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FRACTAL EVALUATION OF GRAIN BOUNDARIES BRANCHING IN THE STRUCTURE OF WELD METAL OF LOW-ALLOY STEELS

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ABSTRACT

Nonmetallic inclusions, which are an integral part of welds, can facilitate the reduction in the sizes of structural grains, playing the role of crystallization centers of the weld pool metal. This helps to increase the strength values of the weld metal on the one hand. On the other hand, the crystalline lattice of grains on the grain boundaries is influenced by the force fields of both tangent crystallites, saturated with nonmetallic inclusions, impurity atoms, dislocations, vacancies, has an increased energy of grain boundaries. These circumstances contribute to the fact that namely grain boundaries are the places of the highest probability of crack origination and propagation. For the numerical description of the dualism of the influence of nonmetallic inclusions on the weld metal structure, it is proposed to use methods of fractal analysis and metallographic analysis based on artificial intelligence.

KEYWORDS: low-alloy steel, welding, weld metal, microstructure, fractal analysis, metallographic analysis, MIPAR software

INTRODUCTION

The structure of steels used for manufacture of welded metal structures is characterized by a polycrystalline structure. In polycrystalline materials, grains or subgrains of different orientation and/or composition are separated from each other by interfaces (boundaries). Depending on the angle of inclination to each other, in the metal structure, small-angle (up to 15°) or large-angle (more than 60°) boundaries are determined. In some cases, when not all, but only individual boundary atoms coincide, the so-called "special" boundaries are formed. These "inner" interfaces play an important and most often dominant role in determination of mechanical properties of materials [1]. It is known that the main mechanical properties of the weld metal of low-alloy steels are tensile strength, ductility and fracture toughness, where grain refinement is a particularly important mechanism that provides the required level of properties. Branching of grain boundaries provides some advantages in terms of strength and fracture toughness, both at room and negative temperatures [2].

The crystalline structure of low-alloy steel consists of many individual crystallites connected with each other by grain boundaries. On these boundaries, the atomic structure of two connected crystalline lattices is strongly damaged, so grain boundaries usually have a high energy, which significantly affects the mechanical properties of the material. The impact of grain boundaries is the basis, for example, of the Hall–Petch ratio, which establishes the dependence of metal strength on grain size (the more branching of grain boundaries, the stronger the metal), but they also determine the indices of their ductility and crack resistance.

$$\sigma_y = \sigma_0 + Kd^{-1/2}, \quad (1)$$

where σ_0 is a certain friction stress required for sliding dislocations in the single-crystal; K is the constant individual for each material, which is also called "Hall–Petch ratio"; d is the grain size in the metal structure.

The whole technological process of welding steels is based on understanding the mechanisms of control of welded metal structure and structure parameters (sizes of grains, phases and inclusions) in the structure of welded joints metal. The more control is performed over this process, the higher level of their mechanical properties may be obtained.

There are two different categories of inner interfaces distinguished in crystalline materials: homophase boundaries and heterophase boundaries. The first are usually called grain boundaries, and the latter are often referred to as heterophase boundaries. Grain boundaries include boundaries of twins and domain boundaries. Heterophase boundaries, on the contrary, divide crystallites of two thermodynamically different phases. For heterophase boundaries, unlike grain boundaries, it is necessary to take into account their tendency to chemical reactions and diffusion processes. The behaviour of steels during fracture, for example, changes significantly as a result of segregation of certain impurities (especially sulphur, phosphorus) to the grain boundaries, which change adhesion between adjacent crystallites. If an increase in branching of grain boundaries is accompanied by improved strength values of metal, then the presence

of liquation elements and nonmetallic inclusions on the boundaries, as a rule, causes a decrease in its resistance against brittle fracture [2].

Moreover, to determine the degree of elements liquation along the grain boundaries and the binding energy of alloy boundaries is a difficult task. It is known that grain boundaries are a thin layer of about one nanometer thick with a low level of the orderly arranged atoms [3, 4], which divides two regions of the crystalline lattice with different orientation. During etching of the specimens of low-alloy steels, grain boundaries appear to be much wider, which indicates both the high level of dislocation density in these regions, as well as the presence of segregated elements and nonmetallic inclusions in these regions [5]. I.e., it seems that it is possible to establish a relation between the width of grain boundaries, the degree of their alloying and the energy of boundaries.

