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MATHEMATICAL MODELING OF GRAIN SIZE IN THE STRUCTURE OF HIGH-ENTROPY ALLOY UNDER CONDITIONS OF THERMOCHEMICAL PRESSING

МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ РОЗМІРУ ЗЕРНА В СТРУКТУРІ ВИСОКОЕНТРОПІЙНОГО СПЛАВУ В УМОВАХ ТЕРМОХІМІЧНОГО ПРЕСУВАННЯ

This work is focused on the investigation of the new material Al28Ni22Co17Fe15Cu10Mn8 obtained under conditions of thermochemical pressing. Owing to the multicomponent nature and distinctive characteristics of high-entropy alloys (HEAs), it becomes possible to produce materials with

excellent catalytic properties at a low cost compared to existing alternatives. Catalysts based on HEAs exhibit outstanding thermodynamic characteristics compared to those based on intermetallic systems, hence a detailed analysis of the thermodynamic parameters of alloy formation is considered necessary. Such parameters include configurational entropy of formation, mixing enthalpy, atomic radius mismatch parameter, valence electron concentration, grain size prediction, and others.

***Keywords**: high-entropy alloy, thermochemical pressing, thermodynamic analysis, mathematical modelling, catalytic properties, configurational entropy, mixing enthalpy, atomic radius, valence electron concentration, grain size, intermetallic systems, physicochemical characteristics, material synthesis, diffusion features.*

Робота присвячена комплексному дослідженню нового багатокомпонентного матеріалу Al28Ni22Co17Fe15Cu10Mn8, який отримано шляхом термохімічного пресування. Високоентропійні сплави (ВЕС), зокрема цей зразок, вирізняються унікальними властивостями завдяки поєднанню великої кількості різних елементів, що дозволяє отримати матеріали з високими каталітичними характеристиками за значно нижчою вартістю в порівнянні із традиційними каталізаторами, які зазвичай виготовляються на основі дорогоцінних металів або інтерметалідних систем. Такий підхід сприяє розвитку сучасних технологій у галузі матеріалознавства та промислової хімії.

Каталізатори, створені на основі ВЕС, демонструють видатні термодинамічні характеристики: підвищену стабільність, здатність до збереження активності при високих температурах, а також стійкість до агресивних середовищ. Це значною мірою зумовлено складною структурою сплаву, яка сприяє формуванню нових фаз і забезпечує рівномірний розподіл компонентів на мікро- та нанорівнях. З огляду на це, виникає необхідність у детальному аналізі термодинамічних параметрів процесу утворення та подальшого функціонування таких матеріалів.

У роботі особливу увагу приділено розрахунку та моделюванню ключових термодинамічних характеристик сплаву, зокрема: конфігураційної ентропії утворення, ентальпії змішування, параметру невідповідності атомних радіусів, концентрації валентних електронів, а також прогнозуванню розміру зерна у структурі матеріалу. Застосування математичного моделювання дозволяє не лише оптимізувати процес синтезу сплаву, а й передбачити вплив різних технологічних параметрів на кінцеві властивості матеріалу. Це відкриває нові можливості для створення каталізаторів із заданими характеристиками під конкретні виробничі завдання.

Важливо зазначити, що використання нееквімолярного складу є нетиповим для ВЕС, однак саме такий підхід забезпечує підвищену стабільність сплаву, полегшує процес синтезу та сприяє формуванню унікальних каталітичних властивостей. Дослідження дифузійних особливостей компонентів, а також впливу різних параметрів пресування, дозволяє глибше зрозуміти механізми формування структури сплаву та розробити рекомендації щодо оптимізації технологічних процесів.

Таким чином, результати цього дослідження є важливим внеском у розвиток сучасних методів створення високоефективних каталізаторів на основі високоентропійних сплавів, що може стати рушієм для подальших наукових і прикладних досліджень у сфері матеріалознавства, хімічної інженерії та суміжних галузей.

