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Mathematical modeling of the structure and properties of low-carbon alloys

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Issues related to the determination of the numerical values of the qualitative characteristics of Fe -C alloys by interpreting the spectrum of elements of its structure by the spectrum of fractal dimensions are considered. This is due to the fact that the geometric configuration of many elements of iron-carbon alloys is complex, and it is not enough to use Euclidean geometry for its identification. Therefore, the fractal theory was applied to estimate the structure of Fe-C alloys. The results of experimental studies are presented, where it was found that the most sensitive to the fractal dimension of pearlite are the indicators of strength and hardness, which is confirmed by their physical-mechanical interaction and the obtained mathematical models. The indicators of plasticity were most sensitive to the fractal dimension of ferrite and grain boundaries, which is also consistent with the main provisions of their structure formation processes and is confirmed by the corresponding models. The obtained results can be interpreted as a technique for evaluating the quality criteria of the Fe-C alloy based on the analysis of the fractal dimension of its microstructure.

Keywords : Fe-C alloy, fractal, ferrite, pearlite, grain boundaries, quality criteria.

Математичне моделювання структури та властивостей низьковуглецевих сплавів. *Д.Б. Глушкова, В.М. Волчук*

Розглянуто питання, пов'язані з визначенням чисельних значень якісних характеристик сплавів Fe-C шляхом інтерпретації спектру елементів його структури спектром фрактальних розмірностей. Це обумовлене тим, що геометрична конфігурація багатьох елементів залізовуглецевих сплавів складна та для її ідентифікації недостатньо використовувати геометрію Евкліда. Тому для оцінки структури сплавів Fe–C застосовано теорію фракталів. Наведено результати експериментальних досліджень, де виявлено, що найбільш чутливими до фрактальної розмірності перліту являються показники міцності та твердості, що підтверджується їх фізико-механічною взаємодією та отриманими математичними моделями. Найбільш чутливими до фрактальної розмірності фериту та меж зерен виявилися показники пластичності, що також узгоджується з основними положеннями процесів їх структуроутворення і підтверджується відповідними моделями. Отримані результати можна інтерпретувати як методика оцінки критеріїв якості сплаву Fe-C на основі аналізу фрактальної розмірності його мікроструктури.

1. Introduction

The problem of assessing the structure and qualitative characteristics of metals and alloys based on them has been solved for a considerable period of time by the methods and means of solid state physics, mechanics, chemistry, materials science, and other scientific disciplines [1-3]. The reason for this is that the analysis of the structure and the evaluation of the qualitative characteristics of metals is a time-consuming process and requires a complex approach, which consists in combining traditional methods of evaluating the qualitative characteristics of metals with new methods of evaluating their structure [4-6]. Analysis of traditional methods of electron and optical microscopy, X-ray structural analysis, and quantitative metallography shows that none of these methods can be universal and suitable for solving the full range of tasks of identifying quality characteristics [7-9].

At the same time, the theory of fractals and fractal structures emerged relatively recently, on the basis of which −material scientists draw conclusions regarding the application of this theory of fractals for the analysis of qualitative characteristics of materials [10-12]. Taking into account the fact that until now there is no strict definition of the concept of fractals, we will call them geometric objects (lines, surfaces, bodies) that have a cut structure and have the property of self-similarity on a limited scale. That is, the fractal structure on a small scale repeats this structure on a large scale. By fractal dimensionality, we will understand the compactness of filling the space with an object. As the total length of the grain boundaries increases, their fractal dimension D increases, which follows from the well-known ratio [13]:

$$L \sim \delta^{D}, \quad (1)$$

where L is the length of the broken line (in the case of a grain boundary); δ - the size of the broken link. the fractal dimension has a fractional dimension, which is a quantitative characteristic of the parameters of the structure of metals, for example: grains, grain boundaries, fracture surfaces, concentrations of dislocations, finely dispersed particles of secondary phases, etc.

2. Purpose and tasks

As it follows from the analysis of literary sources, the realization of this goal of establishing the influence of the fractal dimension of the Fe-C alloy structure on the quality criteria requires the following tasks:

1. Establishing the fractality of the Fe-C alloy microstructure.

2. Development of a method for detecting among the existing phase components of the Fe-C alloy the component whose fractal dimension is most sensitive to a specific quality criterion.