It is well known that branching of grain boundaries, on the one hand, as well as their clogging, on the other, significantly affect the mechanical properties of weld metal of low-alloy steels [6]. I.e., the properties of grain boundaries directly determine the properties of both the steels themselves as well as their welded joints, and the further studies of their structure suggest prospective opportunities for the development of new materials. The modern methods of metallographic examinations allow distinguishing the features of dualism of such an impact.

The aim of the work was to study the capabilities of a numerical description of grain boundaries that allows visualizing the dualistic nature of their structure.

PROCEDURE AND RESEARCH MATERIALS

The studies were conducted on the specimens of weld metal, which were manufactured according to the procedure [3] in arc welding in shielding gas environment (82 % Ar, 18 % CO_2) using flux-cored wire of 1.6 mm diameter of type «metalcore» at a direct current of 200 ± 5 A, arc voltage of 30 ± 2 V with input energy of 21 ± 2 kJ/cm. To determine the nature of distribution of nonmetallic inclusions in the weld metal, to a "cold" part of the welding pool, a flux-cored wire of 1.6 mm diameter was introduced, the core of which contained a mixture with 10 % of particles of refractory compounds of 040–0.200 mm and 90 % of iron powder of grade PZhV according to DSTU 9849. As inoculants, the following titanium based compounds were selected: titanium oxide (TiO_2 weld), titanium carbide (TiC weld), titanium nitride (TiN weld), as well as aluminium oxide (Al_2O_3 weld) and silicon carbide (SiC weld). The obtained results were compared with the data from the specimens of the weld metal, produced during welding using flux-cored wire, into the core of which ferrotitanium (Base weld) was introduced.

According to their physicochemical indices, nonmetallic inclusions may affect the formation of grain structure in the process of metal cooling, playing the role of crystallization centers (TiN), microcoolants (TiO_2) and phases that change energy at the crystallization front (Al_2O_3), or inhibit the carbon diffusion during decomposition of austenite (SiC, TiC). Accordingly, nonmetallic inclusions have a different effect on branching of grain boundaries in the structure of weld metal. The aim of the studies was to establish the possibilities of evaluating branching of grain boundaries of the metal matrix using the methods of fractal parametrization.

Metallographic examinations were performed on the transverse sections cut out from welded joints. The structure of the weld metal was examined in the optical microscope Neophot 32. Microstructure in the specimens was revealed by chemical etching in a 4 % alcohol solution of nitric acid. The specimens for examinations were made according to standard procedures using diamond pastes of different dispersion. The size of structural components was determined in accordance with GOST 5639.

The MIPAR (USA) v.4.2.1 software for image analysis was used to determine the structure parameters. The MIPAR software uses the technology of deep learning of artificial intelligence that allows teaching the software to adapt to the obtained microphotos, which are characterized by different contrast, brightness and texture features, as well as the technique of preparing specimens for examinations.

The latest versions of the MIPAR software (later than v.4.2) use a large library of procedures (recipe) to determine grain sizes, volumetric fraction and distribution of phases and inclusions, determination of orientation and heterogeneity of the structure, texture features, etc. The work used standard procedures (recipe) of the MIPAR software for determination of size and branching of grain boundaries in low-alloy steels.

RESEARCH RESULTS

Table 1 shows the results of determining the chemical composition of the metal of the studied welds, and Table 3 shows the content of structural components in the specimens of the welds.

The data of optical microscopy showed that the secondary microstructure of the weld metal consists of a bainitic-martensitic mixture with a small fraction of the ferritic component (Figure 1). The composition of the secondary structure and the size of structural grains are given in Table 2. Bainite is represented by morphological shapes of upper, lower and intragranular bainite and ferrite by torn polygonal precipitates and Widmanstätten ferrite outside the grain boundaries. Martensite was formed as a traditional acicular structure.