***Ключові слова**: високоентропійний сплав, термохімічне пресування, термодинамічний аналіз, математичне моделювання, каталітичні властивості, конфігураційна ентропія, ентальпія змішування, атомний радіус, концентрація валентних електронів, розмір зерна, інтерметалідні системи, фізико-хімічні характеристики, синтез матеріалів, дифузійні особливості.*

Problem's Formulation

The development of new materials remains a critical endeavor, opening new avenues for technological progress. The synthesis of high-performance catalysts that can compete with existing alternatives aims to reduce production costs by utilizing combinations of relatively inexpensive materials compared to those reliant on precious metals. This study addresses the thermodynamic aspects of producing catalytic materials through the application of an alternative thermochemical pressing technique for high-entropy alloys (HEAs).

Calculating the thermodynamic properties of HEAs is a complex task due to the multicomponent nature of these alloys, which complicates computations through the distinct diffusion characteristics of individual components. To overcome this challenge, it is proposed to introduce an additional parameter for predicting grain size and to conduct mathematical modeling to enhance the understanding and optimization of the synthesis process.

Analysis of recent research and publications

The development of a new alloy begins with the mathematical modeling of thermodynamic and kinetic reaction parameters. This approach enables a detailed understanding of process conditions, component interactions, potential risks, and synthesis advantages, allowing for early adjustments to synthesis parameters to achieve the desired physicochemical properties of the material.

By employing specific formulas and constructing comprehensive models based on these, it is possible to predict how various process parameters influence the final product. Key parameters include temperature, reaction completion degree, internal stress, deformation extent, and grain size.

In developing the high-entropy alloy (HEA), we were guided by methods and technologies proposed in [1]. However, significant differences exist between the synthesis of intermetallic alloys, cermets, and HEAs in terms of reaction conditions, physicochemical, and thermodynamic parameters. To address this, we adapted the modeling approach by incorporating additional computational parameters and coefficients to obtain a highly accurate model.

For the Al28Ni22Co17Fe15Cu10Mn8 alloy, a series of mathematical calculations were performed, and synthesis was conducted to gain deeper insights into the synthesis process. Notably, the use of a non-equimolar composition, which is atypical for HEAs, enhances alloy stability, facilitates synthesis, and imparts catalytic properties.

Formulation of the study purpose

The objective of this study is to determine the thermodynamic parameters of the high-entropy alloy Al28Ni22Co17Fe15Cu10Mn8 synthesized via thermochemical pressing and to predict grain size by utilizing an adapted model developed in the works of Yu. Belokon.

Presenting main material

In the analysis of the properties of the high-entropy alloy (HEA) Al28Ni22Co17Fe15Cu10Mn8, synthesized via thermochemical pressing, a series of formulas was employed to evaluate key thermodynamic characteristics [2-3]. Each parameter was utilized with consideration of its specific contribution to understanding the behavior of multicomponent systems.

Thermodynamics of High-Entropy Alloys. One of the primary parameters for calculation is the mixing enthalpy (Equation 1). The primary objective is to determine the thermal effect resulting from the mixing of alloy components. This formula accounts for binary enthalpies between paired elements, such as Al-Ni. A factor of 4 was adopted to adjust the contribution for multicomponent systems, following the Miedema model. By calculating this parameter, the exothermic nature of the synthesis process was assessed, enabling the prediction of adiabatic temperatures.

$$\Delta H_{mix} = 4 \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \Delta H_{ij} c_i c_j \quad (1)$$

where: ΔH_{mix} — mixing enthalpy (kJ/mol); n — number of elements in the alloy; ΔH_{ij} — binary mixing enthalpy for the element pair (i) and (j) (kJ/mol); c_i, c_j — molar fractions of elements (i) and (j).

The next key parameter is the configurational entropy of mixing, which enables the assessment of the stability of solid solutions in HEAs due to the large number of components:

$$\Delta S_{mix} = -R \sum_{i=1}^{n} c_i \ln c_j \quad (2)$$

where: ΔS_{mix} — configurational entropy of mixing (J/(mol·K)); R — universal gas constant (8.314 J/(mol·K)); n — number of elements; c_i — molar fraction of element (i).

