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DESIGN AND THERMODYNAMIC EVALUATION OF A MULTI-COMPONENT HIGH ENTROPY ALLOY CATALYST Al-Ni-Co-Fe-Cu-Mn UNDER THERMOCHEMICAL PRESSING CONDITIONS

РОЗРОБКА ТА ТЕРМОДИНАМІЧНА ОЦІНКА БАГАТОКОМПОНЕНТНОГО ВИСОКОЕНТРОПНОГО СПЛАВНОГО КАТАЛІЗАТОРА Al-Ni-Co-Fe-Cu-Mn В УМОВАХ ТЕРМОХІМІЧНОГО ПРЕССУВАННЯ

High-entropy alloys (HEAs) are multicomponent materials containing five or more elements in near-equiatomic or carefully selected ratios. Using high configurational entropy, HERs stabilize simple crystal structures such as face-centered cubic (FCC) or volume-centered cubic (VCC), which provides

exceptional properties: high mechanical strength, resistance to oxidation at high temperatures, and natural catalytic potential. These qualities make WEC ideal for innovative applications. The compositional flexibility of systems such as Al-Ni-Co-Fe-Cu-Mn allows for fine-tuning of microstructure and surface characteristics, contributing to the creation of stable active centers under thermochemical conditions. Existing research in the field of materials science confirms their superiority over traditional materials.

***Keywords**: high-entropy alloys, configurational entropy, crystal structures, catalytic potential, thermochemical resilience, Al-Ni-Co-Fe-Cu-Mn.*

Високоентропійні сплави (ВЕС) це багатокомпонентні матеріали, що містять п'ять або більше елементів у близьких до еквіатомних чи ретельно підібраних співвідношеннях. Використовуючи високу конфігураційну ентропію, ВЕС стабілізують прості кристалічні структури, такі як гранецентрована кубічна (ГЦК) або об'ємноцентрована кубічна (ОЦК), що забезпечує виняткові властивості: високу механічну міцність, стійкість до окислення при високих температурах і природний каталітичний потенціал. Ці якості роблять ВЕС ідеальними для інноваційних застосувань. Композиційна гнучкість систем, таких як Al-Ni-Co-Fe-Cu-Mn, дозволяє точно налаштовувати мікроструктуру та поверхневі характеристики, сприяючи створенню стійких активних центрів у термохімічних умовах. Наявні дослідження у області матеріалознавства, підтверджують їх перевагу над традиційними матеріалами. Це дослідження зосереджене на розробці та термодинамічній оцінці ВЕС з метою використання у процесах каталітичного відновлення газових фаз. Мета розвитку каталітичних матеріалів у напрямку ВЕС супроводжується необхідністю отримання альтернативи наявним високовартісним платиновим каталізаторам. У дослідженні розглядаються 4 системи різного складу, та порівнюються їх термодинамічні властивості.

***Ключові слова**: високоентропійні сплави, конфігураційна ентропія, кристалічні структури, каталітичний потенціал, термохімічна стійкість, Al-Ni-Co-Fe-Cu-Mn.*

Problem's Formulation

High-entropy alloys (HEA) are materials that have unique physical and chemical parameters due to the richness of the systems, so their research and development are important for further progress. The high configuration entropy of rich component systems with a strong warehouse ensures the formation of a stable crystal lattice such as BCC or FCC, which increases mechanical strength, resistance to oxidation for high temperatures and potency of formation of active catalytic centers. The main goal of this research lies in the development of a system of non-equiatomic high-entropy alloy for thermochemical presing using methods of mathematical modeling of synthesis and assessment of physicochemical and thermodynamic parameters for vicorization in catalyst components in thermochemical processes at high temperatures. The main focus of this achievement is on the selection of the optimal molar ratio of elements to achieve optimal parameters of thermodynamic reactions, ensured phase stability and proximity to ideal dissolution.

Analysis of recent research and publications

Research on high-entropy alloys describes their potential as catalysts due to their multi-element composition, which leads to high configurational entropy and structural stability. The main focus is on studying their thermodynamic properties and catalytic performance in various applications, including gas purification.

