The American Journal of Applied Sciences
ISSN 2689-0992 | Open Access

TYPE Original Research
PAGE NO. 20-26
DOI 10.37547/tajas/Volume07Issue03-04

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# Aspects of modification and ccrystallization of0 high-alloy steels

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OPEN ACCESS

SUBMITED 18 January 2025
ACCEPTED 16 February 2025
PUBLISHED 18 March 2025
VOLUME Vol.07 Issue03 2025

CITATION

Khasanov Abdurashid Solievich, Utkir Mirzakamolovich Khalikulov, & Djeparova Medine Narimanovna. (2025). Aspects of modification and ccrystallization of high-alloy steels. The American Journal of Applied Sciences, 7(03), 20–26. https://doi.org/10.37547/tajas/Volume07Issue03-04



**Abstract:** This article examines current approaches to modification and crystallization, as well as their practical applications in the field of materials science. An analysis of key modification tasks is provided, including the management of material structures, enhancement of their mechanical and chemical properties, and optimization of thermal and electrical characteristics.

An overview of contemporary research dedicated to steel crystallization processes is presented, with an emphasis on the use of rare earth elements, nanoparticles, and computer modeling methods. Experimental techniques for studying crystallization and modification processes, such as X-ray diffraction, scanning electron microscopy, and differential thermal analysis, are discussed.

The article also presents the results of studies on the effect of ultrafine powders on the structure and properties of materials, as well as the determination of the optimal powder concentration in a transporting gas medium. In conclusion, the importance of further improving modification methods to create innovative materials with specific characteristics is highlighted.

**Keywords:** Modification, crystallization, nanoparticles, metallurgy, materials, computer modeling, mechanical properties, rare earth elements, ultrafine powders, structural changes.

**Introduction:** Relevance of studying modification and crystallization processes

The processes of modification and crystallization play a key role in materials science and technological development in various industries. The study of these processes is relevant for the following reasons:

1. Improvement of material quality

• Modern technologies require materials with enhanced mechanical, thermal, and chemical properties.

• Controlled crystallization minimizes defects and improves the strength and wear resistance of materials.

2. Development of high-tech industries

• In metallurgy, modification processes enhance the casting characteristics of alloys.

• In micro- and nanoelectronics, precise control of crystallization is crucial for creating semiconductors and superconductors.

• In medicine, crystallization of biomaterials affects biocompatibility and the longevity of implants.

3. Economic efficiency and resource conservation

• Optimization of crystallization and modification processes reduces production costs.

• The use of modifiers enhances material properties without significantly increasing the cost of production.

4. Adaptation to new challenges and development of advanced materials

• Research in this field contributes to the creation of adaptive and self-healing materials.

• New theoretical models help develop materials with specified properties at the molecular and atomic levels.

Thus, the study of modification and crystallization processes is an essential direction in materials science and engineering, determining the further development of science and technology.

Main tasks and goals of material modification

Material modification aims to improve their properties by changing their structure, phase composition, or chemical composition. This process is widely applied in metallurgy, ceramics, polymers, composites, and other materials.

Main tasks of modification:

1. Control of structure and crystallization

 Control of grain size, shape, and distribution in metals and polymers.

 Formation of amorphous, nanostructured, or crystalline phases with specific properties.

2. Enhancement of mechanical properties

 Increasing strength, hardness, impact toughness, and wear resistance.

 Reducing brittleness and increasing plasticity.

3. Improvement of chemical and corrosion resistance

 Enhancing resistance to oxidation, acids, alkalis, and other aggressive environments.

 Creating protective coatings and barrier layers.

4. Optimization of thermal and electrical properties

 Regulation of thermal conductivity and heat capacity of materials.

 Improving electrical conductivity or, conversely, creating dielectric materials.

5. Creation of special functional materials

 Development of superconductors, magnetic, optical, piezoelectric, and biocompatible materials.

 Production of materials with changeable or adaptive properties (e.g., self-healing coatings).

6. Economic efficiency and resource conservation

 Reducing the need for expensive and rare earth elements.

 Increasing the service life of materials and reducing replacement costs.

Main goals of modification:

1. To impart new or improved properties to materials

2. To increase the service life of products

3. To create competitive materials for high-tech industries

4. To reduce production and operational costs

5. To minimize environmental impact by creating eco-friendly materials

Thus, material modification is a key tool for creating innovative solutions in various fields of science and technology.

