UDC 620.175.2:669.15

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PREDICTION OF MECHANICAL PROPERTIES OF 40KHMFA STEEL BASED ON MULTIFRACTAL ANALYSIS OF MICROSTRUCTURE

Purpose. *The purpose of the study is to develop and scientifically substantiate a method for quantitative assessment and prediction of mechanical properties (tensile strength, yield strength, relative elongation) and resistance to hydrogen sulfide corrosion-mechanical destruction of 40KHMFA steel based on multifractal analysis of the parameters of its bainite-martensitic microstructure after various heat treatment regimes.*

Research methods. *The research was carried out on 40KHMFA steel (0.42% C; 0.87% Cr; 0.25% Mo; 0.14% V). The samples were quenched from 860 °C in oil with subsequent high tempering in the temperature range of 660–740 °C (step 20 °C) with holding times of 5, 30, 60 and 90 minutes. Mechanical tests included static tensile testing on standard cylindrical samples, determination of impact strength on Charpy samples with a V-shaped notch and hardness measurements by the Rockwell and Vickers methods. Microstructural analysis was performed using optical metallography after mechanical grinding, polishing, electrolytic polishing and etching in 4 % nital. Multifractal analysis of microstructure images was performed by calculating the generalized Renyi dimensions (Dq), the singularity spectrum f(α) and the derived parameters:* D_0*,* Δ*, K and the spectral width* $\Delta f(\alpha)$ *separately for the bainite and martensitic components. Resistance to hydrogen sulfide cracking was assessed according to standardized methods in an environment saturated with* H_2S*.*

Results. *With increasing temperature and duration of tempering, a regular decrease in strength characteristics (*$\sigma_в$ *and* σ_t*) and an increase in plasticity (*δ_5*) is observed. Multifractal parameters sensitively reflect the evolution of the microstructure: a decrease in* D_0 *contributes to improving plasticity, and an increase in the parameters* Δ *and K – to increasing resistance to plastic deformation. Regression models with high coefficients of determination (*R^2 *= 0.86–0.95) have been developed, which allow reliable prediction of mechanical properties exclusively from the multifractal characteristics of the microstructure. It is shown that long-term tempering at 700 °C preserves the acicular morphology, but is accompanied by coagulation growth of carbide particles.*

Scientific novelty. *The scientific novelty of the work lies in the first systematic application of multifractal analysis for the quantitative characterization of the bainite-martensitic microstructure of 40KHMFA steel in order to predict its mechanical properties and resistance to hydrogen sulfide corrosion-mechanical destruction. For the first time, quantitative correlations between the parameters* D_0*,* Δ*, K,* $\Delta f(\alpha)$ *and the indicators of strength and ductility were established, and regression dependencies were developed that allow for non-destructive assessment of material properties. The higher informativeness of the multifractal approach compared to traditional methods of quantitative metallography in the analysis of substructural changes was proven.*

Practical value. *The developed multifractal method and regression models can be used to create digital systems for non-destructive quality control and predict the durability of pipelines and structural elements operating in aggressive hydrogen sulfide environments of the oil and gas and nuclear power industries. The proposed optimal heat treatment regime − of quenching from 860 °C in oil with subsequent tempering at (700 ± 10) °C for 90 minutes − provides a rational balance of strength, ductility and corrosion resistance of 40KHMFA steel. This makes it possible to reduce the volume of destructive mechanical tests in the production of dual-purpose pipes.*

Key words: *multifractal analysis, 40KHMFA steel, bainite-martensitic structure, heat treatment, mechanical properties, hydrogen sulfide corrosion-mechanical destruction, regression modeling, forecasting, non-destructive testing, pipeline steels.*

Introduction

Resistance to hydrogen sulfide corrosion cracking (HSCC) is one of the main problems for pipeline steels operated in aggressive environments of the oil and gas industry. HSCC occurs due to the combined action of corrosion, mechanical stresses and diffusion of atomic hydrogen into the metal, which leads to the formation of

DOI 10.15588/1607-6885-2026-2-4

cracks and premature failure of structures. Low-alloy steels of the 40KHMFA type (analogs of Cr-Mo-V steels) are particularly sensitive to this type of failure due to the peculiarities of the phase composition, the presence of non-metallic inclusions and microstructural inhomogeneities.

