ADVANCED PREDICTIVE MODELLING OF MULTIPHASE CARBIDE PRECIPITATION IN FE–CR–C ALLOYS: INTERRELATION OF THERMODYNAMIC STABILITY FIELDS AND KINETICALLY GOVERNED MICROSTRUCTURAL EVOLUTION

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Аннотация. В данном исследовании с применением продвинутого термокинетического моделирования проанализировано образование многофазных карбидов и их микроструктурная эволюция во времени в сплавах Fe–Cr–C. На основе подхода CALPHAD с использованием программ Thermo-Calc и TC-PRISMA определены термодинамические области стабильности, механизмы зарождения и кинетика роста карбидов. Путём сравнения сплавов с содержанием 18% и 28% Cr показано влияние хрома на диффузионные процессы, фазовую устойчивость и морфологию карбидов. Полученные результаты позволяют прогнозировать формирование свойств и оптимизировать режимы термической обработки износостойких высокохромистых чугунов.

Ключевые слова: Термодинамика, карбид, кинетика, износостойкий чугун, металлическая основа

Abstract. This study employs advanced thermo-kinetic modeling to evaluate the formation of multiphase carbides and their time-dependent microstructural evolution in Fe–Cr–C alloys. Using the CALPHAD approach with Thermo-Calc and TC-PRISMA, the thermodynamic stability fields, nucleation mechanisms, and growth kinetics of carbides were determined. Comparative analysis of alloys containing 18% and 28% Cr reveals the influence of chromium on diffusion behavior, phase stability, and carbide morphology. The results provide a predictive basis for optimizing heat-treatment regimes and improving the performance of high-chromium wear-resistant cast irons.

Keywords: Thermodynamics, carbide, kinetics, wear-resistant cast iron, metallic matrix.

Annotatsiya. Ushbu tadqiqotda ilg‘or termo-kinetik modellashtirish usullari qo‘llanib, Fe–Cr–C qotishmalarida ko‘p fazali karbidlarning shakllanishi va ularning vaqt o‘tishi bilan mikrostrukturaviy rivojlanishi baholandi. Thermo-Calc va TC-PRISMA dasturlari yordamida CALPHAD yondashuvi asosida karbidlarining termodinamik barqarorlik sohalari, yadrolanish mexanizmlari va o‘sish kinetikasi aniqlandi. 18 % va 28 % xrom tarkibiga ega qotishmalarni taqqoslash xromning diffuziya xatti-harakatlari, faza barqarorligi va karbid morfologiyasiga ta’sirini ko‘rsatdi.

ISSN 3030-3907

Kalit so‘zlar: Termodinamika, karbid, kinetika, yeyilishga bardoshli cho‘yan, metall Matritsa.

Introduction.

Materials science examines the relationship between mechanical properties and the structural transformations that occur in metals during their production and heat treatment. The manufacturing of metals and alloys, the formation of their microstructures, and their chemical composition are all closely interconnected with crystallography, kinetics, and thermodynamics [1]. In recent years, advances in computational tools have enabled the prediction of these properties and their interrelations in advance. For instance, the CALPHAD (Computer Calculation of Phase Diagrams) approach, widely used in computational thermodynamics, serves as a fundamental theoretical method for determining the thermodynamic properties of complex multicomponent and multiphase systems. Thermo-Calc is extensively utilized for thermodynamic modeling of various alloys, analyzing phase transformations, studying time–temperature dependencies of microstructural changes, determining the sizes and volume fractions of phases, and calculating enthalpy and entropy values [2], [3].

The TC-PRISMA module is developed to support the systematic design of alloy compositions and heat-treatment regimes required to achieve a desired microstructure. It is tightly integrated with Thermo-Calc and uses CALPHAD-based databases to obtain accurate thermodynamic and kinetic data for alloys. This study demonstrates the capabilities of TC-PRISMA in modeling complex microstructural reactions—such as various growth mechanisms, particle size distribution of precipitates, and nucleation behavior—that occur during heat treatment.