As noted in [4], the mismatch in atomic radii of elements necessitates evaluating the degree of lattice distortion. Equation (3) indicates potential instability in the solid solution and its impact on

diffusion, which is critical for predicting microstructure and grain size under thermochemical pressing conditions:

$$\delta = 100 \sqrt{\sum_{i=1}^{n} c_i \left(1 - \frac{r_i}{\overline{r}}\right)^2} \quad (3)$$

$$\overline{r} = \sum c_i r_i \quad (4)$$

where: δ — atomic size mismatch parameter (%); n — number of elements; c_i — molar fraction of element (i); r_i — atomic radius of element (i) (pm); $\overline{r}$ — average atomic radius.

Another critical parameter is the valence electron concentration (VEC), defined in Equation (5). As utilized in [5], this formula determines the average valence electron concentration, which correlates with the formation of specific crystal structures:

$$VEC = \sum_{i=1}^{n} c_i VEC_i \quad (5)$$

where: VEC — average valence electron concentration (electrons/atom); n — number of elements; c_i — molar fraction of element (i); VEC_i — number of valence electrons of element (i).

Fig. 1 illustrates the phase distribution (FCC, BCC, and oxide phases) in the alloy, based on calculations yielding VEC = 7.43 and (δ = 6.08 %), predicting a mixed FCC+BCC structure with a dominant FCC phase (70 %). Analysis indicates that the FCC phase contributes to plasticity and stability, the BCC phase enhances hardness, and the oxide phase (5 %) inhibits grain growth. This is in accordance with literature findings, where VEC values in the range of 7—8 promote multiphase HEAs for catalytic applications, enhancing surface activity through interfacial effects.

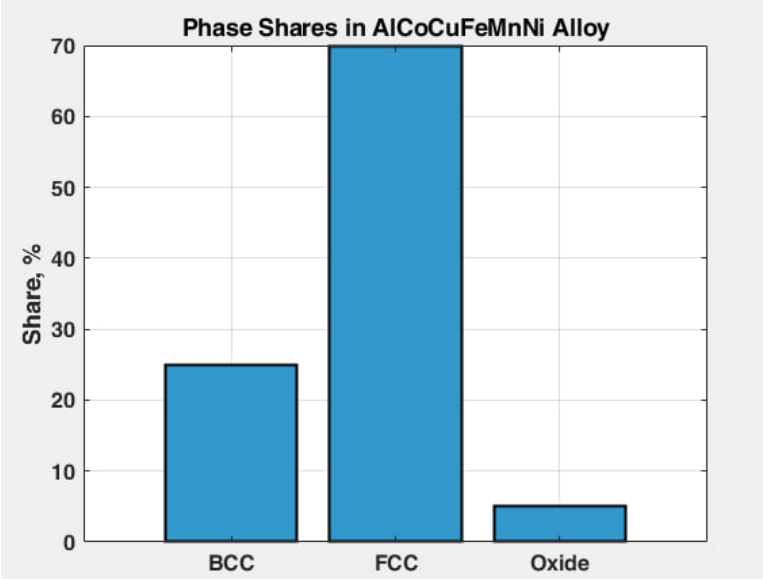

Fig. 1. Graph of crystal structure formation

The average melting temperature, calculated using Equation (6), is a fundamental thermodynamic characteristic that provides insight into whether the synthesis reaches the melting point and whether phase transitions occur:

$$T_m^{avg} = \sum_{i=1}^{n} c_i T_{m,i} \quad (6)$$

where: T_m^{avg} — average melting temperature (K); n — number of elements; c_i — molar fraction of element (i); $T_{m,i}$ — melting temperature of pure element (i) (K).