Heat treatment significantly affects the balance of strength and ductility of such steel, as well as its corrosion resistance. Therefore, it is urgent to find effective methods for quantitative assessment of the microstructure, which would allow predicting operational properties without conducting destructive mechanical tests.

Analysis of research and publications

The mechanical and corrosion properties of alloyed steels depend on the microstructure, distribution of alloying elements and non-metallic inclusions. Sulfides and oxides often become the sites of crack initiation in environments containing H_2S.

NACE TM0177 and TM0284 are used to assess resistance to SCR and hydrogen cracking. Studies show that tempering in the range of 700–715 °C provides the best compromise between strength and embrittlement resistance for Cr-Mo steels.

Recently, fractal and multifractal methods have been actively used for quantitative characterization of complex structures, corrosion defects and failure mechanisms. Multifractal analysis, unlike classical fractal, allows for a more detailed assessment of the heterogeneity, order and regularity of the microstructure through the spectrum of generalized Renyi dimensions (Dq) and the spectrum of singularities f(α).

Despite the significant number of works on fractal analysis of corrosion and inclusions, there is a lack of systematic research on the application of the multifractal approach specifically to 40KHMFA steel for predicting resistance to SCR. This necessitates the development of an appropriate methodology. The performance characteristics and durability of alloyed steels are largely determined by the features of their microstructural structure, phase composition, the nature of the distribution of alloying components, as well as the presence and morphology of non-metallic inclusions [1–5]. Inclusions of non-metallic nature, in particular sulfide and oxide particles, play the role of local stress concentrations and can act as centers of crack initiation in environments containing hydrogen sulfide. This, in turn, intensifies localized corrosion processes and contributes to the accumulation of diffuse hydrogen in the metal [1, 2]. It has been established that hydrogen sulfide corrosion cracking is activated in aggressive acidic environments (pH < 4) under conditions of increased partial pressure of H_2S (over 0.0034 bar), when atomic hydrogen penetrates the crystal lattice of steel and causes its brittle fracture [7, 8].

To quantify the resistance of materials to this type of fracture, standardized test methods are widely used, in particular NACE TM0177 (uniaxial tensile method) and NACE TM0284 (determination of susceptibility to hydrogen-induced cracking, HIC). These approaches are focused on determining both mechanical characteristics and corrosion resistance of the material [2, 7, 8]. In particular, for low-alloy steels, it has been shown that an increase in the nickel content above 1 wt.% can lead to a decrease in the SCR resistance due to the formation of unstable phase components [1, 9]. At the same time, for Cr-Mo steels, a significant effect of the tempering temperature on the formation of the martensitic-bainite structure and the corresponding susceptibility to fracture has been established: the optimal range of 700–715 °C provides a favorable combination of strength and ductility with a reduction in the risk of embrittlement [10].

In modern research, digital approaches to materials analysis are becoming increasingly widespread, including mathematical modeling, the concept of digital twins, and machine learning methods. Such tools allow predicting the behavior of materials under operating conditions with increased accuracy [6, 9]. Among them, fractal and multifractal methods occupy a special place, which are used to quantitatively describe the complexity of the microstructure, the geometry of corrosion damage, and the mechanisms of fracture [11–13].

The fractal approach, in particular the use of fractal dimension D, is effectively used to analyze heterogeneous corrosion processes in pipeline steels. For example, for steel grade X80, it was found that the parameters of the fractal geometry of corrosion defects allow estimating the fracture pressure and predicting the development of cracks [14–18]. Similarly, when studying the corrosion behavior of 316L stainless steel, a clear relationship was found between the value of the fractal dimension and its resistance to hypochlorite environments [19].