MATERIALS AND METHODS. The chemical compositions selected for this study are presented in Table 1. Thermo-Calc software (version 2025b, educational) along with its integrated TC-PRISMA module was used to model and evaluate the thermodynamic stability of phases, phase transformations, and nucleation processes.

Table 1.

Chemical composition of the materials

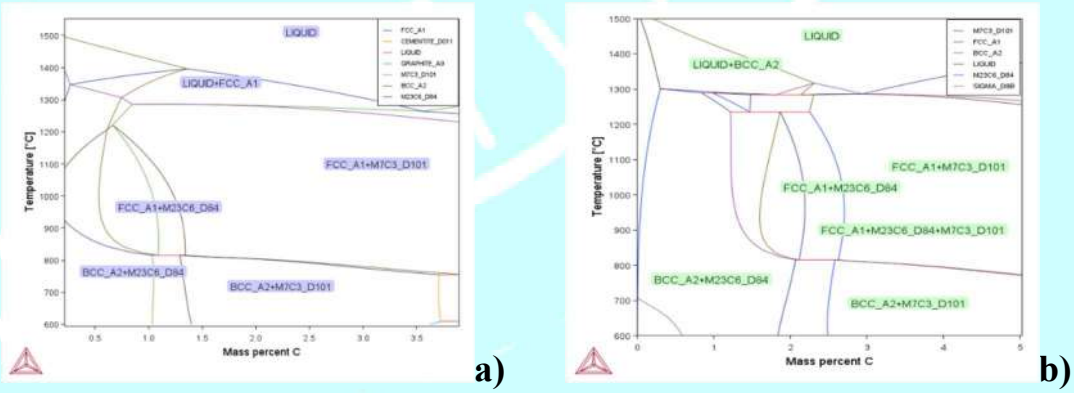
№	C	Si	Cr	Mn	Mo	Ni	P	S	Cu	B
1	2,6	0,66	18.0	0,7	0,04	0,71	0,016	0,011	0,12	0.006
2	2,6	0,58	28.0	0,52	0,032	0,74	0,016	0,011	0,12	0.006

The TC-PRISMA module is based on the Langer–Schwartz theory, which makes it possible to calculate the simultaneous processes of nucleation, growth, and coarsening of dispersed phase precipitates within the microstructure. To accurately describe these processes, the Kampmann-Wagner numerical method is

ISSN 3030-3907

employed, providing high precision in modeling time and temperature-dependent kinetic transformations. In addition, an isothermal heat-treatment simulation at 930 °C was performed for the alloys with the chemical compositions listed above.

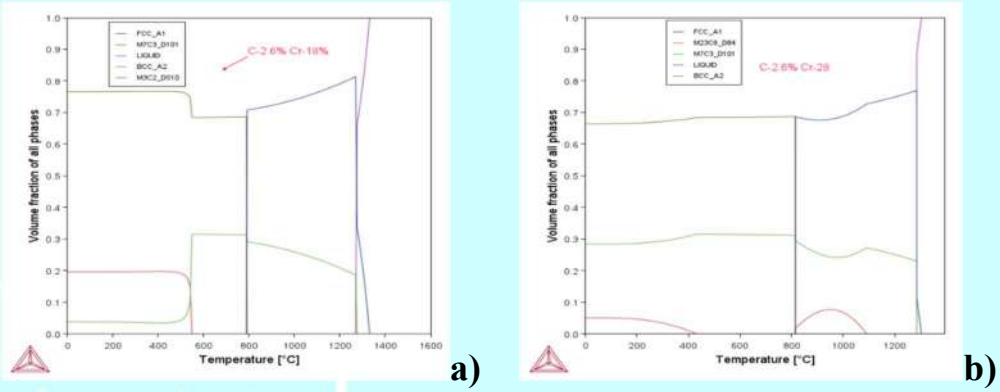
RESULTS AND DISCUSSION. The phase diagrams of the investigated alloys are presented in Figure 1. In both cases, the primary phase constituents are austenite, ferrite, and the carbides of the M_7C_3 and $M_{23}C_6$ types. For the alloy containing 18% chromium, a pronounced expansion of the austenite and M_7C_3 carbide formation region is observed. Such a phase structure is regarded as optimal for abrasive wear because it ensures a favorable balance of strength and wear resistance. The temperature-dependent phase constituents formed in the system, along with their corresponding volume fractions, are presented in Figure 2. In both alloy compositions, ferrite forms the primary metallic matrix; however, the carbide phases appear in different volumetric proportions. Specifically, in the first alloy, the $M_{23}C_6$ carbide accounts for approximately 20% of the total volume, whereas in the second alloy, the M_7C_3 carbide dominates, reaching up to 0.3 mol, which corresponds to roughly 30% of the system.