3. The choice of a method of formalized description of a mutually unambiguous correspondence between the qualitative characteristic of the metal and the fractal dimension of the phase, which is most sensitive to this characteristic.

4. Development of a method for determining the mechanical properties of the Fe-C alloy using analysis of the fractal dimension of its structure.

3. Results and their discussion

Solving the task consisted of two main parts. The first part is confirmation of the existence of a mutual correspondence between the fractal dimension of the microstructure of the Fe–C alloy and its quality characteristics. And if such an assumption is confirmed, conduct a direct experiment with the development of an appropriate methodology for evaluating quality characteristics based on the analysis of the fractal dimension of the microstructure.

The first part of the work was carried out using data previously developed in the prehistory of materials science (selection of properties, photographs of the structure, chemical composition) [14].

Since the microstructure of steel is determined by various structural components and inclusions, and each element of this structure (ferrite, pearlite, bainite, martensite, grain boundaries, etc.) has its own fractal dimension, so each element of this structure is responsible for its specific quality indicator. Therefore, we will consider the microstructure of steel as a multifractal, where each element characterizes its quality indicator. To detect such an element, a method based on determining the sensitivity of its fractal dimension to a specific mechanical property of the metal has been proposed [14]. This method is based on the fact that at *a minimum* deviation of the alloy quality criterion– ΔX, determined at two different points of the structure, *the maximum* possible deviation of the fractal dimension is calculated ΔD and the sensitivity coefficient (2) is determined:

$$K_i = |D_i - D_{i+1}| / |\mathrm{X}_i - \mathrm{X}_{i+1}| = \Delta D/\Delta \mathrm{X} \quad (2)$$

where D_i and D_{i+1} – the fractal dimension of the structural component of the alloy, calculated at different points of the structure; X_i and X_{i+1} – criterion of metal quality at these points.

Thus, the element of the metal structure that best integrates a specific quality criterion is revealed. Since the existing methods for determining the fractal dimension (cellular and point) have their advantages and disadvan-

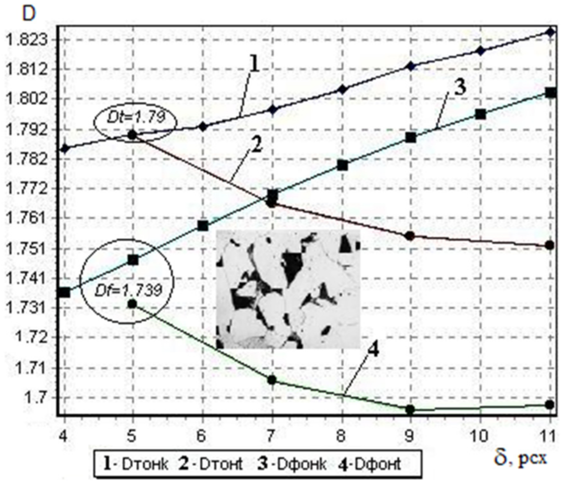


Fig. 1. Calculation of the fractal dimension *D* of pearlite based on the convergence of cellular and point dimensions

tages, the method [14] was used, according to which the fractal dimension is determined by the best convergence between them (see Fig.1).

In Figure 1, lines 1 and 2 show changes in the values of the fractal dimension of dark inclusions of structural elements (pearlite) depending on the iteration step (depending on the size of the cell covering the image of the microstructure). A similar operation is performed for light inclusions – ferrite (lines 3 and 4). Where there is the greatest convergence of the values of the fractal dimension of the structural components, which is calculated using the cellular and point method, its average characteristic is determined. As can be seen from Figure 1, the greatest convergence of the values of the fractal dimension of structural components was observed at the fifth stage of iteration.

The passive experiment was conducted on three Fe-C alloys of English production (Table 1). The choice of these grades of steel is due to the fact that the literature has accumulated many photographs of the structures of these metals with the corresponding mechanical qualities (hardness) calculated for the given areas of the structure, for example [14].

