

Prediction of phase-structural state of as-cast high-entropy alloys

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The structural and chemical heterogeneity of two Al-based complex concentrated alloys Al – Cr – Mn – Fe – Ni – Cu and Al – Cr – Mn – Fe – Co – Ni – Cu – Zn was investigated in the as-cast condition in order to evaluate the predictive capability of commonly used high-entropy alloy (HEA) descriptors. Integral thermodynamic parameters (ΔS_{mix} , ΔH_{mix} , δ , VEC, Ω , $\Delta\chi$) calculated for both compositions fall within ranges typically considered favorable for solid-solution formation in HEA and complex concentrated alloys. In particular, ΔH_{mix} and δ satisfy empirical stability criteria, while Ω exceeds commonly proposed thresholds for solid-solution formation. However, microstructural characterization reveals that these descriptors alone do not reliably predict the actual phase constitution in as-cast state.

SEM/EDS analysis showed that both systems form a chemically heterogeneous dendritic-like morphology, accompanied by pronounced chemical partitioning between chemically distinct microstructural regions. In the Al – Cr – Mn – Fe – Ni – Cu alloy, two chemically distinct microstructural constituents were identified; however, both of them may correspond to B2-type intermetallic phases with a BCC-related lattice. Although VEC values fall within ranges associated with BCC or mixed BCC/FCC tendencies in Al-rich multicomponent alloys, experimental evidence indicates that the dominant structural constituents correspond to ordered intermetallic phases rather than disordered solid solutions.

In contrast, the Al – Cr – Mn – Fe – Co – Ni – Cu – Zn alloy exhibits significantly higher chemical and morphological heterogeneity. Addition of Co and Zn leads to increased microstructural complexity and decrease of Cu-driven chemical separation. Local enrichment in Cu and Zn was detected in chemically distinct regions, indicating a strong tendency toward chemical separation and suggesting the formation of brass-type intermetallic phases.

Keywords: complex concentrated alloys, HEA, lightweight alloys, casting, microstructure, phase formation, thermodynamic parameters, SEM.

High-entropy alloys (HEAs) have established a new direction in modern materials science by proposing an alternative concept of alloy design based on the use of several principal (multiprincipal) elements in comparable atomic concentrations instead of the traditional scheme of a “base element + minor alloying additions”. Such an approach significantly expands the space of possible compositions and enables the purposeful design of properties combinations that are difficult to achieve in conventional alloys. The concept of multicomponent systems

was systematized at the beginning of the 21st century and quickly attracted attention due to its potential for the development of next-generation materials [1].

The scientific relevance of HEAs and multicomponent concentrated alloys (MCAs) research is also associated with the need to reconsider fundamental concepts of phase formation and thermodynamics in a concentrated multicomponent systems. In contrast to conventional binary and ternary phase diagrams, the behavior of such alloys is governed by complex multivariate interactions between constituent elements, which influence phase stability, diffusion processes, deformation mechanisms, and ordering phenomena. For this reason, HEAs are regarded not only as a new class of structural materials but also as model systems for the development of physical metallurgy [2]. From a practical standpoint, HEAs/MCAs are of considerable interest because certain systems demonstrate advantageous combinations of mechanical properties, including high strength combined with sufficient ductility and fracture resistance, as well as the retention of fracture toughness at low temperatures, making these materials promising for operation under extreme conditions [3].

Early concepts of HEAs associated their phase stability primarily with the high configurational entropy of mixing and the expected formation of relatively simple solid-solution phases (FCC or BCC). However, subsequent studies have shown that the actual structural and phase state is determined by a complex interaction of thermodynamic and kinetic factors, as well as by local chemical composition and the possibility of ordered phase formation. In this context, HEAs are increasingly considered within the broader paradigm of complex concentrated alloys (CCAs) or multicomponent concentrated alloys (MCAs), where the key aspect is the multicomponent design itself rather than the magnitude of configurational entropy alone [2]. For preliminary prediction of phase formation in HEAs/CCAs, a number of empirical and semi-empirical parameters are widely used, including the entropy and enthalpy of mixing, the atomic size mismatch parameter δ , the valence electron concentration (VEC), the Ω parameter, and the electronegativity difference ($\Delta\chi$). These indicators are useful for the initial screening of compositions and for estimating the likelihood of forming solid solutions or intermetallic phases; however, they primarily reflect the averaged thermodynamic state of the system.