The use of fractal analysis to assess the influence of non-metallic inclusions on the properties of structural steels, in particular of the S355J2 type, has shown a close correlation between the fractal characteristics of the structure and the indicators of strength and impact toughness [2]. Similar results have been obtained in the study of surface-modified materials: fractal modeling after ion-plasma chromium plating or TiN-type coatings indicates an increase in wear resistance, which is due to changes in the morphology of the surface layer [20, 21].

Multifractal analysis is a further development of the fractal approach and allows the study of complex heterogeneous systems by determining the spectrum of singularities f(α) and generalized dimensions Dq. This provides a deeper characterization of the structure, including the degree of its homogeneity, order, and statistical regularity [6, 13]. In the field of pipeline transport, such methods have already demonstrated their effectiveness in analyzing the failure processes of composite pipes and predicting their mechanical behavior [6].

DOI 10.15588/1607-6885-2026-2-4

However, despite a significant number of studies, the issue of using multifractal analysis to assess the resistance to hydrogen sulfide corrosion cracking of 40KHMFA steels remains insufficiently addressed. This is especially important given the specificity of their bainite-martensitic microstructure and the role of non-metallic inclusions in the fracture processes [20–22]. Traditional analysis methods often do not take into account the complex multifractal nature of corrosion damage, which can lead to underestimation of the risk of crack initiation [22–24].

In this context, the application of a multifractal approach to predicting the mechanical properties and resistance of 40KHMFA steel to hydrogen sulfide based on the analysis of its microstructure opens up new prospects for optimizing heat treatment regimes and improving the efficiency of quality control systems in industry.

Purpose of work

The aim of the work is to develop a method for predicting the mechanical properties and resistance to hydrogen sulfide corrosion-mechanical destruction of 40KHMFA steel based on the multifractal characteristics of its bainite-martensitic microstructure.

To achieve the goal, the following tasks were solved:

- conduct heat treatment of 40KHMFA steel (quenching from 860°C in oil and high tempering in the range of 660–740°C with different holding times) and perform microstructural analysis;
- apply multifractal analysis to bainite and martensitic components and establish correlations between the parameters D_0, Δ, K, Δf(α) and mechanical characteristics ($\sigma_в$, σ_t, δ_s);
- develop regression models for predicting properties exclusively based on multifractal indicators and assess their accuracy.

Research material and methodology

The object of the study was 40KHMFA steel with the following chemical composition (wt. %): C – 0.42; Mn – 0.59; Si – 0.26; Cr – 0.87; Ni – 0.30; Mo – 0.25; V – 0.14.

The samples were quenched from 860 °C in oil, after which they were tempered at temperatures of 660, 680, 700, 720 and 740 °C with holding times of 5, 30, 60 and 90 min. The temperature was controlled by a thermocouple built into the sample.

Mechanical tests included tensile testing on standard cylindrical specimens, determination of impact strength on Charpy V-notch specimens, and Rockwell and Vickers hardness measurements.

The microstructure was studied after mechanical grinding, polishing, electrolytic polishing and etching in 4% nital. The size of the former austenite grain was determined by etching in picric acid with the additive "Sintol". Resistance to SCR was assessed according to standardized methods in an environment saturated with hydrogen sulfide.

Research results

With increasing temperature and duration of tempering, there is a natural decrease in strength (**$\sigma_в$** and σ_t) and an increase in plasticity (δ_5). At temperatures around 700 °C, the effect of holding time on strength is less pronounced due to the acceleration of diffusion processes (Fig. 1).

