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A study on the influence of composition and fractal structure of the Fe-Cr-Ni alloy on its properties

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This study employed a multifractal approach to assess the heterogeneous structure of the Fe-Cr-Ni alloy. The calculation of the spectrum of dimensionalities for microstructural elements (pearlitic matrix, carbides, and graphite) was conducted using the Rényi formula. New relationships were established between the structure and properties of the alloy (such as hardness and impact strength), which are described by models allowing prediction of properties from microstructure images. Most of the derived correlations exhibit a linear nature, indicating that not only does the percentage content of a particular structural element influence its properties, but also the shape of the element, as characterized by its fractal dimension, contributes to those properties.

Keywords: Fe-Cr-Ni alloy, properties, composition, structure, multifractal, model.

Дослідження впливу складу та фрактальної структури сплаву Fe-Cr-Ni на його властивості. *Д.Б. Глушкова, В.М. Волчук*

У роботі використано мультифрактальний підхід до оцінки неоднорідної структури сплаву Fe-Cr-Ni. Розрахунок спектра розмірностей елементів мікроструктури (перлітною матрицею, карбідами та графітом) проводився за допомогою формули Реньї. Встановлено нові закономірності між структурою і властивостями сплаву (твердістю, ударною міцністю), що описуються моделями, які дозволяють прогнозувати властивості за фотознімками мікроструктури. Більшість отриманих залежностей мають лінійний характер, що свідчать про те, що не тільки відсотковий зміст того чи іншого елемента структури впливає на його властивості, а й форма самого елемента, виражена через фрактальну розмірність, також впливає на властивості.

1. Introduction

The deterministic approach, commonly used to assess the properties of metals and alloys, especially in analyzing cause-and-effect relationships, is not always feasible [1-3]. This is due to the numerous technological parameters that affect the quality of alloys, including chemical composition, alloying elements, cooling conditions, casting methods, and other factors [4-6]. These parameters determine the formation of structural elements that are often closely interrelated. Additionally, localized and bulk heat treatment has a significant impact on the properties of alloys [7-9].

As a result, there is a need to find and develop new scientific approaches to evaluate the properties of alloys. Materials science often relies on various modeling techniques to monitor and predict material quality criteria [8-10]. Particularly popular are models based on ana-

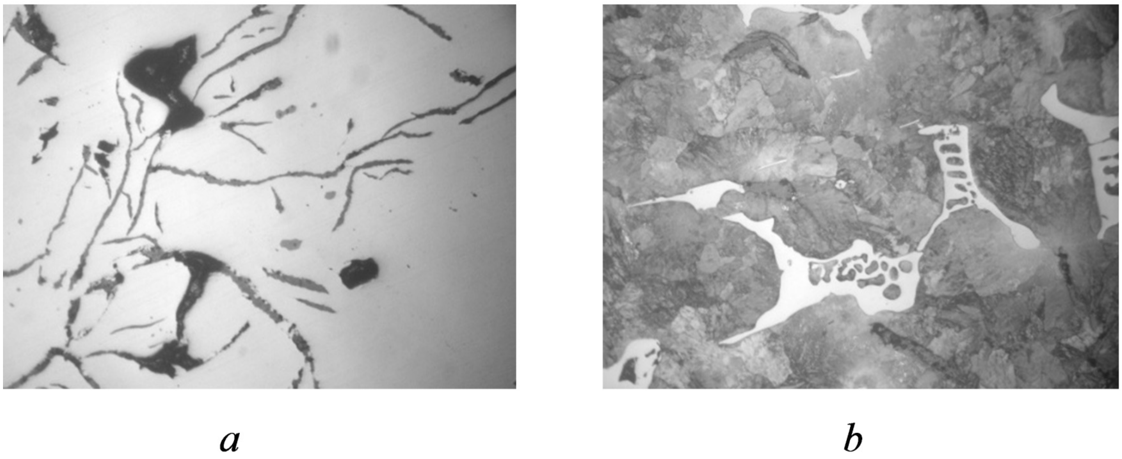


Fig. 1. Microstructure of the Fe-Cr-Ni alloy in the as-cast condition, at a distance of 10 mm from the surface: graphite before etching (a, b), pearlite-graphite-carbide constituents after etching (c, d) (×200).

lyzing the impact of chemical composition (for example, [11-14]), as well as those that consider structure and its effect on alloy properties [15-17].