One of the advantages of multicomponent alloy systems is the possibility of simultaneously activating several strengthening mechanisms, including solid-solution strengthening, lattice distortion strengthening, and phase strengthening (dispersion hardening), which potentially allows an increase in strength without a critical loss of ductility [4]. Multicomponent compositions may also create conditions for improved corrosion resistance due to the formation of stable passive films and changes in the character of localized corrosion. In such systems, microstructural heterogeneity can significantly influence electrochemical behavior and may provide opportunities to tailor corrosion properties through optimization of alloy composition [5]. Another important characteristic is the potential thermal stability of HEAs, which may manifest itself in the ability to retain phase composition and microstructure at elevated temperatures. Although thermal stability strongly depends on the specific composition and phase state,

multicomponent alloys demonstrate considerable potential for applications in high-temperature environments and aggressive service conditions [6].

In summary, HEAs/MCAs combine fundamental scientific interest with broad possibilities for practical application, which determines the need for further investigation of structural and phase relationships as well as material properties depending on composition and processing conditions [7].

A distinct and rapidly developing research direction is represented by aluminum-containing high-entropy, middle-entropy and complex concentrated alloys (Al-containing HEAs/MEAs/CCAs). These materials are considered particularly promising because aluminum addition prones a simultaneous reduction in density and control over the crystal structure type (FCC–BCC/B2) as well as the dispersion of ordered phases. Literature analysis for such systems as AlCoCrFeNi, AlCrMnFeCoNi and similar ones shows that an increase in aluminum content reduces the predominance of the FCC structure and promotes the formation of a BCC/B2 component. At the same time, the morphology of the cast microstructure changes and chemical heterogeneity between dendritic and interdendritic regions becomes more significant. This combination of effects makes aluminum a key regulator of the phase state and, consequently, of the mechanical and corrosion behavior of these alloys, while simultaneously increasing the sensitivity of the resulting structure to the precise composition and processing conditions [8].

In last studies, the role of aluminum in multicomponent alloys is interpreted as a result of the interaction between electronic, thermodynamic, and structural factors that determine the stability of solid solutions and the way of phase formation. It has been shown that in systems such as Al_xCrFeCoNi, variation in aluminum concentration may lead not only to a transition between predominant crystal structures (FCC or BCC) but also to modifications of the local chemical order (short-range order, SRO), which arises from the competition between enthalpic and entropic contributions to interatomic interactions. Such ordering may be weakly reflected in X-ray diffraction results because this method mainly characterizes the average crystal structure; however, SRO can significantly affect the energy conditions of the system, the thermodynamic stability of phases, and the tendency toward phase separation or the formation of ordered structures during heat treatment. This highlights the importance of interpreting the microstructure of cast alloys while considering the combined influence of equilibrium thermodynamic factors and kinetic processes of solidification and diffusion that ultimately determine the final structural and phase state [9].

At the same time, for aluminum-containing HEAs/CCAs the key practical challenge is not alloying in the traditional sense but the compositional design of lightweight multicomponent alloys in which low density represents a target parameter, while the HEA approach is used as a methodological framework for constructing multiprincipal systems. Within such an approach, each component (including Cu, Zn, and Co) is considered a full compositional element influencing the solidification pathway, the tendency toward ordering or phase separation, and the degree of chemical heterogeneity.