In general, the HES effect is achieved through the interaction between elements, which affects catalytic activity and stability. Pt-containing HESs demonstrate high activity in HER and MOR due to multiple active sites and fast electron transfer [3]. Platinum-free catalysts such as CoFeNiGaZn achieve 98 % conversion of *CO* to CO_2 at 500 °C, which is explained by the transfer of electrons from nickel to adsorbed *CO* and O_2 molecules [1]. The CoNiCuRuPd system in the form of a surface layer based on TiO_2 demonstrates high activity in the hydrogenation of CO_2 with a CH_4 selectivity of 68.3 % at 400 °C, which is associated with the release of hydrogen [2]. Thus, WPPs as a class can carry out *CO* oxidation and related reactions involving *CO*, VOCs and H_2S.

To design a catalyst, a necessary step is to determine the general thermodynamic properties. The method of calculating the enthalpy of mixing is to use the Miedema model; the result of the calculations

should be enthalpy values from -22 to 7 kJ/mol, which contribute to the formation of a solid solution. For HEA, $\Delta S_{mix} > 1.5R$ (approximately 12.47 J/(mol-K)) stabilises disordered phases [6].

Coke gas purification requires catalysts capable of handling the complex gas composition (55—60 % H_2, 23—27 % CH_4, 5—8 % CO, 1.5—3 % CO_2, 2—4 % C_nH_m) and meeting strict standards (e.g. sulphur ≤ 0.1 mg/nm³, phenols ≤ 1 mg/nm³) [7]. Current research on HEA catalysts for high-temperature processes with gaseous phases is limited, especially for *Mn*-containing alloys. Main fuction of *Mn* is improving redox properties, as in the case of nanoporous HEAs for CO oxidation [8]. However, there is a lack of data on Al-Ni-Co-Fe-Cu-Mn systems at 900—1300 °C, but there are calculations of the reduction intensity for intermetallic systems [9]. For example, *PtPdCoNiMn* shows high activity in oxygen reduction [4], but there is a lack of high-temperature tests relevant to coke production and the general type of platinum catalysts is the opposite direction of development from this study.

Empirical and semi-empirical methods, such as the CALPHAD method and first-principles calculations, are used to obtain data on the stability of HEAs [6]. HEA with moderate ΔH_{mix} and high ΔS_{mix} are resistant to phase decomposition. However, the use of non-equimolar compositions, such as $Al_{25}Ni_{15}Co_{15}Fe_{15}Cu_{15}Mn_{15}$, has not been sufficiently studied, and there is a lack of information on the use and optimisation of HEA composition for high-temperature gas cleaning. It should be noted that the lack of experimental data on the role of *Mn* at 900—1300 °C limits the understanding of its contribution to the conversion of *CO* and H_2S

Formulation of the study purpose

The purpose of this study is to develop and preliminary thermodynamically evaluate a highly entropy system of Al-Ni-Co-Fe-Cu-Mn with different molar configurations of molar composition, which aims to create a catalytic highly entropy alloy for gas phase purification. The main task is mathematical modeling and calculation of key parameters of the formation of a highly entropic alloy such as enthalpy — ΔH_{mix} and entropy — ΔS_{mix} mixing, free Gibbs energy — ΔG_{mix} to assess phase stability and catalysis ability in the temperature range 900—1300 ° C. The Miedema model for binary compounds and their interaction is used as the main one for calculations.

Presenting main material

For the thermodynamic analysis of the properties of high-entropy alloys, the following formulas were used:

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

where: R — the universal gas constant, R=8.314 J/(mol\K); ∑ =1n c_i — summation from i=1 to, where n is the number of components in the alloy; c_i— the molar fraction of the i-th component in the alloy.

ln c_i — the natural logarithm of the molar fraction of the i-th component.

$$\Delta H_{mix} = 4 \sum_{i=1}^{4} \sum_{j=i+1}^{5} c_i c_j H_{ij}, \quad (2)$$

where: c_i is molar fraction of the i-th component; c_j is molar fraction of the j-th component; H_{ij} is mixing enthalpy between the i-th and j-th components, measured in kJ/mol.

$$\Delta G_{mix} = \Delta H_{mix} - T \cdot \Delta S_{mix}\,, \quad (3)$$

where: ΔG_{mix} — the Gibbs free energy of mixing (measured in kJ/mol); ΔH_{mix} — the mixing enthalpy (from Formula 2); T — the temperature (measured in Kelvin, e.g., T=298 K for room temperature); ΔS_{mix} — the mixing entropy (from Formula 1)

$$VEC_{HEA} = \sum_{i=1}^{n} c_i \, (VEC)_i\,, \quad (4)$$

where: c_i — the molar fraction of the i-th component; $(VEC)_i$ — the valence electron concentration of the i-th component (number of valence electrons).