a) b)

Figure 1. Phase diagrams of the alloys: a) C–2.6% Cr–18%, b) C–2.6% Cr–28%

It should be noted that the diagrams provided represent the thermodynamically stable state of the system.

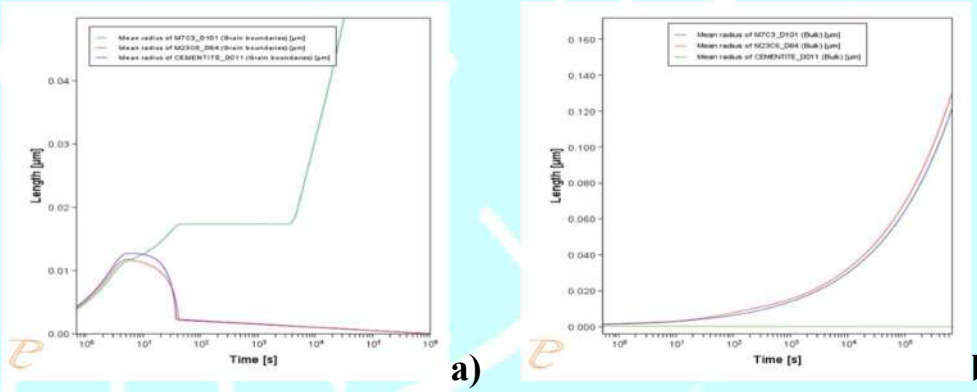


a) b)

Figure 2. Phase formation in alloys as a function of temperature: (a) C–2.6% Cr–18%, (b) C–2.6% Cr–28%.

ISSN 3030-3907

Under crystallization conditions, the initial phase observed is austenite with a face-centered cubic (FCC) lattice. In both samples, the stability range of this phase extends up to 800 °C. As a result of the heat treatment of high-chromium cast irons, in addition to eutectic and primary carbides, secondary carbides-chemical compounds of carbon with metal-also form within the metallic matrix. Their sizes are generally very small; however, over time they may grow and eventually completely dissolve [4], [5]. The nature of this process is illustrated in Figure 3. At the heat treatment temperature of 930 °C, the secondary carbide phases selected in the system were M_7C_3, $M_{23}C_6$, and M_3C. In Sample 1, during the first 100 s, all three phases grow at nearly the same rate; however, by 10^6 s, their amount completely disappears. The M_7C_3 carbide increases in size over time, and this phase, forming within the metallic matrix, acts as a protective barrier between the material surface and the abrasive wear zone [6].



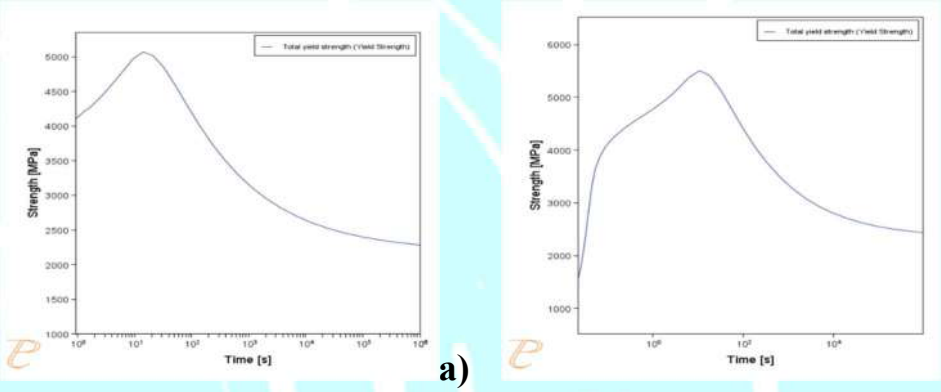
a) b)

Figure 3. Time-dependent growth rate of the precipitated carbide phases under isothermal treatment: (a) alloy C-2.6% Cr-18%; (b) alloy C-2.6% Cr-28%.