Table 1. Chemical composition of weld metal

Weld	Chemical element, wt.%										
	C	Si	Mn	S	P	Cr	Ni	Mo	Cu	Al	Ti
Base	0.050	0.290	1.32	0.024	0.014	0.16	2.19	0.27	0.36	0.039	0.019
TiC	0.054	0.263	1.28	0.025	0.011	0.13	2.22	0.26	0.49	0.035	0.009
TiN	0.035	0.317	1.40	0.019	0.009	0.14	2.29	0.26	0.56	0.036	0.011
SiC	0.066	0.370	0.92	0.016	0.024	0.14	1.72	0.23	0.54	0.021	0.005
TiO_2	0.035	0.405	1.24	0.016	0.021	0.11	1.97	0.27	0.72	0.032	0.015
Al_2O_3	0.034	0.424	1.40	0.017	0.023	0.12	2.15	0.29	0.60	0.023	0.030

Table 2. Composition of secondary structure of weld metal

Weld	Averaged fraction of components in the microstructure of welds, vol.%				Size of structural grains, μm
	Lower bainite	Upper bainite	Martensite	Ferrite	
Base	50	30	10	10	15 ± 1
TiN	30	57	10	3	15 ± 0.7
SiC	30	50	10	10	19 ± 1
TiO_2	25	45	10	10	20 ± 1
Al_2O_3	15	50	15	15	16 ± 1
TiC	25	60	10	5	18 ± 1

For fractal analysis, five optical images of the secondary structure at a magnification ×1000 for each weld metal were selected (Figure 1). After processing with the use of the ImegeJ software, binary images of the corresponding structures (Figure 2) were obtained, for which the fractal parameter was determined. The results of fractal parameterization are given in Table 3.

The cell method was used to calculate fractal dimensions. [7]. According to this method, the prepared fractal image (Figure 1) is covered with grids of square cells ("box counting method") with the grid step d scaled to 1px = 0.0377 μm and a number of cells $N(d)$ is calculated, in which information boundary (grain boundary) of the investigated fractal object — structure was captured. The fractal dimensions of the image D are determined as a result of approx-

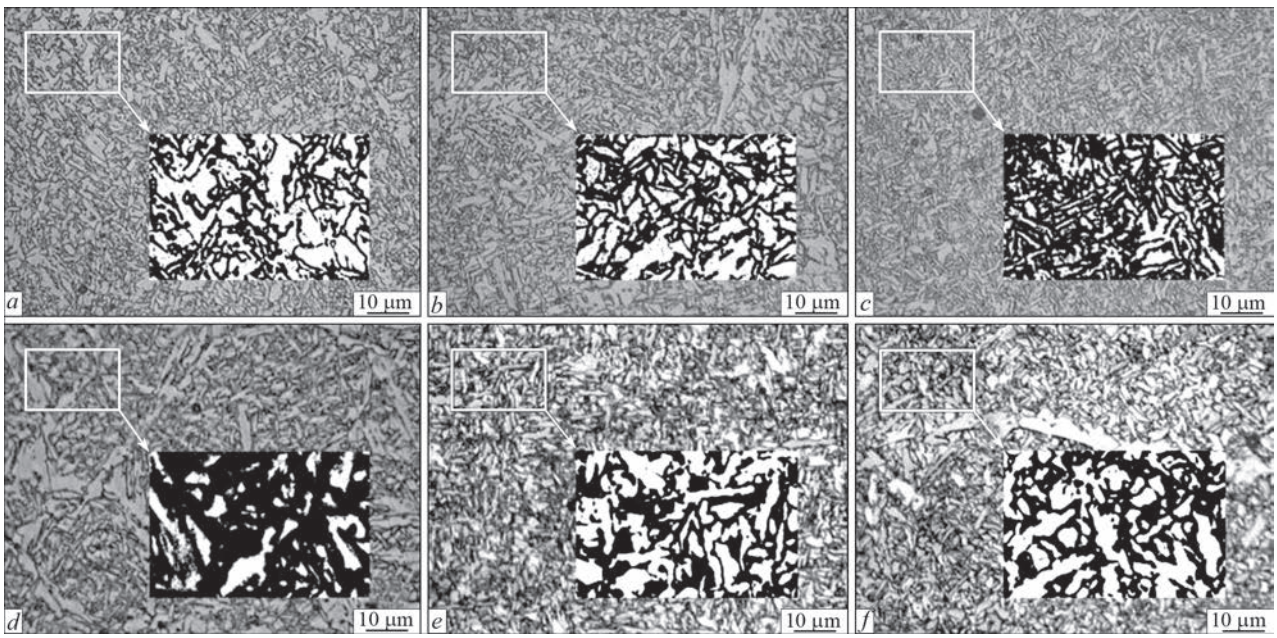

Figure 1. Microstructure of metal and binarized weld microstructure: *a* — base; *b* — SiC; *c* — TiN; *d* — TiC; *e* — TiO_2; *f* — Al_2O_3