These formulas enabled the evaluation of key alloy parameters that influence its phase stability and crystalline structure. Specifically, ΔS_{mix} reflects the degree of disorder in the system, a defining characteristic of high-entropy alloys. ΔH_{mix}, which depends on pairwise elemental interactions, aids in assessing the energetic contribution to alloy formation, though accurate values require experimental H_{ij} data. ΔG_{mix} integrates entropic and enthalpic contributions, facilitating predictions of phase

thermodynamic stability at a given temperature [5]. Finally, the valence electron concentration (VEC_{HEA}) indicates the potential coexistence of FCC and BCC phases, but in this study, we focused on modeling both structures separately to gain deeper insight into their individual contributions [6].

Table 1. ΔHmix calculated for binary systems using the Miedema model

─	Al	Ni	Co	Fe	Cu	Mn
Al	─	-22	-19	-11	-7,6	-19
Ni	-22	─	-9	-2	3,6	-8
Co	-19	-9	─	-1	6	-5
Fe	-11	-2	-1	─	13	5
Cu	-7,6	3,6	6	13	─	4
Mn	-19	-8	-5	-5	4	─

Four alloys were selected for the calculation of the required high-entropy system intended for use in catalytic processes:

– Al20Ni20Co20Fe20Cu20
– Al28Ni22Co17Fe15Cu10Mn8
– Al32Mn23Ni17Fe8Cu8Co12
– Al32Ni15Co13Mn15Fe10Cu15

One of the primary conditions for achieving a solid solution in a high-entropy system is adherence to the following condition:

$$13{,}4 \leq \Delta S_{\text{mix}} \leq 22 \left(\frac{J}{mol \cdot K}\right). \quad (5)$$

Based on data obtained from open sources, mathematical modeling of several systems with varying molar configurations was conducted. This was done to determine the optimal composition of a high-entropy alloy (HEA) that would meet the specified parameters required for synthesis and subsequent performance as a catalytic product. For the synthesis of the HEA, the Al-Ni-Co-Fe-Cu-Mn system was selected. A detailed analysis of this system necessitates an explanation of the choice of specific elements.

The foundation of the HEA is aluminum, which promotes the formation of the BCC phase due to its low valence electron concentration (VEC = 3) and enhances oxidation resistance by forming protective Al_2O_3 layers. Additionally, *Al* tends to segregate to the surface under high temperatures, facilitating the formation of catalytically active sites.

Nickel is a key element with VEC = 10, forms the FCC phase, characterized by a dense atomic arrangement and, consequently, a high number of catalytic sites. In the ternary Ni-Co-Fe system, *Ni* significantly enhances catalytic activity and plays a pivotal role in *CO* oxidation reactions.

Other chemical elements serve as auxiliary components, enhancing the physicochemical properties of the HEA: cobalt improves the mechanical properties and is active in *CO* reactions; iron (*Fe*) stabilizes the mixed FCC+BCC phase and forms Fe_2O_3 oxides that can act as active centers; copper increases the alloy's plasticity and exhibits a tendency for surface segregation; manganese enhances high-temperature stability and forms oxides that serve as catalytically active centers. All selected elements possess either BCC or FCC lattices, a critical factor in HEA formation.

Among numerous options, the following compositions were chosen: Al28Ni22Co17Fe15Cu10Mn8, Al32Mn23Ni17Fe8Cu8Co12, Al32Ni15Co13Mn15Fe10Cu15, and Al20Ni20Co20Fe20Cu20. Analytical review of existing literature suggests that equiatomic compositions, such as Al20Ni20Co20Fe20Cu20, are optimal for HEA formation. However, challenges arise in synthesizing this material via thermochemical pressing due to *Al* high reactivity, which initiates reactions and requires a higher concentration. Thus, the Al20Ni20Co20Fe20Cu20 configuration was taken as a reference for ideal conditions.