**Review of Modern Research Directions in Steel Crystallization**

Currently, there is no universal theory that explains the modification process for all melt treatment methods. The main reason for this is the lack of a comprehensive crystallization theory. Modern approaches to studying crystallization rely on various theories of the structural state of Fe-C alloys, which determine the mechanism of formation of crystallization centers and the corresponding modification theories. Each of these is generally experimentally validated through the development of new types of modifiers [2].

To date, there are more than 10 modification theories for Fe-C alloys [1], which are closely linked to crystallization theories. The foundations of metal crystallization theory were laid by D.K. Chernov in the 1870s when he first introduced the concept of crystallization rate [3]. In the early 20th century, G. Tamman expanded these studies by formulating the concept of the rate of formation of crystallization centers and establishing their dependence on the degree of undercooling.

Modification and crystallization processes play an important role in the development of modern materials, ensuring their optimal physical-mechanical and operational characteristics. Crystallization is the process of a substance transitioning from an amorphous state to a crystalline one, which is regulated by various factors such as temperature, pressure, and the presence of impurities. Modification, in turn, involves changing the properties of materials through alloying, heat treatment, or the introduction of nanoparticles. Research in this area has a wide range of applications, from metallurgy to biomedical technologies.

Steel crystallization research focuses on improving its properties, such as strength, corrosion resistance, impact toughness, and wear resistance. Modern directions in this field include:

- Application of molecular dynamics and machine learning methods for predicting grain growth;
- Development of digital models for thermodynamic solidification processes;
- Introduction of rare-earth elements (e.g., niobium, vanadium, titanium) to control grain boundary processes;
- Optimization of chemical composition to enhance mechanical properties;
- Use of nanoparticles in crystallization processes;
- Addition of nanostructured modifiers to control the size and orientation of crystallographic grains;
- Study of the influence of carbon and oxide nanoparticles on crystallization rate;
- Heat treatment and accelerated crystallization methods;
- Application of directed hardening and controlled cooling for the formation of ultrafine-grained structures;
- Use of electromagnetic influence and ultrasonic technologies to control solidification;
- Additive manufacturing technologies and rapidly quenched alloys;
- Development of laser and electron-beam surfacing methods for creating high-strength steel structures;
- Investigation of crystallization processes under rapid cooling conditions, characteristic of additive manufacturing.

**Experimental Methods:**

Differential thermal analysis (DTA) to study the kinetics of crystallization.

X-ray diffraction analysis to determine phase composition.

Scanning electron microscopy (SEM) to analyze the morphology of structures.

**Theoretical Approaches:**

Computer modeling (Monte Carlo method, molecular dynamics) for predicting the nucleation and growth of crystals.

Thermodynamic calculations of the influence of various additives on structure formation.

Materials modification methods:

Alloying of steels with rare-earth elements to improve mechanical properties.

Introduction of nanostructured additives to enhance corrosion resistance.

Use of ultrasonic treatments to regulate grain sizes in metals.

In the study to select the optimal composition for modifying chromium-molybdenum steel, ultradispersed powders of molybdenum (Mo), vanadium (V), and aluminum (Al) were used. The method chosen for synthesizing ultradisperse powders was the production of fine-disperse metallic, oxide, nitride, and carbide powders using the electrical explosion of a conductor (metallic wire with a diameter of 0.1-1.0 mm) by passing a powerful current pulse (duration of 10^-5 to 10^-7 s) with a current density of 10^4-10^6 A·mm^-2 through the wire. Vanadium wires (0.28 mm in diameter and 40 mm in length) were selected as consumables. The voltage for the graphite electrode was set to 30 kV. Molybdenum wire (0.30 mm in diameter and 60 mm in length) at 30 kV and aluminum wire (0.30 mm in diameter and 130 mm in length) at 21 kV were also used as starting materials.

Further, micrographs of the obtained ultradispersed powders produced by the electrical explosion of the conductor were taken using an electron-optical metallographic microscope (OEM ODM) (Fig. 1).