In particular, copper is often characterized by limited mutual solubility with several constituent elements, which promotes the formation of Cu-enriched regions during solidification [10]. The addition of zinc to systems such as AlCrFeCoNi may modify electronic and chemical interactions, alter the phase composition, and further complicate structural prediction [11]. The effect of cobalt is also composition-dependent: with variation in aluminum content, the system may have transition between FCC- and BCC/B2-dominated states, accompanied by corresponding changes in phase morphology and properties [10].

Prediction of the phase state in multicomponent HEA/CCA type alloys is a multilevel task because widely used indicators (ΔH_{mix} , ΔS_{mix} , δ , VEC, Ω , $\Delta\chi$) are suitable mainly for preliminary compositional screening but do not provide a reliable description of the actual as-cast microstructure. This limitation arises from their insufficient consideration of local chemical ordering, the competition between ordering and phase separation processes, and the kinetics of solidification and diffusion [9, 12, 13]. This issue is particularly pronounced in Al-containing systems with Cu and/or Zn, where experimental data remain limited due to the strong sensitivity of phase composition to synthesis conditions and the pronounced dendritic microsegregation that complicates comparison of results even for similar nominal compositions [10, 11]. It is therefore essential to distinguish between the average alloy composition and the local compositions of individual structural constituents, since local chemistry ultimately determines the crystal structure type, phase morphology, and the tendency toward ordering or phase separation [8]. In this context, a key scientific problem remains the lack of consistent experimental data that would allow a direct correlation between calculated thermodynamic parameters and the real cast microstructure (segregation, formation of B2-type phases, appearance of enriched phases, etc.) in Al-contained multicomponent systems with lowered density [9, 12].

The aim of the present investigation is to evaluate the possibility and limitations of predicting the phase-structural state of lightweight aluminum-containing multicomponent alloys designed according to the HEA/CCA concept by comparing calculated thermodynamic parameters with the actual cast microstructure based on SEM/EDS analysis. This approach enables verification of the cause-and-effect relationships between compositional design, thermodynamic indicators, and the structural state of the material, considering the decisive role of solidification processes and microsegregation.

Chemical compositions of the investigated experimental alloys were designed based on the specified atomic concentrations of the constituent elements. The actual chemical composition after melting was determined using local elemental analysis by energy-dispersive X-ray spectroscopy (EDS). The correspondence between the designed and obtained compositions was evaluated by comparing the nominal and experimentally measured concentrations of the elements, which made it possible to assess possible losses of alloying components during melting as well as the produced materials degree chemical homogeneity. The nominal and measured compositions of the alloys, that was further used for the calculation of thermodynamic parameters of the system are presented in Table 1.

Table 1

Nominal charge composition and actual composition of the Al – Cr – Mn – Fe – Ni – Cu (1) and Al – Cr – Mn – Fe – Co – Ni – Cu – Zn (2) alloy systems after melting

Element		Al	Cr	Mn	Fe	Co	Ni	Cu	Zn
1	Nominal composition, at. %	50.00	7.00	9.00	7.00	–	7.00	20.00	–
	Actual composition (XRF), at. %	53.95	3.65	7.57	5.40	–	6.16	23.27	–
2	Nominal composition, at. %	39.20	7.60	7.42	7.27	7.47	7.06	16.90	7.08
	Actual composition (XRF), at. %	57.23	2.71	6.16	3.44	1.38	5.15	17.53	6.40

The alloys were produced by melting in a laboratory resistance furnace using alumina crucibles. Melting was carried out in air without the use of a protective atmosphere. To reduce oxidation of the melt surface and to minimize the loss of volatile components, a covering flux of the LiCl – LiF (1:1) was used.

Pure metals and concentrated master alloys (in particular Al – Cu) were used as starting materials. The components were sequentially added into the melt considering their melting temperatures and mutual solubility. Zinc was added at the middle stage of melt preparation process. Melt temperature before pouring was approximately 950 °C in order to minimize evaporation losses and to provide full solubility of the components. No additional degassing treatment was applied.