Although the chemical composition remains constant, the molar ratio plays a crucial role in selecting the optimal system. Among the four variants, the system must meet specific physicochemical and thermodynamic criteria: ΔS_{mix} should range from 13.4 to 22 J/(mol·K), the phase should be FCC, BCC, or a combination thereof, and the alloy must exhibit stability and capability for *CO* oxidation and potentially CO_2 hydrogenation.

The selected systems share similar characteristics, but each warrants individual evaluation to justify the choice. The Al20Ni20Co20Fe20Cu20 system is equiatomic, a significant advantage for HEA formation, but its near-minimum ΔS_{mix} value makes it less favorable. The Al28Ni22Co17Fe15Cu10Mn8 system, with high *Ni* (22 %) and *Co* (17 %) content, plays a critical role in oxidation and hydrogenation reactions. Its $T \cdot \Delta S_{mix}$ value indicates good high-temperature stability, essential for catalytic applications. With a VEC of 7.43, it suggests a mix of FCC and BCC phases, ensuring a high diversity of catalytic sites. Additionally, its ΔS_{mix} is sufficiently high for successful HEA formation. The Al32Mn23Ni17Fe8Cu8Co12 system has an adequate ΔS_{mix}, but its key elements, *Al* and *Mn*, are more relevant for volatile organic compound (VOC) oxidation than *CO* catalysis. The Al32Ni15Co13Mn15Fe10Cu15 system exhibits the highest ΔS_{mix} among the selected variants, but its key elements and application variations indicate it is unsuitable for the intended purposes. Detailed modeling results are presented in Tabl. 2.

Table 2. Comparative characteristics of key HEA parameters for determining the optimal composition

Alloy configuration	**ΔS_{mix}**	**$T \cdot \Delta S_{mix}$**	**VEC**	**Phase**	**Key elements**	**Using**
Al20Ni20Co20Fe20Cu20	13,38	21,40	8,2	FCC	Ni, Co, Cu	Hydration CO_2, oxidation CO
Al28Ni22Co17Fe15Cu10Mn8	14,20	22,71	7,43	FCC+BCC	Ni, Co, Cu	Hydration CO_2, oxidation CO
Al32Mn23Ni17Fe8Cu8Co12	13,82	22,11	6,87	BCC або FCC+BCC	Al, Mn	Oxidation VOC, combustion
Al32Ni15Co13Mn15Fe10Cu15	14,25	22,79	7,13	FCC+BCC	Cu, Ni, Mn	CO_2 hydrogenation, reforming

After conducting a series of mathematical calculations and analyzing literature sources related to the development of high-entropy alloys, it was hypothesized that the most advantageous and suitable system for our purposes has the configuration Al28Ni22Co17Fe15Cu10Mn8. Detailed results are presented in Tabl. 3.

Table 3. Table of Gibbs energy change dependence on temperature for the Al28Ni22Co17Fe15Cu10Mn8 alloy

Temperature, K°	ΔH_{mix} , kJ/mol	ΔS_{mix} , kJ/mol	ΔG_{mix} , kJ/mol	$T\ \Delta S_{mix}$ kJ/mol
400	-14,59	14,20	-20.27	5.67
600			-23.11	8.51
800			-25.95	11.35
1000			-28.79	14.19
1200			-31.63	17.03
1400			-34.47	19.87
1600			-37.31	22.71

High *Ni* and *Co* content ensures active catalytic sites, while *Cu* (10 %) may segregate to the surface, enhancing efficiency. High-temperature stability is confirmed by a $T \cdot \Delta S_{mix}$ value exceeding 20 kJ/mol at 1400 K and above.

Fig. 1 illustrates that the Al28Ni22Co17Fe15Cu10Mn8 alloy is thermodynamically stable across a wide temperature range; however, varying *Al* content may destabilize the phase at lower temperatures. This underscores the importance of optimizing the composition for specific operating conditions, particularly for high-temperature applications such as catalysis. Regions where the surface properties change abruptly may indicate temperatures or compositions at which phase transitions (e.g., FCC → BCC) could occur, necessitating further analysis using diffraction data.

