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High-entropy alloys and the periodic table of elements

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Abstract. To select the compositions of high-entropy alloys (HEA) consisting of five or more elements, it is necessary to use methods that take into account many variables and the complexity of assessing the relationships between them. Based on chemical information approaches to the analysis of Web of Science databases, data on the frequency of use of chemical elements in the described HEAs were obtained, which allow us to determine trends in the research and development of new materials.

Keywords: high-entropy alloys, composition, chemical elements, frequency of application, Web of Science databases, chemical information analysis

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Краткое сообщение

Высокоэнтропийные сплавы и периодическая таблица элементов Д.И. Менделеева

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Аннотация. Показано, что для решения задачи выбора составов высокоэнтропийных сплавов (ВЭС), состоящих из пяти и более элементов, необходимо использовать методы, учитывающие множество переменных и сложность оценки взаимосвязей между ними. На основе химико-информационных подходов к анализу баз данных Web of Science получены сведения о частоте применения химических элементов в описанных ВЭС, которые позволяют определить тренды в исследовании и разработке новых материалов.

Ключевые слова: высокоэнтропийные сплавы, состав, химические элементы, частота применения, базы данных Web of Science, химико-информационный анализ

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The development of a new type of alloy designated as “High-Entropy Alloys” (HEA) [1] containing five or more elements in a relatively equiatomic ratio has enjoyed a certain success in the creation of structural materials.

According to Scopus, there has been a rapid growth in the number of HEA-related publications. 289 papers were published in 2015 and 1,393 in the first 10 months of 2020. After expansion of the concept of HEA and the emergence of the new idea of high-entropic materials (HEM), there has been a manifold increase in the number of publications [2].

In [3], an examination of the prospects for improving only one property (corrosion resistance) has revealed a significant number of combinatorial possibilities in HEA. Therefore, the use of informatics will be required in order to resolve the issue of selecting compositions with specific properties. This is due to the multitude of variables and the complexity of assessing all relationships.

The chemical and information approach and its use in the study of complex systems has been described in a number of works [3 – 7]. This includes studying the thermodynamic characteristics, in order to describe the principles of formation of HEA structures with the required functional characteristics [8].

This report considers the frequency of use of various chemical elements in HEA composition. The analysis used all the Web of Science databases in which a query “high entropy alloy” was created on 01.01.2021. Thus, a problem-oriented database (POB) containing 13,426 records was obtained. Using this array of records, an analysis of occurrence of chemical elements in HEA was carried out. Records containing the name of the chemical element in the Mendeleev's periodic table were identified and the following were determined: N – number of records corresponding to this element in the total array; i – amount of information equal to log2N.

Figure 1 shows the dependence of the amount of information (i) for each chemical element on its atomic number (Z) in the Mendeleev table.

Despite the cyclic change of i with an increase of the element atomic number, typical for many properties of elements and reflected in Mendeleev’s fundamental law on the cyclic change of properties depending on the value of nuclear charges of their atoms, we can observe a reduction of the frequency of use in HEA of elements, along with an increase in their atomic number. Experimental value of the linear correlation coefficient (r) of the dependence $i = f(Z)$, equal to 0.609 in the absolute value, exceeds the critical value of 0.28 for the confidence probability of 0.99 and the number of freedom degrees of 82. It testifies to reliability of the decrease in the frequency of use in HEA of elements along with an atomic number increase in the Mendeleev table.

Allocation of points above and below the trend line $i = f(Z)$ allows a series of the most and least frequently used elements in the composition of HEA to be constructed

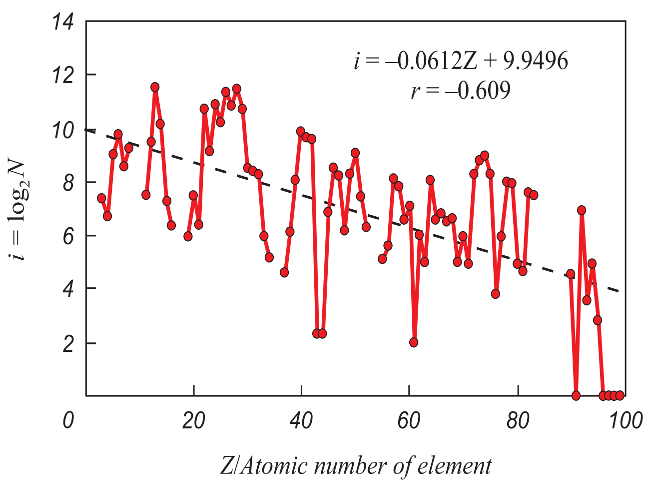

Fig. 1. Dependence of amount of information on elements of the periodic table used as a part of HEA (data as of 01.01.2021 in Web of Science database)

Рис. 1. Зависимость количества информации по элементам таблицы Д.И. Менделеева, используемым в составе ВЭС (данные на 01.01.2021 в базе данных Web of Science)

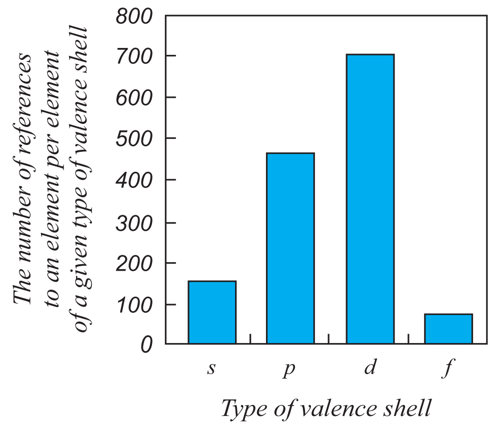

Fig. 2. Influence of the type of chemical element valence shell on frequency of its use as part of HEA

Рис. 2. Влияние типа валентной оболочки химического элемента на частоту его применения в составе ВЭС

and be taken into account by researchers in the selection of HEA components.

The most frequently encountered elements in HEA composition (data above the trend line) can be arranged in order of descending i:

$$Al > Ni > Fe > Cr > Co > Cu > Ti > Mn > Si > Zr >$$
$$> C > Nb > Mo > Mg > V > Sn > W > Ta > Zn >$$
$$> Pd > Ga > Hf > Re > In > Ge > Ag > La > Gd >$$
$$> Y > Pt > Au > Ce > Pb > Bi > Sb > Nd > U > Dy >$$
$$> Er > Tb > Pr > Ho > Yb > Ir > Pu > Th.$$

The least frequent elements in HEA composition (data below the trend line) in order of increasing i are arranged as follows:

$$Pa < Cm < Bk < Cf < Es < Pm < Tc < Ru < Am <$$
$$< Np < Os < Rb < Tl < Lu < Hg < Eu < Tm < Cs <$$
$$< Se < Ba < K < As < Sm < Sr < Cd < Te < S < Sc <$$
$$< Be < Rh < P < Li < Na < Ca < N < B < O.$$

Among all the elements considered, d-elements are most frequently referred to in the composition of HEA, followed by p-elements and much less by s- and f-elements (Figure 2).

Thus, the data obtained clearly indicates the presence of certain trends in research into new materials and the prospects of the proposed chemical and information approach to the analysis of relations between chemical elements and properties of HEA. It allows the number of objects for research to be limited. This is particularly important when developing models aimed at prediction of properties.

Conclusions

The proposed analysis approach to the large arrays of experimental results as applicable to complex multicomponent systems, in particular HEA, has both theoretical and practical value. It is aimed at developing alloys with a given set of performance indicators.

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