination number may vary as a result of reactions to external conditions – temperature and mechanical loads.

The governing parameter of steels susceptibility to intergranular destruction is the ability to form pores at the grain boundaries under the action of external loads, which increases in the presence of grain-boundary phases with low melting temperature. In this regard, an important task of the grain boundaries structural engineering is to determine boundary changes of alloys microstructure quantitative parameters on the basis of model description in order to maintain such corrective processes during the manufacture and work of parts that can provide a given level of vacancies in the crystal grid at grain boundaries in conditions of products exploitation.

Prediction of resistance to intercrystallic destruction of steels, choice of rational technological solutions for its elimination requires monitoring and systematic analysis of the correlation

relationships between the structural and phase composition of the internal division boundaries of the structural and functional properties of steels as well as use of computer simulation to determine the optimal parameters of the structural and energetic state of intergranular surfaces

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