The melt was poured into steel molds at temperatures ~ 950–980 °C. Samples were cut from the as-cast ingots and subjected to standard metallographic preparation. The surfaces were ground using abrasive materials with progressively finer grit sizes and subsequently polished to obtain a mirror-like surface suitable for analysis in the backscattered electron (BSE) mode and for performing EDS measurements. Metallographic etching was not applied; therefore, dendritic-related terms in this work are used as a conditional description based on BSE contrast and EDS elemental redistribution rather than as a direct result of etched relief observation.

Bulk chemical composition was determined using X-ray fluorescence analysis (XRF). Local elemental distribution and compositional variations between chemically distinct microstructural regions were analyzed using scanning electron microscopy (SEM) equipped with an energy-dispersive X-ray spectroscopy (EDS) system. Elemental mapping was used to evaluate the spatial heterogeneity of component distribution between grains and intergranular regions. Local chemical analysis was applied to determine the chemical composition of individual structural constituents and to generate a dataset for comparison with the nominal alloy composition.

To evaluate the tendency of the investigated compositions toward the formation of solid solutions or multiphase structures, the following parameters were calculated: configurational entropy of mixing (ΔS_{mix}), enthalpy of mixing (ΔH_{mix}), atomic size mismatch parameter (δ), valence electron concentration (VEC), thermodynamic stability parameter (Ω), electronegativity difference ($\Delta\chi$), calculated density (ρ).

The calculations were performed both for the nominal compositions (charge compositions) and for the compositions determined after melting based on the experimental data obtained from EDS analysis. Such an approach makes it possible to assess the sensitivity of integral HEA/CCA criteria to actual compositional deviations and to correlate the calculated indicators with the real cast microstructure.

Binary mixing enthalpies ΔH_{ij} required for the calculation of ΔH_{mix} in multicomponent systems were taken from generalized data obtained within the framework of the Miedema model and systematized in the work of Takeuchi and Inoue [14], which are widely used in the design and analysis of high-entropy and complex concentrated alloys. The calculated values of these parameters are presented in Table 2.

Table 2
Calculated physicochemical parameters of the Al – Cr – Mn – Fe – Ni – Cu (1) and Al – Cr – Mn – Fe – Co – Ni – Cu – Zn (2) alloys

Calculated physicochemical parameter		$\Delta S_{\text{mix}}^{\circ}$, $\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$\Delta H_{\text{mix}}^{\circ}$, $\text{kJ}\cdot\text{mol}^{-1}$	δ , %	VEC	Ω	$\Delta\chi$	ρ , $\text{g}\cdot\text{cm}^{-3}$
1	Nominal composition	12.00	-8.60	6.02	6.01	1.71	0.136	3.52
	Actual composition (XRF)	10.96	-7.43	5.86	5.98	1.80	0.138	3.15
2	Nominal composition	15.09	-8.50	5.79	6.82	2.17	0.135	5.59
	Actual composition (XRF)	11.62	-7.23	5.30	5.92	1.97	0.128	4.66

Comparison of the nominal charge composition with the actual composition after melting (based on SEM/EDS data) indicates noticeable deviations in the concentrations of individual elements, which is typical for cast multicomponent Al-containing systems, especially in the absence of a protective atmosphere during melting and in the presence of components prone to losses due to oxidation or evaporation. For the Al – Cr – Mn – Fe – Ni – Cu system alloy, an increase in the fractions of Al and Cu and a decrease in the concentrations of Cr, Fe, and Ni after melting were observed (Table 1). A similar tendency is also observed for the Al – Cr – Mn – Fe – Co – Ni – Cu – Zn alloy, where a significant increase in the fraction of Al after melting is accompanied by a decrease in the concentrations of transition metals, most noticeably for Co and Cr (Table 1). Considering that the actual composition was determined by the local EDS method, the obtained values represent an average of measurements performed over selected regions of the cast microstructure and may additionally depend on the level of microsegregation (dendritic microsegregation) within the sample. Therefore, for the subsequent analysis of thermodynamic parameters and interpretation of phase formation, both the nominal compositions (charge compositions) and the compositions “after melting” obtained from EDS data were used. This approach makes it possible to evaluate the sensitivity of calculated criteria to real compositional deviations and to structural heterogeneity characteristic of the as-cast state.