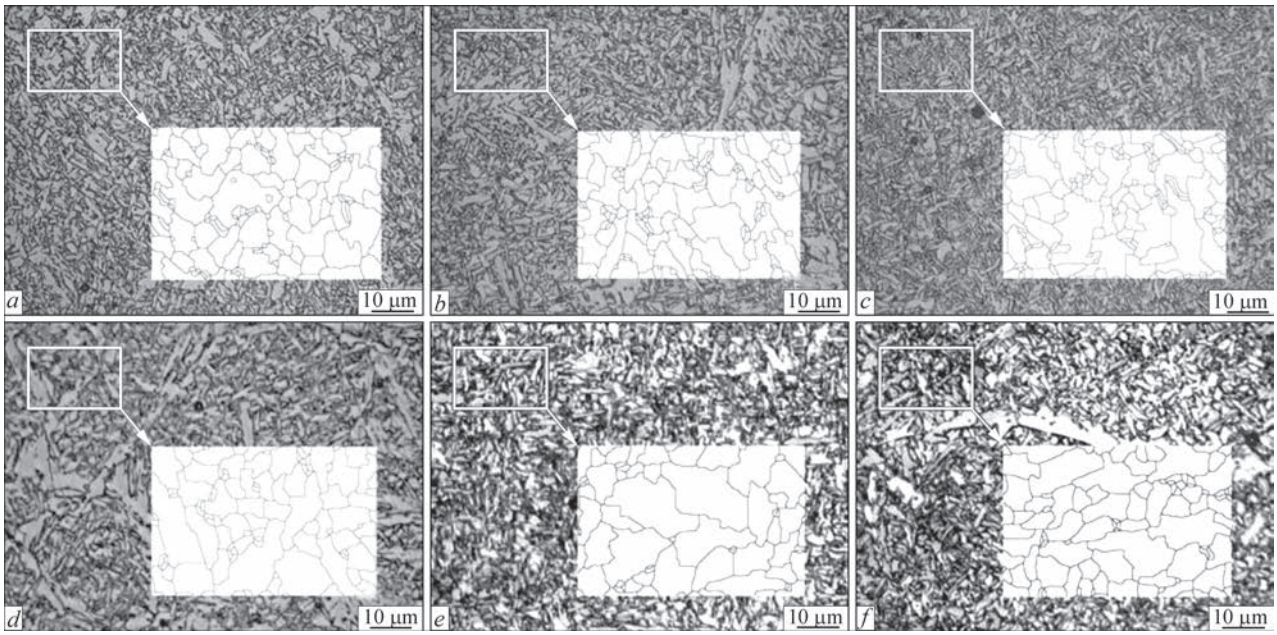

Figure 2. Microstructure and grain boundaries of weld metal modified by compounds: *a* — base; *b* — SiC; *c* — TiN; *d* — TiC; *e* — TiO_2; *f* — Al_2O_3

imation of the obtained set of points using the least squares method according to the expression (2).

$$D = \lim_{d \to 0} \frac{\ln N(d)}{\ln \frac{1}{d}}. \quad (2)$$

The results of the analysis of optical images of the metal structure of the studied welds according to the MIPAR software (Figure 2), which allowed determining the total length of grain boundaries, are given in (Table 4).

DISCUSSION OF RESEARCH RESULTS

The fractal parametrization of the structure is preceded by the binarization of its black and white images, which is based on the determination of a certain level of black colour as a carrier of information. Therefore, the images shown in Figure 1 should be considered as information grain boundaries. In the images, black colour shows the regions of metal corrosion of elevated intensity in the process of etching. Due to the fact that etching pits coincide with the places of elevated concentration of dislocations and liquation elements, the highlighted boundaries can be considered as regions with an increased tendency to brittle fracture of the metal.