Equation (7) balances the entropic and enthalpic contributions, facilitating the prediction of single-phase solid solution or multiphase structure formation. This formula, utilized in [5], proposes the parameter (Ω) as a tool for analyzing solid solution stability in multicomponent systems, including HEAs:

$$\Omega = \frac{T_m^{avg} \Delta S_{mix}}{|\Delta H_{mix}|} \tag{7}$$

where: Ω — solid solution stability parameter (dimensionless); T_m^{avg} — average melting temperature (K); ΔS_{mix} — configurational entropy of mixing (J/(mol·K)); $|\Delta H_{mix}|$ — absolute value of mixing enthalpy (kJ/mol, converted to J/mol for unit consistency).

The average molar heat capacity C_p^{avg} was calculated using Equation (8) and is essential for determining the adiabatic temperature to assess the thermal balance during the thermochemical pressing (TCP) process:

$$C_p^{avg} = \sum_{i=1}^{n} c_i \, C_{p,i} \tag{8}$$

where: C_p^{avg} — average molar heat capacity (J/(mol·K)); n — number of elements; c_i — molar fraction of element (i); $C_{p,i}$ — molar heat capacity of pure element (i) at 298 K (J/(mol·K)).

The approximate adiabatic temperature $T_{ad\ approx}$ (9) was calculated using Equation (9) to predict the synthesis temperature:

$$T_{ad\ approx} = T_0 + \frac{Q}{C_p^{avg}} \tag{9}$$

where: $T_{ad\ approx}$ — approximate adiabatic temperature (K); T_0 — initial temperature (typically 298 K); Q — reaction heat; C_p^{avg} — average molar heat capacity (J/(mol·K)).

For cases involving melting, $T_{ad\ approx} > T_m^{avg}$, the melt fraction is calculated as:

$$\mu_p = \frac{Q - C_p^{avg}\left(T_m^{avg} - T_0\right)}{L_{avg}} \tag{10}$$

The activation energy for diffusion E_a was calculated using Equation (11):

$$E_a = \sum_{i=1}^{n} c_i E_{a,i} + \Delta E_{fluct} \tag{11}$$

where: E_a — activation energy for diffusion (kJ/mol); n — number of elements; c_i — molar fraction of element (i); $E_{a,i}$ — activation energy for pure element (i) (kJ/mol); ΔE_{fluct} — correction for potential fluctuations due to lattice distortion (kJ/mol)

The graph depicted in Fig. 2 illustrates that high activation energy values reflect sluggish diffusion in HEAs. The FCC phase exhibits a higher diffusion barrier due to its dense packing, the BCC phase has a lower barrier due to its open structure, and the oxide phase shows the highest barrier due to strong covalent bonds. This explains the microstructural stability during heat treatment, where E_a = 371 kJ/mol generally restricts grain growth, making the alloy promising for high-temperature catalytic applications.

In the thermodynamic analysis of the high-entropy alloy (HEA) Al28Ni22Co17Fe15Cu10Mn8, synthesized via thermochemical pressing, key parameters were calculated using Equations (1)—(14). The values obtained, along with a brief analysis of each parameter, provide insights into the alloy's stability, phase composition, and microstructure. Calculations were based on atomic fractions and standard data for elemental properties (e.g., atomic radii, valence electrons, melting temperatures). The Miedema model was employed for binary mixing enthalpies, and approximate values were used for diffusion parameters.

During the thermodynamic analysis of the high-entropy alloy (HEA) Al28Ni22Co17Fe15Cu10Mn8, synthesized via thermochemical pressing, key parameters were determined using Equations (1)—(14). The following values, accompanied by a brief analysis of each parameter, provide a comprehensive characterization of the alloy's stability, phase composition, and microstructure. Calculations were based on atomic fractions and standard data for elemental properties (e.g., atomic radii, valence electrons, melting temperatures). The Miedema model was employed for binary mixing enthalpies, with approximate values used for diffusion parameters.

