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High-Entropy Alloys and the Periodic Table

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Abstract—In order to solve the problem of choosing the compositions of high-entropy alloys (HEAs) consisting of five or more elements, it is necessary to use methods that considers many variables and the complexity of estimating the relationships between them. Based on chemical-information approaches to the analysis of Web of Science databases, information on the frequency of use of chemical elements in the described HEAs has been obtained, which make it possible to identify 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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INTRODUCTION

The creation of high-entropy alloys (HEA) [1] was a successful development of a new type of alloy in structural materials, containing five or more elements in a relatively equiatomic ratio.

According to Scopus, the growth in the number of publications related to HEAs is growing rapidly: in 2015, 289 papers were published, and in 10 months of 2020 their number was 1393. After the expansion of the concept of HEA and the emergence of a new concept of high-entropy materials (HEM), the number of publications has increased many times [2].

In [3], when discussing the prospect of improving only one property (corrosion resistance), it was noted that there are a large number of combinatorial possibilities in HEAs. Therefore, to solve the problem of choosing of compositions with specific properties, it will be necessary to use informatics, considering many variables and the complexity of assessing all relationships.

The chemical information approach and its application to the study of various complex systems is described in a number of works [3–7], including the study of thermodynamic characteristics to describe the principles of formation of HEA structures with the necessary functional characteristics [8].

RESULTS AND DISCUSSION

This report discusses the frequency of application of various chemical elements in the HEAs. For the analysis, all Web of Science databases were used, in which the query of "high entropy alloy" was formed on January 1, 2021. Thus, a problem-oriented database (POD) containing 13426 records was obtained. In this array of records, an analysis was made regarding the occurrence of chemical elements in the composition of known HEAs, for which the records containing the name of the chemical element of the periodic table of the elements were selected and the following were determined: N is the number of records corresponding to this element in the total array; i is the amount of information equal to $\log_2 N$.

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

Despite the periodic change in i with an increase in the serial number of the element, which is typical for many properties of elements and is reflected in the fundamental law of D.I. Mendeleev on the periodic change in properties depending on the magnitude of the charges of the atom nuclei, in general, there is a decrease in the frequency of using elements in HEA with an increase in their serial number in the periodic table. The experimental value of the coefficient of linear correlation (r) of the dependence $i = f(Z)$, equal in absolute value to 0.609, exceeds the critical value of 0.28 for a confidence probability of 0.99 and the number of degrees of freedom of 82. This indicates the reliability of a decrease in the frequency of using elements in HEA with an increase in their serial number in the periodic table of the elements.

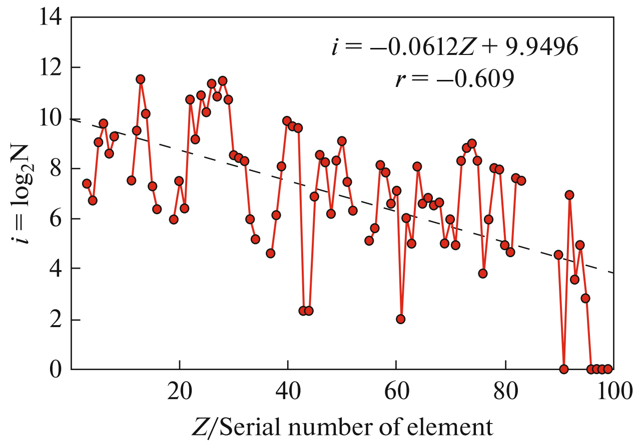

Fig. 1. The dependence of the amount of information on the elements of the periodic table, used as part of HEA (data as of 01/01/2021 in the Web of Science database).

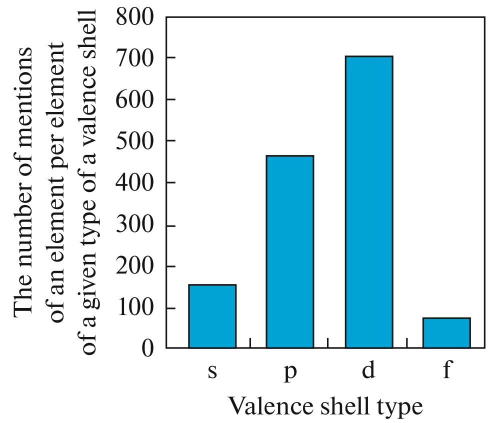

Fig. 2. Influence of the type of the valence shell of a chemical element on the frequency of its use in the HEA.

The selection of points above and below the trend line $i = f(Z)$ allows one to build series of the most and least frequently used elements in the HEA and can be considered by researchers in the selection of HEA of components.

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

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

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

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

Among all the considered elements, *d*-elements are most often mentioned in the HEA composition, then *p*-elements, and much less *s*- and *f*-elements (Fig. 2).

Thus, the data obtained clearly indicate the presence of certain trends in the development of research of new materials and the prospects of the proposed chemical information approach for analyzing the relationships between chemical elements and HEA properties. The data obtained make it possible to limit the number of objects for study, which is important, in particular, when developing models aimed at predicting properties.

CONCLUSIONS

The proposed approach to the analysis of large arrays of experimental results in application to complex multicomponent systems, in particular HEA, has theoretical and practical significance and is aimed at developing alloys with a given set of performance characteristics.

CONFLICT OF INTERESTS

The authors declare that they have no conflicts of interest.

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