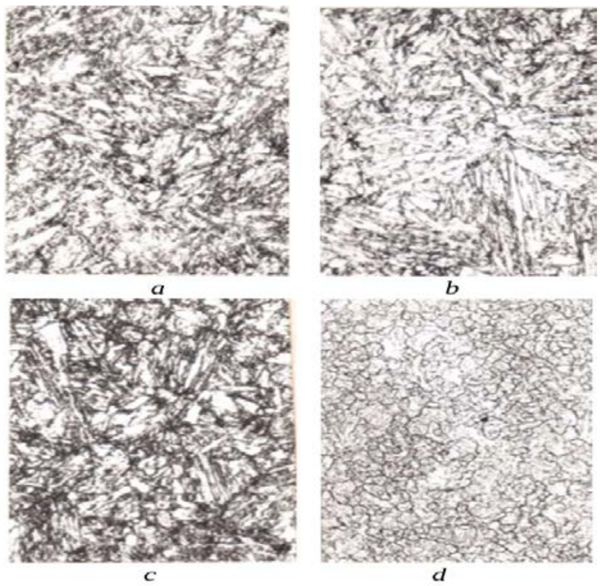

Figure 1. Structure of 40KHMFA steel after heat treatment : *a* – 630 …660 ° C ; *b* – 650…670 ° C ; *c* – 670…690 ° C , ×1250; *d* – austenitic structure , ×400

With increasing tempering temperature and holding time, there is a systematic decrease in strength characteristics and a corresponding increase in ductility. At higher tempering temperatures, the effect of holding time on the decrease in strength is less pronounced compared to lower temperatures. In the as-delivered state, the steel had a tempered acicular bainite-martensitic structure. Long-term tempering leads to coarsening of carbide particles, but retains the acicular morphology (Fig. 2).

The results of mechanical tests are shown in Fig. 3 (the relative elongation after heat treatment was ~ ~ 65–70 % and therefore was not shown in the graphs).

DOI 10.15588/1607-6885-2026-2-4

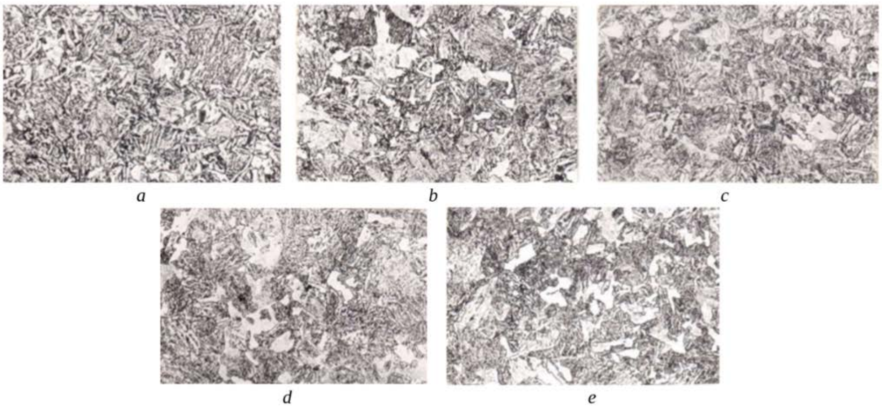

Figure 2. Microstructure of 40KHMFA steel in the as-delivered state and after tempering at 700 °C (holding time × 500-fold increase): *a* – as-delivered state; *b* – 5 min; *c* – 30 min; *d* – 60 min; *e* – 90 min

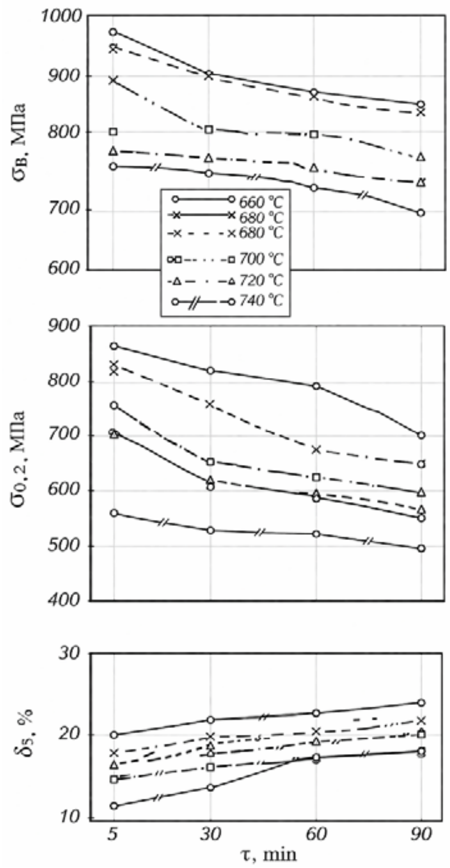

Figure 3. The relationship between tempering temperature, holding time on the mechanical characteristics of 40KHMFA steel after quenching

Multifractal analysis of the microstructure was performed using Renyi dimensions :

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

where δ –the size of the side of the square cell (box) that covers the studied image of the microstructure (in classical notation this parameter corresponds to ε); p_i –the probability that a certain part of the object (e.g., pixel intensity, area of a particular phase or structural element) falls into the i -th grid cell; q –the order of the statistical moment (exponent), which can take on any real values in the range from –∞ to +∞.