The MIPAR software detects "pure" idealized grain boundaries. The total length of grain boundaries calculated based on this software can be used to find the medium grain size (d) in the formula (1) to determine the values of metal strength.

The analysis of the obtained results showed (Figure 3) that there is a fairly simple dependence between the fractal parameter D_{gb} of grain boundaries branching and the total length of grain boundaries L_{gb} (correlation coefficient $R^2 = 0.93$), which can be described by a quadratic expression. I.e., at a relatively low level of the fractal parameter $D_{gb} \leq 1.86$, its change has almost no impact on the total perimeter of grain boundaries, whereas when approaching this parameter to $D_{gb} = 2.0$, the total perimeter of boundaries increases sharply.

The results of the analysis shown in Figure 3, allow visualizing the dualism of the impact of nonmetallic in-

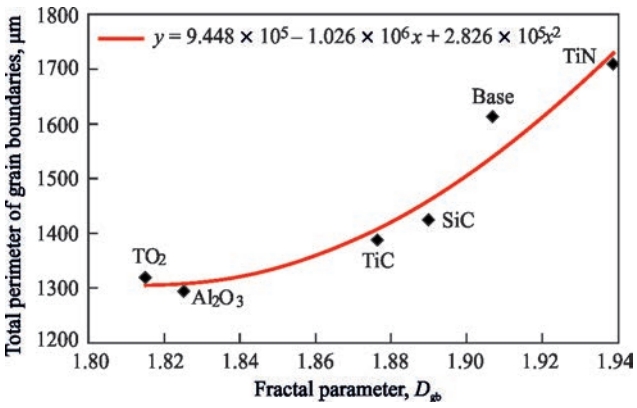

Figure 3. Impact of the fractal parameter on the total perimeter of grain boundaries

Table 3. Fractal parameter D_{gb} of grain boundaries branching obtained as a result of analysis of optical images of weld metal structure

Weld	Base	SiC	TiN	TiC	TiO_2	Al_2O_3
Fractal parameter (D_{gb})	1.9069	1.8916	1.9387	1.8765	1.8149	1.8252

Table 4. Total length of grain boundaries (L_{gb}) in the regions of weld metal

Weld	Base	SiC	TiN	TiC	TiO_2	Al_2O_3
L_{gb}, μm	16112.14	14226.94	17078.15	13893.75	13174.61	12949.53

clusions on the indices of grain boundaries in the structure of weld metal. Thus, for example, during inoculation of TiO_2 and Al_2O_3 particles to the welding pool, both the total perimeter of the boundaries, as well as the size of the region with an increased tendency to brittle fracture are noticeably reduced compared to the Base variant. The introduction of TiN particles to the welding pool leads to an increase in these two indices relative to the Base variant. The presence of SiC and TiC particles in the welding pool make it possible to raise the index L_{gb} without a significant growth in the index D_{gb}.

Thus, the given example of the system analysis indicates the possibility of expanding the knowledge base on the features of the impact of nonmetallic inclusions on grain boundaries in the structure of weld metal and making a more reasonable choice of welding consumables in the manufacture of metal structures of high-strength low-alloy steels.

CONCLUSIONS

The studies on the visualization of the dualism of the influence of nonmetallic inclusions on the indices of grain boundaries in the structure of weld metal of low-alloy steels were carried out. To analyze the impact of nonmetallic inclusions TiO_2, TiC, TiN, SiC, Al_2O_3 and TiO_2, the procedure of fractal analysis and the MIPAR software were involved. As a result of the conducted investigations, it was found that:

1. Involvement of the MIPAR software for analyzing optical images of the structure allows carrying out a numerical description of boundaries of structural grains by setting the value of the total perimeter of boundaries L_{gb}.
2. The methods of fractal analysis can be used to perform a numerical description of grain boundaries through the fractal parameter D_{gb}.
3. Parameter L_{gb} describes the idealized ("pure") size of grain boundaries.
4. Parameter D_{gb} describes information grain boundaries.
5. The system analysis of indices L_{gb} and D_{gb} allows expanding the idea of dualism of the influence of nonmetallic inclusions on the structure of grain boundaries.

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CONFLICT OF INTEREST

The Authors declare no conflict of interest

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