The calculated values of thermodynamic and electronic parameters (ΔS_{mix} , ΔH_{mix} , δ , VEC, Ω , $\Delta\chi$) presented in Table 2 for both alloys systems shows that the integral indicators based on the average composition fall within ranges that are often associated in the literature with an increased probability of solid-solution formation in HEA/CCA compositions. In particular, the values of ΔH_{mix} lie within the range generally considered favorable for the formation of solid solutions (approximately -15 to 5 kJ/mol), while the parameter δ for both systems does not exceed 6% , corresponding to typical threshold estimates of atomic size compatibility. The Ω parameter exceeds 1.1 , which within widely used semi-empirical approaches is also interpreted as thermodynamic favorability for the formation of solid solutions. At the same time, the VEC values for both compositions lie within a range characteristic of BCC or mixed BCC/FCC structures, which is expected for Al-based multicomponent systems with increased Al content and a potential BCC/B2 component. Comparison of the parameters for the “charge” and “after melting” states reflects changes in configurational entropy and calculated density ρ according to the actual (EDS) composition. However, these integral criteria alone do not describe the local chemistry of structural constituents in the cast state; therefore, in this work they are considered as tools for preliminary assessment that must be interpreted together with SEM/EDS results and manifestations of microsegregation.

SEM observations show that the microstructure of the as-cast experimental Al – Cr – Mn – Fe – Ni – Cu alloy exhibits chemically heterogeneous near-dendritic morphology (Fig. 1). EDS elemental mapping confirms the presence of chemical heterogeneity between chemically distinct regions, particularly with an increased local concentration of Cu in certain microstructural areas. Local point analysis (Table 3) reveals at least two chemically distinct groups of regions: (1) areas with increased Cu content and elevated Ni concentration, and (2) regions enriched in Al with the simultaneous presence of Cr, Mn, and Fe. Such a distribution is typical for multicomponent systems in which the elemental distribution is governed by microsegregation during solidification. Unambiguous identification of crystal structures (FCC/BCC/B2) requires phase identification using diffraction methods, but,

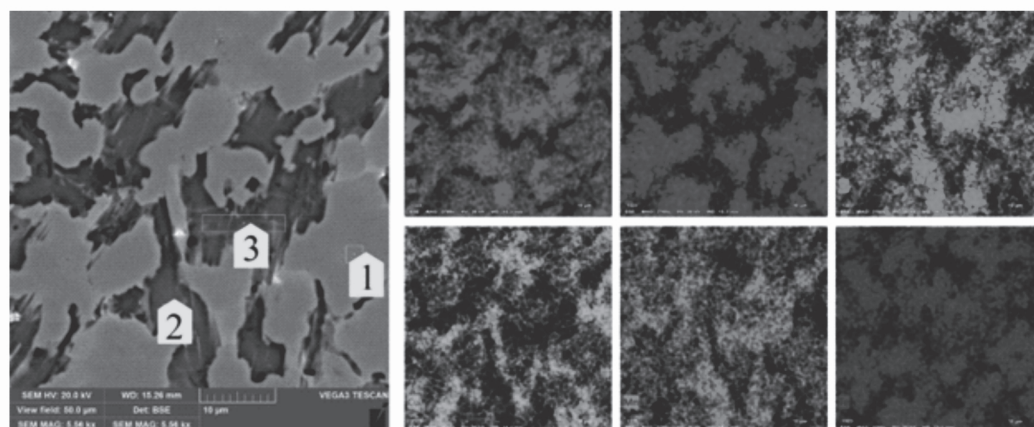


Fig. 1 SEM microstructure of the Al – Cr – Mn – Fe – Ni – Cu alloy and EDS elemental distribution maps.