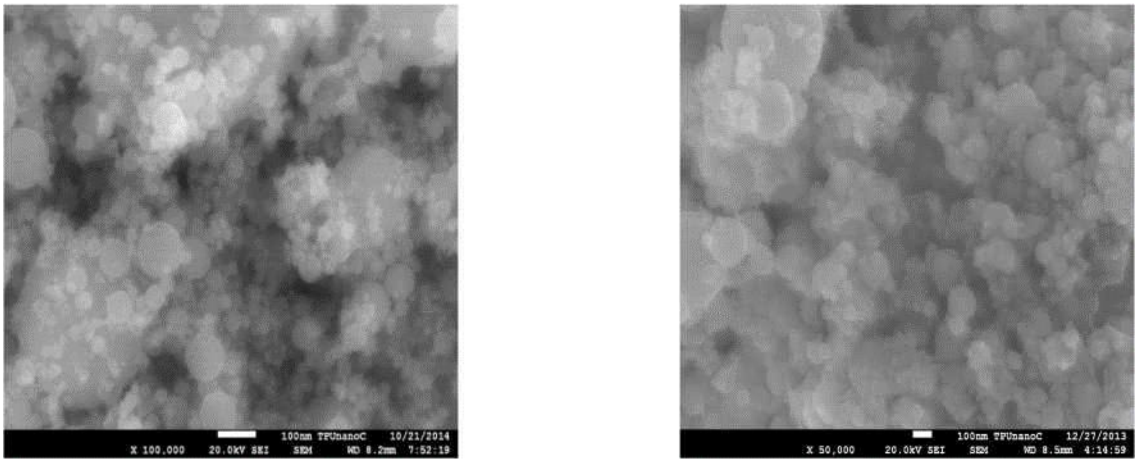


**Figure 1. Micrographs obtained in the electron-optical metallographic microscope OEM ODM of vanadium and molybdenum electropowders.**

Based on the results of this electron-optical analysis, a table was created for the data of the ultradispersed powders (Table 1), which were used as modifiers.

**Table 1. Properties of Modifiers**

| Powder Modifier | Specific surface area, $m^2/g$ | Particle diameter, nm |
|---|---|---|
| Vanadium | 2,56 | 123 |
| Molybdenum | 4,73 | 128 |
| Aluminum | 15,4 | 146 |

It should be noted that the synthesis method using electrical explosion utilized aluminum powders as the starting material for aluminum oxyhydroxide. Accordingly, the micrographs of aluminum oxyhydroxide are presented in Figure 2.

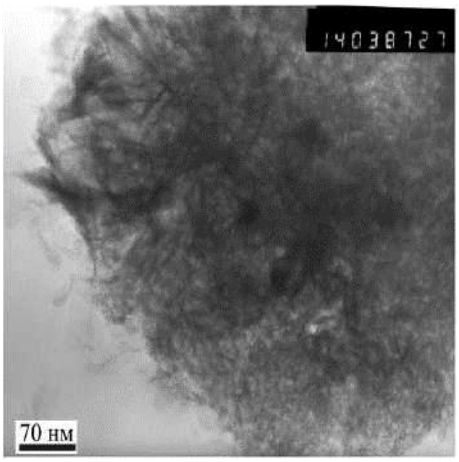


**Figure 2. Micrographs obtained in the electron-optical metallographic microscope OEM ODM of aluminum oxyhydroxide.**

## RESULTS

The studies showed that the introduction of modifying additives significantly affects the rate and nature of crystallization.

Key results include:

Alloying aluminum alloys with zirconium and titanium reduced the grain size by 30%, which improved their mechanical properties.

The use of silica nanoparticles in polymer materials increased their thermal stability by 20%.

The application of computer modeling confirmed theoretical assumptions about the effect of activators and inhibitors on crystallization, which allows for the prediction of material properties with high accuracy.

Study of the optimal concentration of ultradispersed powders in the transporting gas. During the work, studies were conducted to determine the optimal concentration of ultradispersed powders in the transporting gas. The rationalization of the concentration was carried out based on the following technological parameters:

1. Dendrite Thickness SSS (µm)
2. Dendrite Width eee (µm)
3. Volume of the Electrode Metal Droplet vvv (mm³)

To determine the optimal concentration of modifier powders in the transporting gas, a dimensionless function was calculated using the following formula:

$$f= S_6 \bullet еб\ V_6, \qquad (1)$$

Where: S6, is the dimensionless dendrite thickness,; еб - is the dimensionless dendrite width; V6 - is the dimensionless volume of the electrode metal droplet.