An analysis of literature dedicated to the study of alloy structure and properties (for example, [18]) led the authors to the idea of using fractal theory to investigate the influence of the composition and fractal structure of Fe-Cr-Ni alloys on their properties [19]. This approach could open new perspectives in understanding the relationship between composition, structure, and alloy properties, which is highly relevant to their application in various industrial fields.

Objective and problem statement

1. Develop an approach to assess the heterogeneous structure of the Fe-Cr-Ni alloy using fractal formalism.
2. Establish a relationship between the spectrum of statistical dimensions of the structural elements in the Fe-Cr-Ni alloy and its properties, such as strength, hardness, and toughness.

2. Experimental

The chemical composition of the Fe-Cr-Ni alloy varied within the following ranges (in % by mass): 2.60–3.57 C, 0.50–0.94 Si, 0.32–0.80 Mn, 0.108–0.310 P, 0.031–0.150 S, 0.30–1.41 Cr, 0.30–0.76 Ni.

The following properties were chosen as criteria: tensile strength (σ_B), impact toughness (KC), and hardness (HSD).

Figure 1 shows the structure of the Fe-Cr-Ni alloy, featuring a pearlitic matrix.

In the Fe-Cr-Ni alloy, the composition of the carbides, which have a complex configuration in the form of cementite inclusions from ledeburitic eutectic, varied from 8% to 37%. The inclusions of flake graphite ranged from 2% to 3%, with a grade of PGD45-PGD180 according to DSTU 3443.

3. Results and discussion

The study established a connection between the structure and properties of the Fe-Cr-Ni alloy. The importance of this study stems from the difficulty in determining a clear correlation between structural elements and their associated properties. This challenge arises because the structural elements often have complex geometric shapes [20]. To establish a relationship between the structural elements of the Fe-Cr-Ni alloy—such as pearlite, graphite, and carbides—and specific properties, including tensile strength, bending strength, impact toughness, and hardness, the multifractal formalism approach was utilized.

The multifractal theory suggests that the most suitable method for quantifying and qualifying most real structures is to approximate them with fractal geometries, rather than Euclidean shapes. According to the proposed methodology, based on the multifractal formalism, each heterogeneous object, such as most metallic structures, can be characterized by a spectrum of Rényi statistical dimensions.

The study demonstrated that the calculation of the statistical dimension spectrum for each structural element was conducted using a specially developed and implemented computer algorithm. This algorithm calculated the spectrum of statistical dimensions according to a specific formula (1), which follows the methodology illustrated in Figure 2.

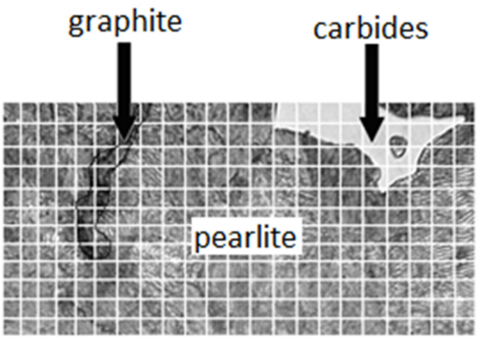


Fig. 2. To the calculation of the spectrum of fractal dimensions in the microstructure of the Fe-Cr-Ni alloy.

This approach allows for a more precise assessment of complex geometric structures and establishes a link between structural elements and mechanical properties, providing insights that could aid in enhancing alloy characteristics and their industrial applications.

$$D(q) = \frac{1}{q-1} \cdot \lim_{\delta \to \infty} \frac{\ln \sum_{i=1}^{N} p_i^q}{\ln \delta}, \qquad (1)$$

where p_i is the probability that a point within the object falls into the i-th cell of a square grid with size δ.

Figure 3 presents a graph illustrating the calculation of fractal dimensions for structural elements.