Table 3
Chemical composition of probable constituents in the Al – Cr – Mn – Fe – Ni – Cu alloy system

Chemical composition in a point, at. %	Al	Cr	Mn	Fe	Ni	Cu	Probable constituent
1	49.48	2.63	6.57	6.26	9.66	25.40	B2-Al(Cu ,Ni)
2	54.76	7.77	13.07	6.72	2.43	15.26	B2-Al(Cu, Mn)
3	56.98	7.41	11.00	4.96	2.23	17.43	B2-Al(Cu, Mn)

according to chemical composition, the phases were identified as probable constituents, as shown in Table 3.

The phase (Point 1) with approximately 50 at. % Al is most likely an ordered aluminide with a B2 crystal structure. Such phases are structurally similar to NiAl-type intermetallic compounds and are characterized by a wide substitutional solubility of transition metals in the metallic sublattice. Therefore, the observed phase can be described as a multicomponent aluminide of the type (Cu,Ni,Fe,Mn,Cr)Al or solid solution of Cr,Mn and Fe in B2-Al(Cu,Ni). The phases (Point 2 and 3) with approximately 55 at. % Al most likely also correspond to probable multicomponent aluminide constituents with B2-related structure, and may be described as B2-Al(Cu, Mn).

The microstructure of the Al – Cr – Mn – Fe – Co – Ni – Cu – Zn alloy is characterized by more pronounced chemical and morphological heterogeneity compared to the alloy without Zn and Co (Fig. 2). EDS elemental mapping demonstrates clear contrasts in the distribution of components, with the formation of regions locally enriched in Cu and Zn, which is confirmed by point analysis (Table 4). The presence of areas with high local concentrations of Cu and Zn adjacent to Al-enriched regions indicates an intensification of microsegregation in the multicomponent system when transitioning from a six-component to an eight-component composition.

For the Al – Cr – Mn – Fe – Co – Ni – Cu – Zn system, a larger number of chemically distinct regions is observed, including areas with high local concentrations of Cu and Zn (Table 4). Provided analysis suggests the

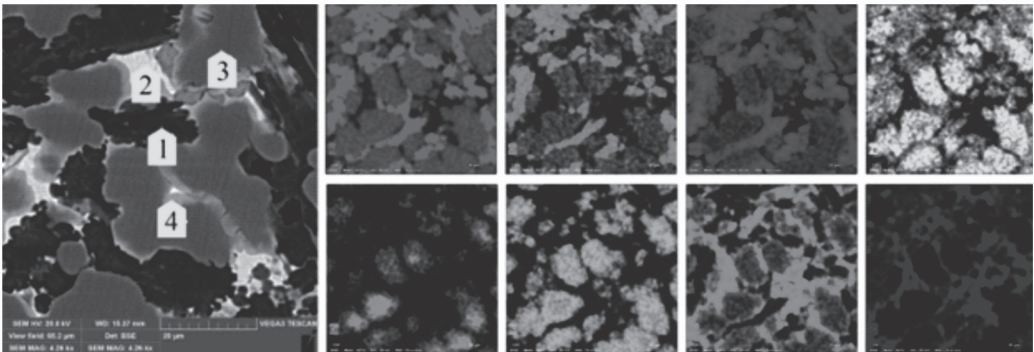


Fig. 2. SEM microstructure of the Al – Cr – Mn – Fe – Co – Ni – Cu – Zn alloy and EDS elemental distribution maps.

Table 4

Chemical composition of probable constituents in the Al – Cr – Mn – Fe – Co – Ni – Cu – Zn alloy system

Chemical composition in a point, at. %	Al	Cr	Mn	Fe	Co	Ni	Cu	Zn	Probable constituent
1	46.5	6.4	11.8	3.92	0.68	1.17	7.44	3.6	B2-Al(Cu, Mn)
2	18.5	0.2	1.05	0.43	0.18	0.57	36.4	42.6	β -brass (BCC)
3	47.4	3.7	6.68	8.12	3.34	11.1	18.6	1.1	B2-Al(Cu, Ni)
4	40.1	0.24	2.08	0.85	0.48	3.49	38.8	14	δ -AlCu [24]

possible formation of three main structural constituents in the alloy – B2 aluminide with saturated transition metals, brass-type CuZn intermetallic, alloyed with Al and δ -AlCu phase, that is ordinary for some kind of brass. B2-like constituents are associated with Al-enriched regions, while the second and fourth constituents are most likely formed from the residual melt during the final stages of crystallization.