Based on a multifactorial experiment that studied the effect of ultradispersed powder modifiers' concentration on the quality of the surface layer, the rational concentration was determined. The minimum value of the dimensionless function

$f$ was 0.2 mg/cm³ for the surface layer.

The obtained results confirm the effectiveness of various modification methods that allow control over the structure and properties of materials. Key points include:

- The use of crystallization activators accelerates the phase transition, ensuring uniform structure formation.
- The application of computational modeling methods has become an indispensable tool for predicting the properties of new materials.

The maximum modification effect of the surface layer is achieved with a concentration of nanostructured powders in the transporting gas of 0.2 mg/m³. A reduction in concentration results in insufficient modification, while an increase in concentration hinders the formation of a defect-free surface layer.

The analysis of the fine structure of the surface layer using atomic force microscopy revealed the presence of particles sized 100–200 nm. These particles are ultradispersed powders that did not dissolve during the high-temperature treatment process, making them effective inoculants that contribute to grain refinement of the metal (Fig. 3).

Studies were conducted to determine the optimal concentration of ultradispersed powders in the transporting gas.

The rationalization of the concentration of ultradispersed powders in the transporting gas was based on the following technological parameters:

1. Dendrite thickness s (µm)
2. Dendrite width e (µm)
3. Volume of the electrode metal droplet v (mm³)

To determine the optimal concentration of ultradispersed modifier powders in the transporting gas, the dimensionless function fff was calculated using the following expression:

$$f= S_6 \bullet еб\ V_6, \quad (1)$$

Where: S6, is the dimensionless dendrite thickness,; еб - is the dimensionless dendrite width; V6 - is the dimensionless volume of the electrode metal droplet.

Based on the conducted multifactorial experiment on the effect of various concentrations of ultradispersed modifier powders in the transporting gas on the quality of the surface layer, the optimal concentration was determined, at which the minimum value of the dimensionless function $f$ was 0.2 milligrams per cubic centimeter of the surface layer.

Discussion. The obtained data confirm the effectiveness of various modification methods that allow for targeted control over the structure and properties of materials. It is important to note that:

- The application of crystallization activators accelerates the phase transition process, ensuring uniform structure formation.
- Computer modeling has become an indispensable tool for predicting the properties of new materials.

- The optimal effect of surface layer modification is achieved with a concentration of nanostructured powders in the transporting gas of 0.2 mg/m³. A decrease in the concentration of ultrafine powders leads to insufficient modification, while an increase in concentration prevents the formation of a defect-free surface layer.
- Analysis of the fine structure of the surface layer using atomic force microscopy revealed the presence of particles sized 100–200 nm. These particles are ultrafine powders that did not dissolve during high-temperature processing and act as effective inoculants, promoting the grain refinement of the metal (Figure 3).