Fractal dimension of pearlite:

$$D_p = tg\alpha = \frac{\ln N(\delta)}{\ln \delta} = \frac{\ln(47{,}7)}{\ln(9)} = \frac{3{,}865}{2{,}20} = 1{,}759$$

Fractal dimension of graphite:

$$D_c = tg\alpha = \frac{\ln N(\delta)}{\ln \delta} = \frac{\ln(30)}{\ln(9)} = \frac{3{,}401}{2{,}20} = 1{,}546.$$

Fractal dimension of carbides:

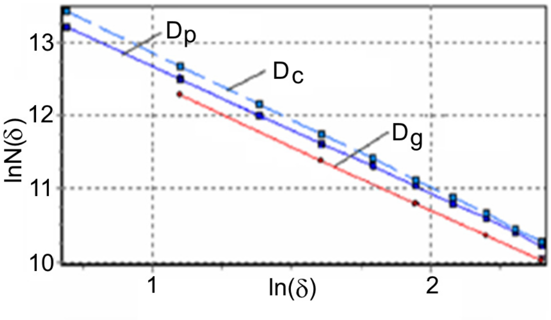


Fig. 3. Fractal dimensions of microstructure elements of the Fe-Cr-Ni alloy: D_p = 1,759; D_g = 1,546; D_c = 1,851.

$$D_g = tg\alpha = \frac{\ln N(\delta)}{\ln \delta} = \frac{\ln(58{,}7)}{\ln(9)} = \frac{4{,}072}{2{,}20} = 1{,}851.$$

When comparing the fractal dimensions of the structural elements in the alloy with their properties, the following relationships were established (Figures 4-6).

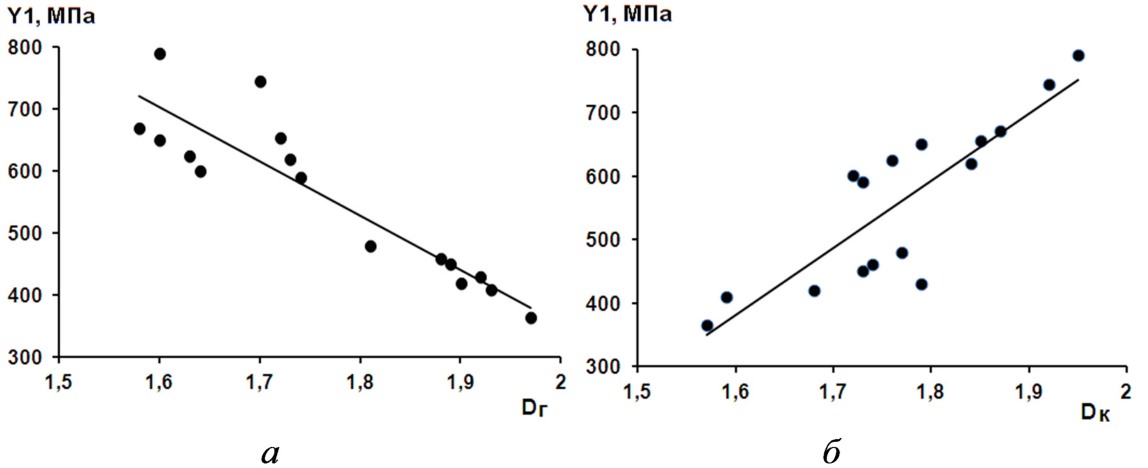
$$\sigma_B = 226{,}11 \cdot D_{-200} - 261{,}26, \qquad R^2 = 0{,}97 \qquad (4)$$