The spectrum of singularities f(α) was obtained through the Legendre transformation:

$$\alpha = d\tau(q) / dq, \qquad (2)$$

$$f(\alpha) = q\alpha - \tau(q). \qquad (3)$$

Based on the spectrum, the parameters of homogeneity, order (Δ), and regularity (K) were calculated.

The results of multifractal characteristics for bainite and martensite are given in Table 1 (the batch numbering corresponds to the different processing regimes).

Table 1 – Multifractal characteristics of the structure of 40KHMFA steel

Batch number	Bainite D_0	Bainite Δ	Beinit K	Bainite Δf(α)	Martensite D_0	Martensite Δ	Martensite K	Martensite Δf(α)
1	1.81	0.55	1.38	0.05	1.68	0.47	1.35	0.11
2	1.85	0.57	1.44	0.02	1.73	0.49	1.40	0.34
3	1.88	0.73	1.51	0.11	1.72	0.52	1.43	0.39
4	1.91	0.68	1.50	0.17	1.77	0.58	1.45	0.36
5	1.90	0.82	1.56	0.18	1.80	0.55	1.52	0.59
6	1.96	0.79	1.60	0.26	1.83	0.59	1.60	0.68
7	1.97	0.85	1.62	0.29	1.88	0.65	1.70	0.69

DOI 10.15588/1607-6885-2025-4-

Regression dependences have been developed:

σ_B = 821.32 – 112.21 D_0 + 111.26 Δ + 216.78 K – 17.24 Δf(α) (R^2 = 0.95) –for martensite;

σ_T = 695.75 – 469.87 D_0 – 190.04 Δ + 573.35 K + 286.82 Δf(α) (R^2 = 0.86) –for bainite;

δ_5 = 20.99 + 16.35 D_0 + 28.03 Δ – 23.15 K + 5.28 Δf(α) (R^2 = 0.88) –for bainite.

The analysis shows that bainite has higher D_0, Δ and K values compared to martensite, indicating greater ordering. With changing processing regimes, the structure becomes more multifractal, which correlates well with changes in mechanical properties.

The proposed models allow for reliable prediction of properties based on microstructural analysis data, which is especially important for non-destructive quality control.

Conclusions

1. Multifractal analysis is an effective tool for quantitatively assessing the bainite-martensitic microstructure of 40KHMFA steel after various heat treatment regimes.

2. The parameters D_0, Δ, K, and Δf(α) sensitively reflect changes in the heterogeneity and ordering of the structure and allow for the prediction of strength and ductility.

3.The developed regression models with high coefficients of determination make it possible to evaluate mechanical characteristics without conducting mechanical tests.

4. The optimum quenching regime for 40KHMFA steel intended for dual-purpose pipes is 860°C in oil followed by tempering at (700 ± 10)°C for 90 minutes. This regime provides the best balance of strength, ductility and resistance to hydrogen sulfide cracking.

5. The multifractal approach surpasses traditional metallographic methods in sensitivity to substructural changes and opens up prospects for creating digital systems for predicting the service life of structural elements operating in aggressive environments.