The obtained results highlight the limitations of applying integral HEA criteria (Table 2), calculated from the average composition, for direct prediction of the phase state in the as-cast condition without considering the local chemistry of chemically distinct regions and the kinetics of solidification.

The results indicate that the calculated integral thermodynamic parameters (ΔS_{mix} , ΔH_{mix} , δ , VEC, Ω , $\Delta\chi$; Table 2) for both systems lie within ranges often considered favorable for solid-solution formation in HEA/CCA compositions [2, 4]. In particular, the values of ΔH_{mix} and δ meet the empirical criteria for “solid-solution stability,” and Ω exceeds the threshold values that semi-empirical approaches interpret as thermodynamic favorability for forming a solid solution. However, recent studies indicate that such integral criteria can overestimate the likelihood of a homogeneous single-phase state, especially in cast alloys where the microstructure forms under nonequilibrium solidification and limited diffusion [15]. In this context, thermodynamic parameters are more useful as comparative metrics for composition selection, but not as direct predictors of the structural-phase state.

SEM examination showed that both systems form a chemically heterogeneous dendritic-like morphology and EDS mapping confirms a significant redistribution of elements between chemically distinct microstructural regions. For the Al – Cr – Mn – Fe – Ni – Cu system, two chemically distinct constituents were identified, but both of them belonged to B2-type phase.

For the Al – Cr – Mn – Fe – Co – Ni – Cu – Zn system, a more complex picture of chemical heterogeneity was observed, including regions locally enriched in Cu and Zn. The transition from a 6-component to an 8-component composition is accompanied by increased chemical contrast and a greater number of locally distinct regions. Literature data indicate that adding Zn to multicomponent Al-based systems can complicate phase interactions and

enhance the tendency for local element partitioning [11], and in combination with Cu can promote the formation of brass-type phases [17]. Thus, the present results confirm that increasing the number of phases and yields a more heterogeneous as-cast microstructure.

The VEC values for the studied systems fall in ranges characteristic of BCC or mixed BCC/FCC tendencies in Al-rich multicomponent alloys, which is consistent with known trends for systems like Al_x (Co Cr Fe Ni) [8, 9]. However, confirmation of lattice types and possible ordering requires diffraction analysis; in the present work these structural assignments should therefore be considered probable and based mainly on local chemical composition [18].

In the studied Al-based HEA/CCA systems one of the key factors for determining the structural and chemical state in the as-cast condition may be crystallization conditions and the associated nonequilibrium partitioning of elements between chemically distinct microstructural regions. The integral parameters (ΔS_{mix} , ΔH_{mix} , δ , VEC, Ω , $\Delta\chi$), while useful for initial alloy design and composition comparison, do not describe the local concentration gradients that define the actual microstructural heterogeneity. Thus, such prediction can be used mainly for preliminary selection of compositions with expected BCC/B2 tendency, Cu- or Cu – Zn-enriched constituents, reduced density, and potentially increased hardness or strength, but not for complete determination of the final as-cast structure.

Therefore, a proper interpretation of the cast-state phase formation requires combining local chemical analysis (SEM/EDS) with phase identification by diffraction (XRD) and, if needed, with thermodynamic and kinetic modeling based on CALPHAD, including Scheil solidification simulations to account for nonequilibrium crystallization and microsegregation effects [19].

Conclusion

1. The Al – Cr – Mn – Fe – Ni – Cu alloy in the as-cast condition is characterized by chemically distinct microstructural regions that, according to SEM/EDS data, can be interpreted as probable B2-like intermetallic constituents with BCC-related lattice type.