$$KC = 3{,}8414 \cdot D_0^{2{,}7778}, \qquad R^2 = 0{,}69 \qquad (5)$$

$$HSD = -87{,}194 \cdot D_0 + 209{,}18, \qquad R^2 = 0{,}84 \qquad (6)$$

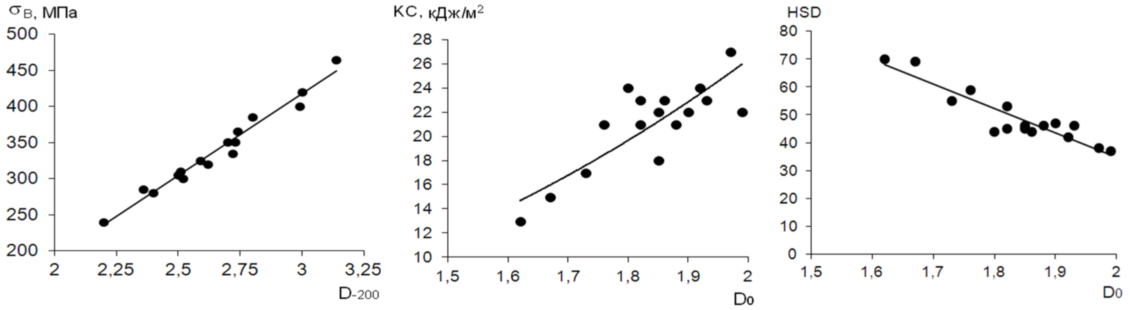
Carbides, in this case cementite, are predominantly formed in the surface layers of rolls during rapid cooling of molten cast iron poured into a mold. They typically exhibit a Shore hardness in the range of 80-100 units, although they also increase the brittleness of the cast iron. The influence of the shape of structural elements on the physical-mechanical properties is not fully understood, but the observed correlations indicate a relationship.

The trend of increasing alloy strength with an increase in the fractal dimension of cementite (Figure 5a, (7)) might suggest that changing



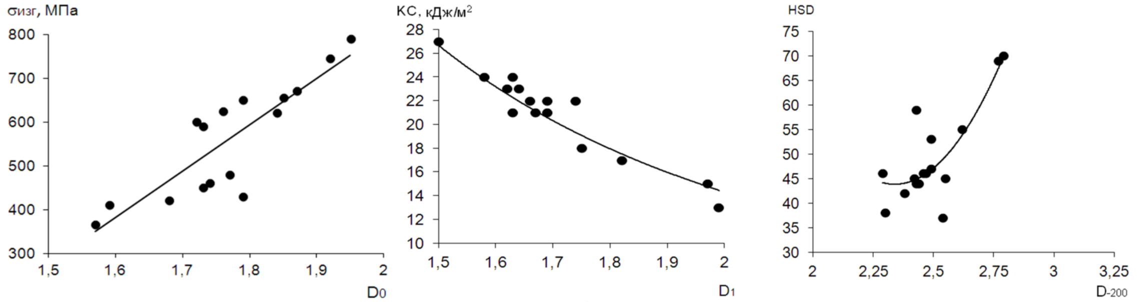
а *б*

Fig. 4. Correlation between tensile strength and the fractal dimension D_g of graphite (a) and carbide D_c (b) inclusions.



a *b* *c*

Fig. 5. Relationships between the properties of the Fe-Cr-Ni alloy and the fractal dimensions of the pearlitic matrix.



a *b* *c*

Fig. 6. Relationships between the properties of the Fe-Cr-Ni alloy and the fractal dimensions of carbides.

its form from geometrically complex to simpler affects these characteristics. The correlation between impact toughness and the information dimension of carbides (Figure 5b), which reflects informational entropy, can be explained from the perspective of the thermodynamics of the structural formation processes. Dependency (8) highlights the degree of impact of carbides on impact toughness.

Figure 5c shows the relationship between the statistical dimension of carbides and hardness, indicating that hardness increases as the density of carbide packing increases (9). These findings suggest that the fractal or statistical dimension can be an important factor in analyzing the structure and properties of alloys, providing a method for predicting mechanical characteristics of materials.

$$\sigma_b = 1055{,}6 \cdot D_1 - 1307{,}1, \qquad R^2 = 0{,}72 \qquad (7)$$

$$KC = 64{,}257 \cdot D_1^{-2{,}1695}, \qquad R^2 = 0{,}86 \qquad (8)$$

$$HSD = 127{,}74 \cdot D_{-200}^2 - 597{,}71 \cdot D_{-200} + 742{,}99, \qquad R^2 = 0{,}68 \qquad (9)$$

4. Conclusion

A new relationship has been established between the spectrum of statistical dimensions of the structural elements in the Fe-Cr-Ni alloy and its properties, such as strength, hardness, and toughness.

Theoretical justification and experimental evidence demonstrate that the fractal dimension of the Fe-Cr-Ni alloy's structural elements correlates with its mechanical properties. This finding allows the use of fractal dimension as an indicator for predicting material properties.

Thus, this approach provides a promising analytical method that can be useful for assessing and improving the characteristics of alloys, particularly when precise determination of properties is critically important for their application in various fields of science and engineering.

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