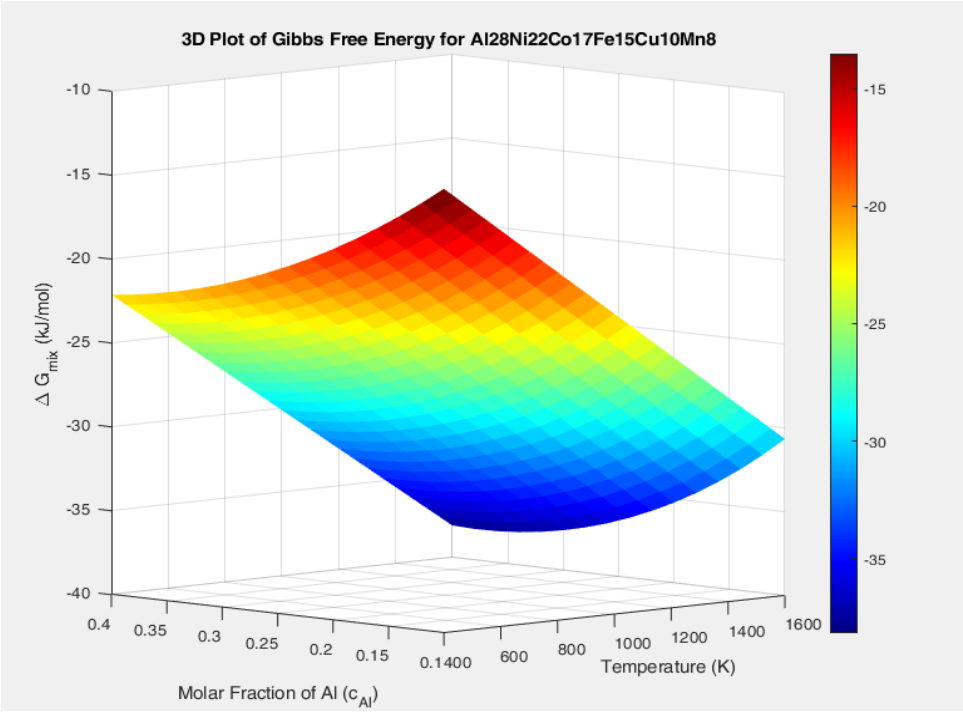


Fig. 1. ΔG_{mix} as a function of temperature T and the molar fraction of one of the elements

Fig. 2 illustrates that a VEC ≈ 7.43 indicates a boundary between FCC and BCC phases (FCC predominates at VEC > 8, BCC at VEC < 6.87). At VEC = 7.43, the alloy may form either FCC or BCC phases, depending on temperature. The graph demonstrates that at low temperatures (400 K), ΔG_{mix} is less negative (≈ −7 kJ/mol), which may favor the formation of the BCC phase, whereas at 1600 K (ΔG_{mix} ≈ −15 kJ/mol), the FCC phase becomes more stable due to the entropic contribution.

For modeling the crystal lattice of Al28Ni22Co17Fe15Cu10Mn8, the VESTA visualization software was employed, significantly aiding in the depiction of the structure. However, to simulate the placement of atoms within BCC and FCC crystal lattices, a custom Python script was developed, which, within the framework of these lattice concepts, randomly positioned the atoms of the elements. The powder diffraction pattern enables confirmation of the crystal lattice by comparing peak positions with expected 2θ values.

Fig. 3 illustrates the three-dimensional FCC crystal lattice model and the powder diffraction pattern of Al28Ni22Co17Fe15Cu10Mn8. Peaks characteristic of FCC (e.g., (111), (200)) confirm that the model accurately reproduces the FCC phase. The shift in peaks due to the supercell (2θ ≈ 10° instead of 42.6°) is expected, as the supercell lattice parameter (a = 7.2 Å) is twice that of the unit cell (a = 3.6 Å). The FCC phase, as demonstrated by thermodynamic calculations, is stable at VEC ≈ 7.43, consistent with the model. This aids in predicting whether the FCC phase will remain dominant under varying conditions (temperature, pressure).