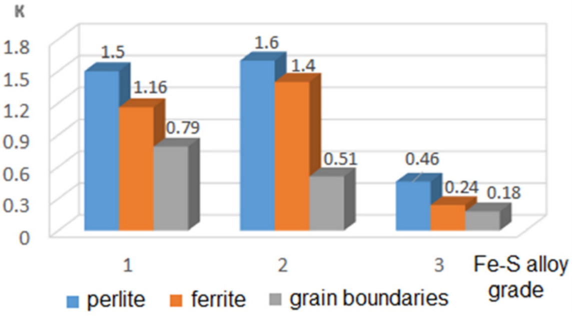


Fig. 2. Histograms of the sensitivity *K* of the hardness indicators of alloys of three grades of Fe-C to the fractal dimension of the structural elements

The histograms in Figure 2 show how the sensitivity factor contributes to determining the impact each structural component for hardness.

As can be seen from the histogram in Figure 2, the hardness indicators of the three studied alloys are the most sensitive to the fractal dimensions of pearlite, as the hardest structural component of the ferrite-pearlite structure, 1.50, 1.60, and 0.46, respectively. Based on the analysis of the results of the passive experiment, a system of equations (3)-(5) was obtained, where the Vickers hardness HV is the objective function, and –the fractal dimension, the most sensitive fractal dimension of pearlite D_n, is the argument.

$$\left\{\begin{array}{lr} HV = 4368D_n^2 - 1560D_n + 14136 \quad - \text{alloy1} & (3) \\ HV = 1341D_n^2 - 4685D_n + 4322 \quad - \text{alloy2} & (4) \\ HV = -3006D_n^2 + 10214D_n - 8419 \quad - \text{alloy3} & (5) \end{array}\right.$$

The analysis of the obtained results confirmed the fact of the existence of a mutually unambiguous correspondence between the quality criteria of low-carbon Fe-C alloys and the fractal dimension of the structure.

The active experiment was carried out on two alloys of domestic production, Splav 4 and Splav 5, also with a ferrite-pearlite structure, which have good weldability and low cost (Table 2).

The structure of the studied alloys is shown in Figure 3.

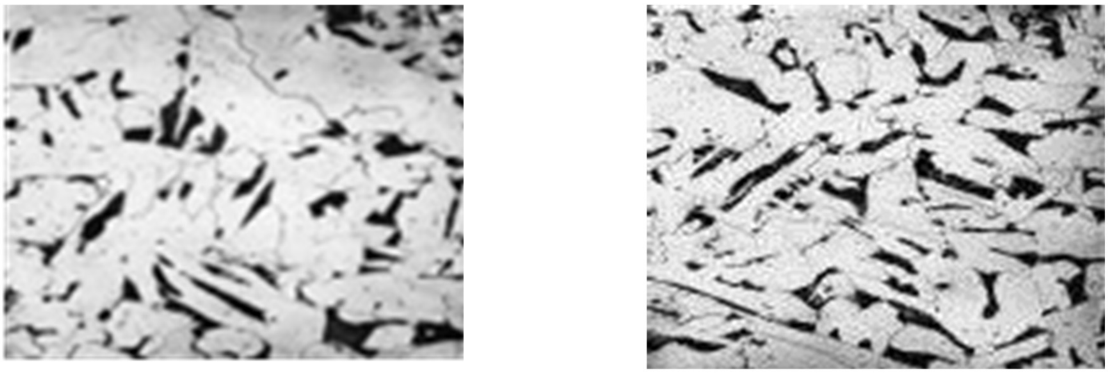
In the course of this work, it was established that the constituent structures (ferrite, pearl-

Table 1. Chemical composition of Fe-C alloys produced in England, % by mass

Fe-C alloy	C	Si	Mn	P	S	Cr	Cu
Alloy 1	0.12	0.29	0.39	0.01	0.03	0.12	0.22
Alloy 2	0.33	0.25	0.55	0.03	0.03	0.14	0.23
Alloy 3	0.44	0.22	0.66	0.02	0.03	0.15	–