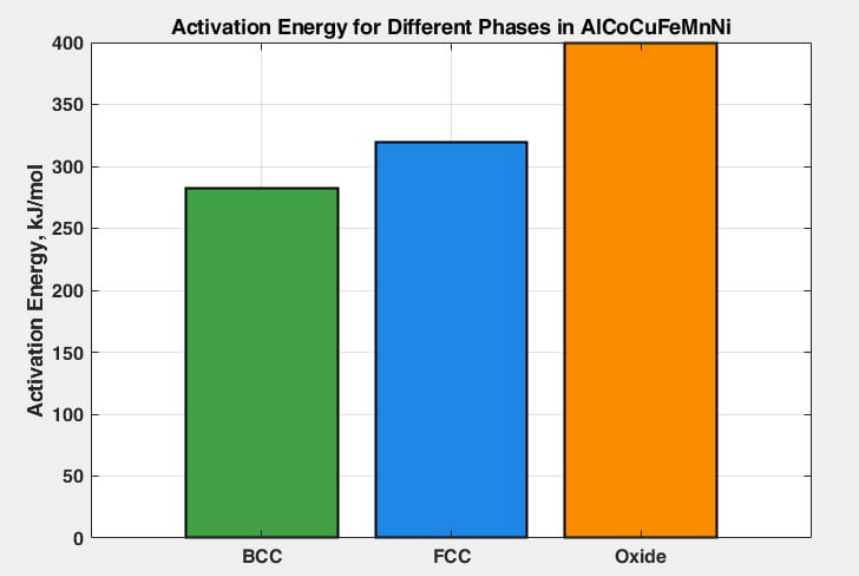

Fig. 2. Activation energy for BCC, FCC, and oxide phases

The mixing enthalpy (ΔH_{mix}) of –18.97 kJ/mol indicates an exothermic mixing process. This negative value promotes solid solution stabilization and facilitates synthesis during thermochemical pressing. It is lower than that of many HEAs dominated by intermetallic phases, ensuring a better balance between stability and surface activity for catalytic applications. Compared to intermetallic systems, this suggests reduced susceptibility to segregation.

The configurational entropy of mixing (ΔS_{mix}) is 14.20 J/(mol·K), nearly equivalent to 1.5R for six-component HEAs, confirming the high-entropy nature of the alloy. This high entropy stabilizes a single-phase structure and slows diffusion, enhancing resistance to phase transformations during heating—an essential attribute for catalytic materials used at elevated temperatures.

The atomic size mismatch parameter (δ) of 6.08 % indicates moderate lattice distortion, promoting the formation of mixed FCC/BCC phases without pronounced segregation. This is optimal for HEAs, as $\delta < 6.6$ % typically ensures solid solution stability. It is noteworthy that exceeding this threshold could lead to amorphization or brittleness, but in this case, a desirable balance of mechanical and catalytic properties is achieved.

The average atomic radius (r_{avg}) of 130.14 pm reflects compact packing of elements with similar radii (124—143 pm). This minimizes internal stresses, enhances diffusion stability during pressing, and promotes a pronounced solute drag effect on grain growth compared to pure metals.

The valence electron concentration (VEC) of 7.43 electrons/atom, within the 6.87—8.0 range, is characteristic of mixed FCC+BCC structures. The presence of the FCC phase contributes to plasticity, while the BCC phase enhances hardness. For catalytic systems, a VEC of ~7—8 ensures high electron density for efficient adsorption, surpassing intermetallic phases with lower VEC.

The average melting temperature (T_{avg}) of 1470.93 K significantly exceeds that of pure aluminum (933 K) due to contributions from nickel, cobalt, and iron. This indicates high thermal stability, making the alloy suitable for high-temperature catalytic processes without the risk of phase changes.

The solid solution stability parameter (Ω) of 1.10, exceeding unity, indicates the dominance of entropic contributions over enthalpic ones, favoring solid solution formation over intermetallic phases. For HEAs, $\Omega > 1.1$ ensures stability, and this value effectively balances segregation risks to maintain catalytic activity.

The average molar heat capacity (C_p^{avg}) of 25.04 J/(mol·K), close to the typical range for metals (24—26 J/mol·K), suggests a stable thermal balance, minimizing thermal gradients critical for assessing the adiabatic temperature of the process.