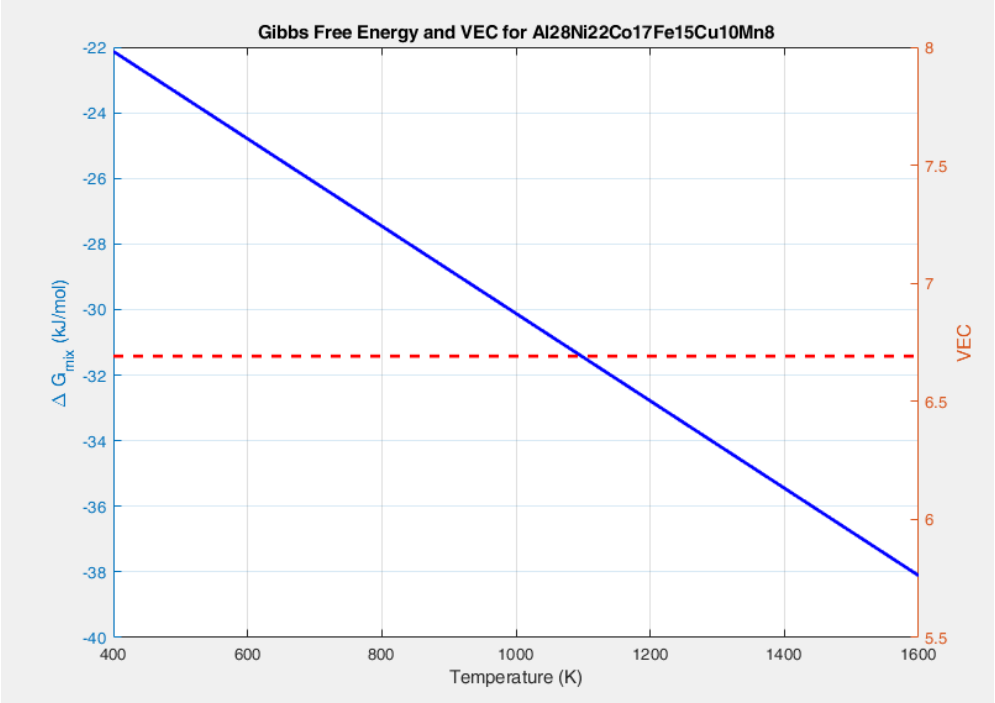
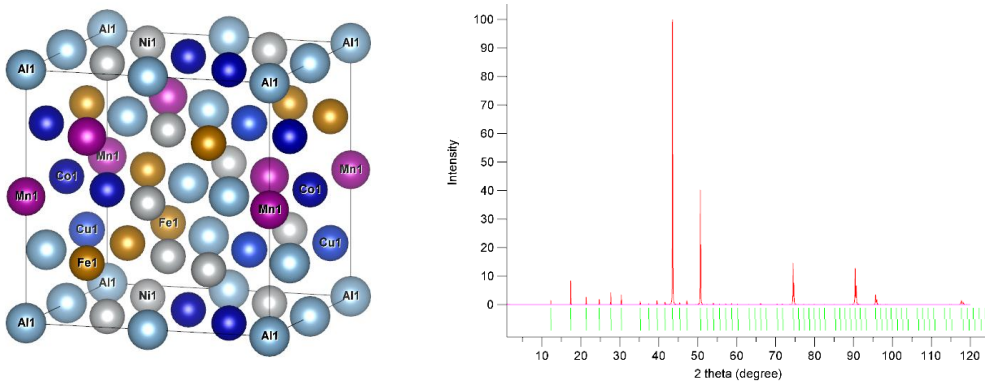