In Sample 2, following heat treatment, little to no cementite precipitation is observed in the metallic matrix. Unlike the first sample, here the M_7C_3 and $M_{23}C_6$ carbides form at the same growth rate. Figure 3b shows that the $M_{23}C_6$ phase is slightly larger; however, the difference is not significant: after a holding time of 100,000 s, the size of the carbide particles is approximately 0.120 µm.

As a result of heat treatment, in addition to structural changes in the materials, changes in their mechanical properties are also observed [7]. Figure 4 shows the dependence of the materials' yield strength on the holding time. The yield strength of the material with the first chemical composition exceeds 5000 MPa, which is achieved within approximately the first 100 s; thereafter, by 10^6 s, it decreases to the range of 2000-2500 MPa. In the second sample, this value is noticeably higher-about 5500 MPa initially and 2500-3000 MPa after the holding time.

ISSN 3030-3907



a) b)

Figure 4. Yield strength of the samples: (a) C–2.6% Cr–18%, (b) C–2.6% Cr–28%.

The main reason for this difference can be attributed to the increased chromium content [8]. Chromium carbides exhibit higher thermodynamic stability, do not dissolve at elevated temperatures, and persist longer, thereby maintaining the alloy's strength over an extended period. Moreover, the increased chromium content slows down diffusion processes, which hinders the coarsening of precipitated phases.

CONCLUSION. Based on the conducted investigations, the following conclusions can be drawn:

In the sample containing 18 % Cr, the maximum strength was observed at the initial stages of isothermal annealing; however, over time, due to the coarsening of precipitated phases and the reduction in their quantity, a decrease in strength was established. It was found that during isothermal quenching, the growth of carbide precipitates is closely related to the chromium content. Specifically, for the alloy with 28 % Cr, it was determined that the high chromium concentration leads to intensive precipitation of $M_{23}C_6$-type carbides along the grain boundaries, and their average radius significantly increases over time. This process indicates the predominance of a growth mechanism controlled by boundary diffusion.

REFERENCES:

1. Хамроев Н.Н. Термодинамический и кинетический анализ формирования и эволюции карбидных фаз в высокохромистых чугунах при термической обработке 930 °c // Universum: технические науки: электрон. научн. журн. 2025. 11(140).

2. Khamroev N. и др. Exploring the influence of the casting process, structural components and heat treatment on the mechanical properties of high chromium cast irons: A review. Samarkand, Uzbekistan, 2024. C. 060021.

3. Safarov, I. I., Teshaev, M. K., Boltaev, Z. I., Kulmuratov, N. R., & Hamroev, N. N. (2019). Own wavesin a spatial viscoelastic cylinder with radial crack. ISJ Theoretical & Applied Science, 12 (80), 341-345.

ISSN 3030-3907

4. Ҳамроев Нурбек Нуриллоевич, Эгамбердиев Илҳом Пулатович, Ашуров Хисрав Хуршид Угли, Буронов Шахзод Болибой Угли Микроструктурный анализ и износостойкость легированных чугунов с марганцем // Universum: технические науки. 2025. №6 (135).

5. Egamberdiyev Ilhom Pulatovich, Yaxshiyev Sherali Namozovich, Ashurov Xisrav Xurshid o‘g‘li, and Hamroyev Nurbek Nurilloyevich. "110G13L po‘latining mikrostrukturaviy tuzilishi va mexanik xossalariga termik ishlov berishning ta’siri" Ilm-fan va innovatsion rivojlanish. Vol. 8, No. 2, 2025, pp. 66–74.

ISSN 3030-3907