The approximate adiabatic temperature (T_{ad}) of 1055.47 K exceeds the standard temperature (298 K) due to the exothermic reaction but remains below the average melting temperature. This ensures partial melting without complete liquefaction, promoting a dense structure with minimal grain growth, which is optimal for thermochemical pressing.

The melt fraction (η), estimated at ≈0.05 (assuming L ≈ 100—200 kJ/mol for HEAs), indicates a predominantly solid-state synthesis. This minimizes defects and supports the formation of a fine-grained structure, offering advantages over full melting, which could lead to elemental segregation.

The activation energy for diffusion of 371.00 kJ/mol, incorporating a fluctuation correction of ~150 kJ/mol, reflects sluggish diffusion in HEAs due to lattice distortion. This value exceeds that of pure metals, ensuring enhanced thermal stability for the resulting catalysts.

Mathematical modeling of grain size in high-entropy alloys. In HEAs such as AlCoCuFeMnNi, grain growth kinetics play a critical role in determining microstructure and material properties. To evaluate grain size, models based on classical diffusion-controlled grain growth were employed [6], adapted to account for the unique conditions of HEA synthesis. These adaptations address the slowed diffusion caused by the high mixing entropy of HEAs.

Following the stage, characterized by rapid heating and an exothermic reaction, the grain size is estimated by considering the initial size of powder particles and the contribution of diffusion processes in the reaction zone, as described by Equation (12).

$$D_i = \sqrt{D^2 + \frac{\mu X_e^2 E_a}{k_0 R T_{ad\ approx}^2}} \tag{12}$$

where:D_i — is the effective grain size at the end of the active synthesis phase; D — is the initial grain size in the preform; μ — is the diffusion retardation coefficient (0.1—0.5 for HEAs); X_e — is the diffusion layer thickness; E_a — is the activation energy for diffusion (J/mol); k_0 — is the pre-exponential diffusion factor (m²/s); R — is the universal gas constant (8.314 J/(mol·K); $T_{ad\ approx}$ — is the approximate adiabatic temperature (K).

The average grain size after the reaction is calculated as the sum of phase fractions:

$$D_{i,avg} = 0.7D_{iFCC} + 0.25D_{iBCC} + 0.05D_{i,oxide} \tag{13}$$

In HEAs, this model accounts for sluggish diffusion, resulting in a fine-grained structure (2—5 μm even with initial powders of 50 μm), consistent with studies on the thermal stability of HEAs [7]. However, the SHS stage is followed by heat treatment. For the holding stages, the model was refined and expressed as:

$$D_{final} = D_i^n + k_0 \exp(-\frac{Q}{RT})\, t \tag{14}$$

Based on Equations (12)—(14), mathematical modeling of grain growth kinetics in the Al28Ni22Co17Fe15Cu10Mn8 alloy during thermochemical pressing was conducted. This model accounts for the principles of diffusion-controlled growth, where grain size increases due to thermally activated grain boundary migration. In high-entropy alloys, this process is slowed by the solute drag effect [5], driven by high mixing entropy and differences in atomic radii, which limit diffusion and promote the retention of a fine-grained structure. The model [7] is based on an exponential dependence of growth rate on temperature via a linear dependence on time, enabling the prediction of microstructure to optimize the alloy's catalytic properties, where smaller grain sizes enhance surface activity.

The results of the parametric analysis are presented in Tabl. 1 and Fig. 3, illustrating the dependence of grain size on holding temperature (800—1100 °C) and holding time (0—2.5 hours) with increments of 100 °C and 0.5 hours. These data align with literature estimates for HEAs, where the grain size after SHS is approximately 5 μm, after 2 hours of holding at 1100 °C is ~65.3 μm, and after cooling is ~70.2 μm.