Fig. 2. ΔG_{mix} and VEC as a function of temperature



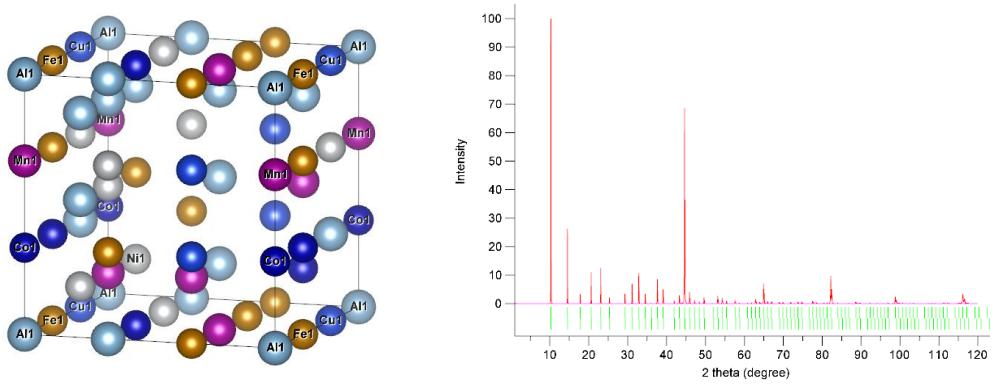
a b

Fig. 3. FCC three-dimensional crystal lattice model(a) and powder diffraction plot(b)

The three-dimensional BCC crystal lattice model and the powder diffraction pattern of Al28Ni22Co17Fe15Cu10Mn8 are depicted in Fig. 4. Peaks characteristic of BCC (e.g., (110), (200)) confirm that the model accurately reproduces the BCC phase. The shift in peaks due to the supercell ($2\theta \approx 10°$ instead of 44.7°) is expected, as the supercell lattice parameters (a = 5.74 Å, c = 11.48 Å) are larger than those of the unit cell (a = 2.87 Å). The BCC phase, as indicated by thermodynamic calculations, is plausible at VEC ≈ 7.43, which aligns with the model.

The diffraction pattern confirms a highly crystalline structure for the Al28Ni22Co17Fe15Cu10Mn8 HEA, with the dominant peak at $2\theta \approx 90°$ corresponding to the (440) plane, consistent with a Heusler-like cubic lattice similar to *Cu_2MnAl*. The narrow peaks and low background underscore excellent material quality, aligning with thermodynamic predictions of phase stability at VEC ≈ 7.43, which supports a mix of FCC and BCC phases. The presence of weaker peaks at lower angles (e.g., $2\theta \approx 30°$) suggests possible minor impurities or secondary phases, such as oxides or residual elemental

phases, which warrant further investigation. To validate the phase composition, comparison with JCPDS database entries for *Cu_2MnAl* and experimental compositional analysis (e.g., EDS) is recommended. The diffraction data reinforces the alloy's potential for high-temperature catalytic applications, but optimization of synthesis conditions may be needed to minimize impurities and ensure phase purity.



a b

Fig. 4. BCC three-dimensional crystal lattice model powder diffraction plot

Conclusions

This study elucidates the thermodynamic and structural attributes of the high-entropy alloy (HEA) Al28Ni22Co17Fe15Cu10Mn8, underscoring its potential as a robust catalytic material for thermochemical applications. Through meticulous mathematical modeling and literature analysis, the alloy's composition was optimized, revealing a high configurational entropy (ΔS_{mix} within 13.4—22 J/(mol·K)) and favorable thermodynamic stability, as evidenced by ΔG_{mix} values ranging from —7 kJ/mol at 400 K to —15 kJ/mol at 1600 K. The valence electron concentration (VEC ≈ 7.43) supports a dual FCC and BCC phase structure, enhancing catalytic site diversity, with high *Ni* and *Co* content driving efficacy in *CO* oxidation. Powder diffraction patterns, modeled using VESTA and custom Python scripts, confirmed the presence of FCC and BCC phases, though minor peaks suggest potential impurities warranting further investigation. These findings position HEAs as a transformative alternative to conventional catalysts, leveraging compositional flexibility to achieve superior resilience. Future research should prioritize experimental validation of phase purity via techniques like EDS and JCPDS database comparisons, alongside optimization of synthesis methods, such as thermochemical pressing, to mitigate *Al* reactivity. Additionally, integrating computational tools, including machine learning, could accelerate the design of tailored HEA compositions, broadening their impact across catalysis, aerospace, and energy sectors.

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Список використаної літератури

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