Table 2. Chemical composition of domestically produced Fe-C alloys, % by mass

Fe-C alloy	C	Si	Mn	P	S	Cr	No
Alloy 4	0.16	0.07	0.61	0.009	0.022	0.02	0.02
Alloy 5	0.22	0.07	0.96	0.020	0.030	0.02	0.02



Alloy 4

Alloy 5

Fig. 3. Ferrite - pearlite structure, ×500

ite, grain boundaries) are fractal objects in a certain scale range (from ×100 to ×500). The error for ferrite and pearlite grains in this case was 0.1÷0.3%. This fact confirms the fractality of the metal microstructure, as one of the main properties is fulfilled – its self-similarity. A further increase in the area of the structure field (more than ×1000) leads to the loss of information about its components, for which the fractal dimension is determined. The last circumstance is related to the appearance of new structural elements in the metal grains due to such an increase.

The obtained results of the active experiment confirm the relationship of the fractal dimension of each structural component (ferrite, pearlite, bainite, martensite, the average value of the structural components and their grain boundaries) with a specific mechanical property. At the same time, it was experimentally established that the hardness of steel is significantly influenced not only by the presence and ratio of ferrite, bainite and martensite phases, but also by the configuration of their structure, which is somehow reflected in the form of their fractal dimension. The increased sensitivity of the fractal dimension of ferrite and grain boundaries is recorded mainly to the properties characterizing plasticity. The increased sensitivity of the fractal dimension of bainite and martensite is observed, mainly, to the mechanical properties characterizing strength.

In the course of this work, it was established that the fractal dimension of the microstructure, which is a multifractal, is sensitive to changes in the mechanical properties of steel, which makes it possible not only to calculate, but also to predict its quality.

As a result of the work performed, equations were obtained that describe the quality criteria of Alloy 1 and Alloy 2 as a function of the fractal dimension of its microstructure and the temperature at the end of accelerated cooling in water from 600 to 680 ^{0}C:

$$\sigma_B = 237.2 + 232.5D_n - 8.17t + 0.007t^2 \quad (6)$$

$$\delta = -711.2 + 582.8\ln D_f + \\ +218.5/\ln D_f + 5.42\cdot 10^{-8}t^3 \quad (7)$$

$$HBR = -1172.2 - 1138.8\ln D_n + \\ + 312.3/\ln D_n + 7.32\times 10^{-8}t^3 \quad (8)$$

$$\psi = -6700 + 150.2e^{-D_g} + 6680.3e^{t/-2016.11} + \\ + 20.4t/\ln t \quad (9)$$

where σ_B – strength limit; δ –relative elongation; HBR – Rockwell hardness; ψ – relative narrowing; D_f – fractal dimension of ferrite; D_g – fractal grain boundary; t – end temperature of accelerated cooling in potable water.

Based on the obtained equations, a knowledge base was created because each equation explained from the point of view of the mechanism of the studied phenomena. As can be seen from equations (6-9), the objective function is the mechanical property of the metal, and the arguments are –the fractal dimension of the structural components and the temperature at the end of accelerated cooling in water.

The error of the method of determining the qualitative characteristics of the metal using the analysis of the fractal dimension of its microstructure is 2÷5%. The total error of the method, including the error arising during mechanical tests, is 6÷8%.

5. Conclusions

The analysis of the results of the experiment confirmed the efficiency of the presented method of determining the qualitative characteristics of Fe-C alloys based on the analysis of the fractal dimension of the structural components and grain boundaries. tasks:

1. The fractality of the Fe-C alloy microstructure has been established.
2. It was found that the indicators of strength and hardness obtained by mathematical models are the most sensitive to the fractal dimension of pearlite. Plasticity indicators were most sensitive to the fractal dimension of ferrite and grain boundaries.
3. A mutually unambiguous correspondence between the qualitative characteristic of the metal and the fractal dimension of the phase, which is most sensitive to this characteristic, is established.

The reliability of the results is ensured by the use of proven methods of optical microscopy, the method of determining the fractal dimension of the metal microstructure, comparison of the obtained results with analogues known in the literature, satisfactory consistency of the obtained results with the corresponding data of field tests. The method can be recommended for analyzing the quality of Fe-C alloys, which should lead to a significant reduction in mechanical tests.

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