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Received 25.03.2026
Accepted 01.04.2026
Published 07.05.2026

УДК 620.175.2:669.15

ПРОГНОЗУВАННЯ МЕХАНІЧНИХ ВЛАСТИВОСТЕЙ СТАЛІ 40ХМФА НА ОСНОВІ МУЛЬТИФРАКТАЛЬНОГО АНАЛІЗУ МІКРОСТРУКТУРИ

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Мета роботи. *Метою дослідження є розробка та наукове обґрунтування методу кількісної оцінки й прогнозування механічних властивостей (межі міцності на розрив, межі текучості, відносного подовження) та стійкості до сірководневого корозійно-механічного руйнування сталі 40ХМФА на основі мультифрактального аналізу параметрів її бейнітно-мартенситної мікроструктури після різних режимів термічної обробки.*

Методи дослідження. *Дослідження проводили на сталі 40ХМФА (0,42 % C; 0,87 % Cr; 0,25 % Mo; 0,14 % V). Зразки піддавали гартуванню з 860 °C в олії з подальшим високим відпуском у діапазоні температур 660–740 °C (крок 20 °C) з витримками 5, 30, 60 та 90 хвилин. Механічні випробування включали статичний розтяг на стандартних циліндричних зразках, визначення ударної в'язкості на зразках Шарпі з V-подібним надрізом та вимірювання твердості за методами Роквелла і Віккерса. Мікроструктурний аналіз виконували за допомогою оптичної металографії після механічного шліфування, полірування, електролітичного полірування та травлення в 4 % ніталі. Мультифрактальний аналіз зображень мікроструктури здійснювали шляхом розрахунку узагальнених розмірностей Реньї (Dq), спектру сингулярностей f(α) та похідних параметрів: D_0, Δ, K і ширини спектру Δf(α) окремо для бейнітної та мартенситної складових. Стійкість до сірководневого розтріскування оцінювали відповідно до стандартизованих методик у середовищі, насиченому H_2S.*

Отримані результати. *Зі збільшенням температури та тривалості відпуску спостерігається закономірне зниження міцнісних характеристик ($\sigma_в$ і σ_t) та зростання пластичності (δ_5). Мультифрактальні параметри чутливо відображають еволюцію мікроструктури: зменшення D_0 сприяє покращенню пластичності, а зростання параметрів Δ та K – підвищенню опору пластичній деформації. Розроблено регресійні моделі з високи-*

DOI 10.15588/1607-6885-2026-2-4

ми коефіцієнтами детермінації (R^2 = 0,86–0,95), які дозволяють достовірно прогнозувати механічні властивості виключно за мультифрактальними характеристиками мікроструктури. Показано, що тривалий відпуск при 700 °С зберігає ацикулярну морфологію, але супроводжується коагуляційним ростом карбідних частинок.

Наукова новизна. *Наукова новизна роботи полягає в першому системному застосуванні мультифрактального аналізу для кількісної характеристики бейнітно-мартенситної мікроструктури сталі 40ХМФА з метою прогнозування її механічних властивостей і стійкості до сірководневого корозійно-механічного руйнування. Вперше встановлено кількісні кореляції між параметрами D_0, Δ, K, $\Delta f(\alpha)$ та показниками міцності й пластичності, а також розроблено регресійні залежності, які дозволяють проводити безруйнівну оцінку властивостей матеріалу. Доведено вищу інформативність мультифрактального підходу порівняно з традиційними методами кількісної металографії при аналізі субструктурних змін.*

Практична цінність. *Розроблений мультифрактальний метод і регресійні моделі можуть бути використані для створення цифрових систем безруйнівного контролю якості та прогнозування довговічності трубопроводів і елементів конструкцій, що працюють в агресивних сірководневих середовищах нафтогазової та атомної енергетики. Запропонований оптимальний режим термічної обробки – гартування з 860 °С в олії з подальшим відпуском при (700 ± 10) °С протягом 90 хвилин – забезпечує раціональний баланс міцності, пластичності та корозійної стійкості сталі 40ХМФА. Це дає змогу скоротити обсяг руйнівних механічних випробувань у виробництві труб подвійного призначення.*

Ключові слова: *мультифрактальний аналіз, сталь 40ХМФА, бейнітно-мартенситна структура, термічна обробка, механічні властивості, сірководневе корозійно-механічне руйнування, регресійне моделювання, прогнозування, безруйнівний контроль, трубопровідні сталі.*

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