2. The Al – Cr – Mn – Fe – Co – Ni – Cu – Zn alloy exhibits higher chemical and morphological heterogeneity, including Cu- and Zn-enriched regions that indicate a tendency toward the formation of brass-type intermetallic constituents.

3. Integral HEA/CCA descriptors are screening tools only. Although ΔS_{mix} , ΔH_{mix} , δ , VEC, Ω , $\Delta\chi$, and ρ (Table 2) fall within ranges frequently associated with solid-solution formation in HEA/CCA screening, these criteria are based on the average composition and do not account for local chemistry. Therefore, they cannot directly predict the as-cast state phase-structural constituents without explicitly considering solidification kinetics and microsegregation. They indicate only the probability of forming certain structural constituents.

4. VEC and Al enrichment indicate a possible BCC/B2 tendency in the studied alloys; however, the experimental SEM/EDS data show that

this tendency is realized mainly through chemically heterogeneous B2-like intermetallic constituents rather than through a homogeneous solid solution.

5. The practical value of the applied prediction approach is the preliminary selection of alloy compositions for obtaining cast materials with expected BCC/B2 constituents, Cu- or Cu – Zn-enriched phases, reduced density, and potentially increased hardness or strength. Final confirmation of such predetermined properties requires additional phase identification and mechanical testing.

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Прогнозування фазово-структурного стану литих сплавів з високою ентропією

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Анотація

Було досліджено структурну та локальну неоднорідність хімічного складу двох комплексних концентрованих сплавів систем Al – Cr – Mn – Fe – Ni – Cu та Al – Cr – Mn – Fe – Co – Ni – Cu – Zn в литому стані. Метою було визначення прогностичної здатності загальноновживаних дескрипторів високоентропійних сплавів (BEC). Інтегральні термодинамічні параметри (ΔS_{mix} , ΔH_{mix} , δ , VEC, Ω , $\Delta\chi$), розраховані для обох складів, знаходились в межах діапазонів, які зазвичай вважаються сприятливими для утворення твердих розчинів у BEC та комплексних концентрованих сплавах. Зокрема, ΔH_{mix} та δ для експериментальних сплавів задовольняли емпіричні критерії стабільності, тоді як значення Ω перевищувало загальнопропоновані межі для утворення твердих розчинів. При цьому, було показано, що ці дескриптори самі по собі не здатні надійно передбачити фактичний фазовий склад у литому стані.

SEM/EDS аналізи показали, що обидві системи формують хімічно неоднорідну дендритоподібну морфологію, що супроводжується помітною хімічною неоднорідністю між хімічно відмінними мікроструктурними областями. У сплаві Al – Cr – Mn – Fe – Ni – Cu було виявлено дві хімічно різні мікроструктурні складові, однак обидві вони можуть відповідати інтерметалідним фазам типу B2 з ОЦК-граткою. Також показано, що хоча значення VEC для цього сплаву знаходились в діапазонах, які визначають ОЦК-тип ґратки, або змішаний тип ОЦК/ГЦК, домінуючі структурні складові в експериментальному сплаві відповідають впорядкованим інтерметалевим фазам, а не невпорядкованим твердим розчинам, на що вказує локальний хімічний склад цих складових.

На противагу цьому, сплав Al – Cr – Mn – Fe – Co – Ni – Cu – Zn демонструє значно вищу хімічну та морфологічну гетерогенність. Додавання Co та Zn призводить до збільшення мікроструктурної неоднорідності та зниження хімічної неоднорідності, зазвичай зумовленої міддю. Поява областей, збагачених Cu та Zn, підтверджує підсилення структурно-фазової неоднорідності та вказує на можливість утворення інтерметалідних фаз, які утворюються в латунях та бронзах.

Ключові слова: складні концентровані сплави, BEC, сплави з пониженою густиною, лиття, мікроструктура, фазоутворення, термодинамічні параметри, SEM.