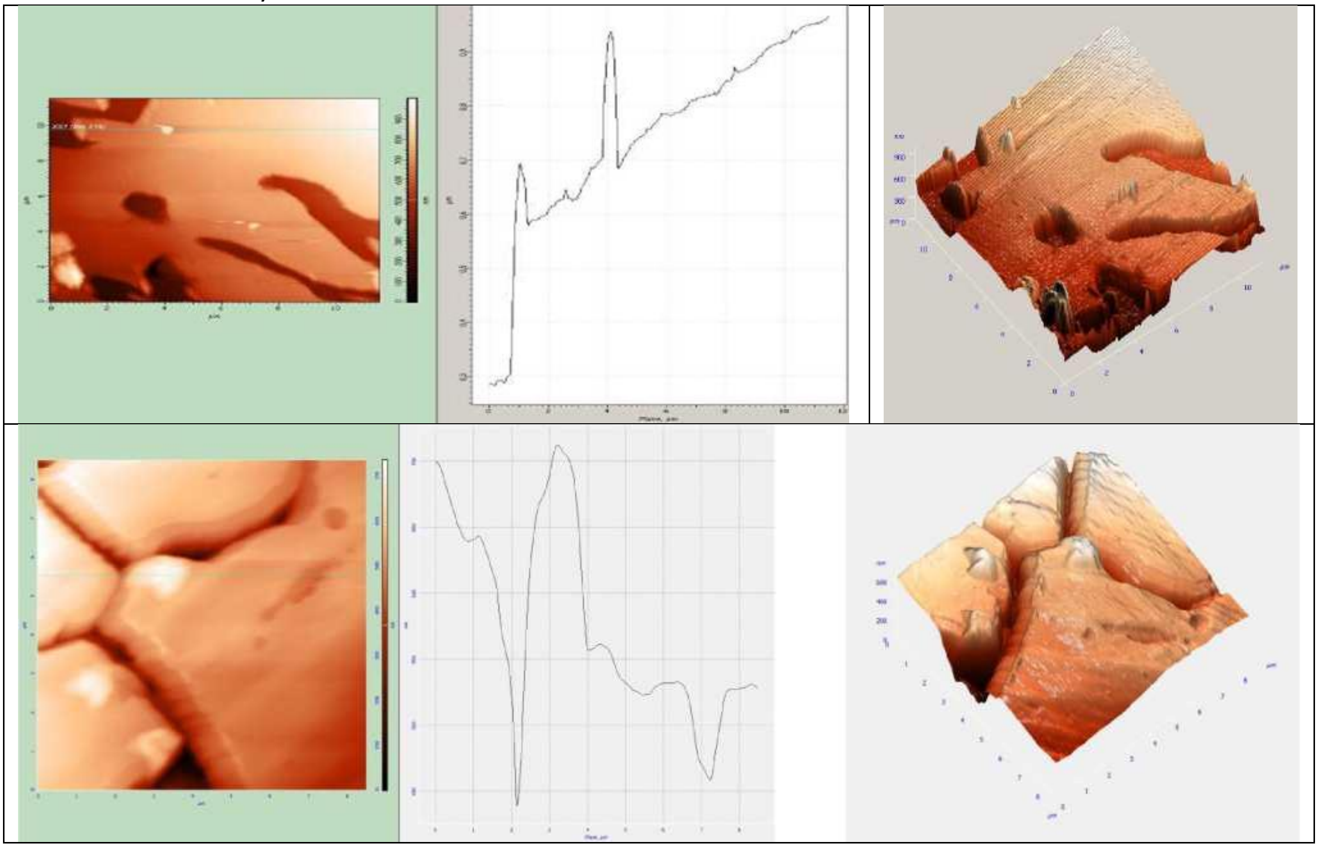

**Figure 3. Results of modification with ultrafine powders of Al2O3 and vanadium.**

Further research should focus on studying the interactions of nanoparticles with the matrix of materials to create composites with enhanced properties.

## CONCLUSION

Modern theories of modification and crystallization significantly expand the possibilities of materials science. The development of experimental methods and computer modeling contributes to the creation of new materials with tailored properties, opening up prospects in metallurgy, the polymer industry, medicine, and other sectors. Further studies in this field will help optimize existing technologies and develop new methods for controlling crystallization and modification processes.

## REFERENCES

Kakhovsky N.I. Electrogas welding of corrosion-resistant ferritic-austenitic steels type 21-3 and 21-5 / N.I. Kakhovsky, K.A. Yushchenko, Z.V. Yushkevich // Automatic Welding – 1963. – No. 12. – pp. 49-57.

Kakhovsky N.I. Welding of corrosion-resistant austenitic chromium-nickel-manganese-nitrogen steel 0Kh17N5G9AB (ZP55) / K.A. Yushchenko, V.G. Fartushny, Z.V. Yushkevich // Automatic Welding – 1963. – No. 7. – pp. 21-28.

Poletika I.M. Formation of corrosion-resistant coatings by cladding in a beam of relativistic electrons / I.M. Poletika, M.G. Golkovsky, M.V. Perovskaya, E.N. Belyakov, R.A. Salimov, V.A. Bataev, Y.A. Sazanov // Prospective Materials – 2006. – No. 2. – pp. 80-86.

Tsvirkun O.A. Hardening and protection of the surface of steel Kh12 by electro-explosive alloying / O.A. Tsvirkun, E.A. Budovskikh, E.E. Rudneva, V.F. Goryushkin, V.E. Gromov // Journal of Fundamental Materials – 2007. – Vol. 1. – No. 3. – pp. 117-119.

Goryushkin I.F. Relative resistance of various tool and corrosion-resistant steels to mechanical and chemical effects from pharmaceutical preparations / I.F. Goryushkin, S.A. Lezhayeva, A.A. Permyakov, N.N. Shevchenko // Bulletin of the Mining and Metallurgical Section of the Russian Academy of Natural Sciences. Metallurgy Division – 2002. – No. 11. – pp. 59-65.