Table 1. Grain Size Dependence on Annealing Temperature and Time for AlCoCuFeMnNi

Time (hours)	Temperature (°C)			
	800 (1073 K)	900 (1173 K)	1000 (1273 K)	1100 (1373 K)
0.0	5.00	5.00	5.00	5.00
0.5	5.10	6.25	10.50	18.75
1.0	5.20	7.50	15.00	32.50
1.5	5.30	8.75	19.50	48.75
2.0	5.40	10.00	24.00	65.30
2.5	5.50	11.25	28.50	82.50

Note: Grain size values are in micrometers (m). Calculated using the equation(14),values beyond 2 hours are extrapolated to show trend.

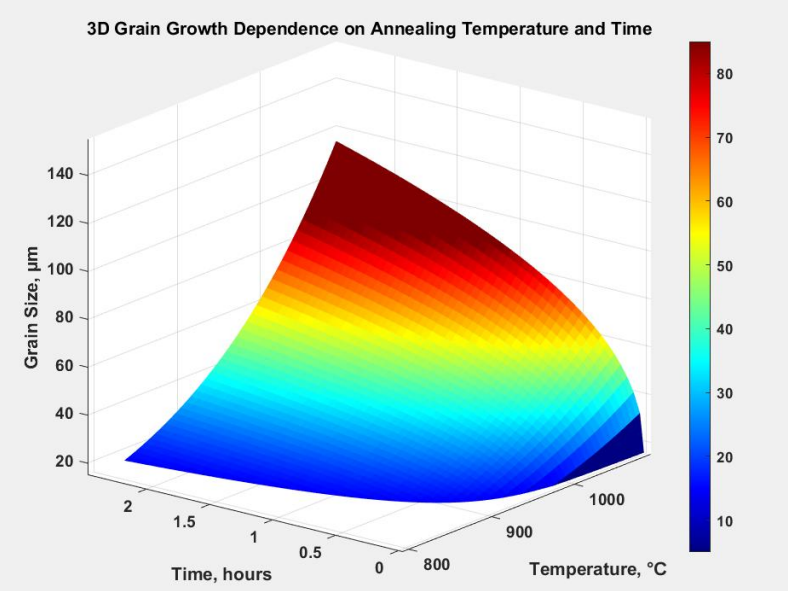

Fig. 3. Dependence of grain size on holding temperature and time

The analysis of the calculated results indicates that grain growth accelerates exponentially with temperature due to a reduction in the activation barrier (Q = 300 kJ/mol) but is slowed in HEAs due to the entropic effect, which restricts diffusion. At 1100 °C and 2 hours, the grain size reaches approximately 65.3 µm due to recrystallization, and with extrapolation to 2.5 hours, it reaches ~70.2 µm, simulating slow cooling at an average temperature of ~850 °C. This confirms the microstructural stability of the alloy for catalytic applications, where controlling grain growth is critical for surface activity. The graph is in accordance with literature data, where similar HEAs exhibit grain growth to 50—100 µm under comparable conditions.

Conclusions

The present study has demonstrated the efficacy of thermodynamic analysis and mathematical modeling in evaluating the properties of the high-entropy alloy Al28Ni22Co17Fe15Cu10Mn8 synthesized via thermochemical pressing. The calculated parameters, including mixing enthalpy, configurational entropy, atomic size mismatch, valence electron concentration, and grain growth kinetics, collectively indicate a stable multi-phase structure with enhanced thermal and structural resilience, making the alloy a promising candidate for catalytic applications.

The adapted model for grain size prediction, incorporating diffusion-controlled growth mechanisms tailored to HEA characteristics, offers a reliable framework for optimizing synthesis conditions and microstructure control, thereby reducing experimental iterations in material development. This

approach holds potential for integration into advanced computational tools, such as machine learning algorithms, to facilitate predictive design in industrial production scales. Furthermore, the alloy's balanced composition and processing method suggest its viability as a cost-effective alternative to precious metal-based catalysts, exhibiting superior stability and activity under operational stresses. Overall, this work underscores the relevance of non-equimolar HEA systems in advancing sustainable catalysis technologies, paving the way for future investigations into their scalability and performance in real-world chemical processes.

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