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THEORETICAL ANALYSIS OF BASIC CHARACTERISTICS OF HIGH-ENTROPY MATERIALS AND PROSPECTS FOR THEIR APPLICATION

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Abstract
This article provides a theoretical analysis of the formation theory, unique lattice characteristics, thermodynamic stability, and mechanical, thermal, physical, and chemical properties of high-entropy materials (HEMs). The study illuminates the properties of high-entropy materials, arising from their multi-component composition's configurational entropy and the interactions between their constituent elements. Furthermore, it explores the potential applications of these materials in military contexts, including armored protection systems, high-temperature resistant mechanisms, corrosion-resistant coatings, and to enhance the performance characteristics of aerospace technologies and specialized technical equipment.

Keywords: high-entropy materials, configurational entropy, crystal lattice, thermodynamic stability, mechanical properties, heat resistance, corrosion resistance.

Introduction

The development of modern materials science is closely related to the creation of a new generation of multi-purpose materials. In particular, one of the urgent tasks today is to combine such properties as high strength, hardness, heat resistance, corrosion resistance and mechanical resistance in a single material.

Traditional metal alloys are usually formed from a single main element and a small amount of alloying elements added to it. However, this approach can degrade the material properties under certain operating conditions. In this regard, high-entropy alloys and materials composed of several main elements are of great interest as a new scientific direction.

The concept of High-Entropy Alloys (HEAs) began to emerge as an independent research area in 2004. The research led by Jien-Wei Yeh and Brian Cantor played a significant role in this area. Their work demonstrated that solid solutions can be formed in multicomponent metallic systems under the influence of high configurational entropy [1]. The main scientific importance of high-entropy materials is that their properties are

determined not only by the properties of individual elements, but also by the interactions of constituent elements, the arrangement of atoms in the crystal lattice and thermodynamic factors [2].

The purpose of this article is to theoretically analyze the main properties of high-entropy materials and shed light on the prospects for their application in the military field on a scientific basis.

LITERATURE ANALYSIS.

Theory of formation of high-entropy materials. High-entropy materials are a class of complex materials consisting of several main components. Their classical representatives are formed as a result of the combination of five or more main elements in certain concentrations [3]. In such materials, each element plays a significant role in shaping the overall properties of the material. Therefore, they need to be studied as multi-component systems, unlike traditional alloys.

Gibbs free energy is important in the formation of high-entropy materials:

$$\Delta G = \Delta H - T\Delta S$$

Here: G – is Gibbs free energy; H – is enthalpy; T – is absolute temperature; S – is entropy.

From this equation, it can be seen that the thermodynamic stability of a material is determined by the relationship between the enthalpy and entropy factors. One of the factors of primary importance in high-entropy materials is the configurational entropy. For an ideal mixture, the configurational entropy is determined by the following formula:

$$\Delta S_{conf} = -R\sum_{i=1}^{n} C_i \ln C_i$$

Here: R – is the universal gas constant; n – is the number of components; c_i – is the molar fraction of the i-th element.

For an ideal system consisting of five elements in equal amounts:

$$\Delta S_{conf} = R \ln 5$$

This value is approximately 1.61R.

Therefore, an increase in the number of components and their balanced distribution in the composition leads to an increase in configurational entropy. However, the presence of high configurational entropy does not always guarantee the formation of a single-phase solid solution The enthalpy of mixing, the difference in atomic radii, the electronic structure and temperature also play an important role.

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ANALYSIS RESULTS

Main properties of high-entropy materials. The unique properties of high-entropy materials are explained by four main theoretical effects [4]. These are the high-entropy effect, strong deformation of the crystal lattice, diffusion retardation, and the complex effect of components (cocktail effect).

High entropy effect (Thermodynamic stability). The high entropy effect is associated with an increase in configurational entropy in multicomponent systems due to the different arrangements of atoms in the crystal lattice. From a thermodynamic point of view, an increase in entropy contributes to a decrease in the Gibbs free energy:

$\Delta G = \Delta H - T\Delta S$

In this case, the importance of the entropy contribution may increase with increasing temperature. As a result, under certain composition and temperature conditions, the formation of solids with a simple crystalline structure instead of complex intermetallic compounds becomes energetically favorable. However, this phenomenon is not considered a universal law for all high-entropy materials. When determining the phase composition, it is also necessary to take into account the chemical affinity between the components and the production conditions.

Elastic deformation of the crystal lattice. In high-entropy materials, elements with different atomic radii and electronic structures are arranged in a single crystal lattice. As a result, local elastic deformations and stress fields arise in the lattice. This phenomenon is called deformation of the crystal lattice.

As a result of crystal lattice deformation, the following are observed:

- Difficulty in movement of dislocations.
- The occurrence of a strengthening effect due to a certain concentration of the mixture .
- In the hardness and strength of the material.
- The complexity of plastic deformation mechanisms.
- Increased mechanical strength in some compositions.

Therefore, the balance between strength and plastic deformation is important when choosing a material composition.

Diffusion retardation effect. In high-entropy materials, the different sizes and chemical environments of different atoms can complicate the conditions for the movement of atoms through the crystal lattice.

The temperature dependence of the diffusion coefficient is usually expressed by the Arrhenius equation:

$D=D_0 \exp(-Q/RT)$

Here: D – is the diffusion coefficient; D_0 – is the previous multiplier for diffusion; Q – is the activation energy; R – is the universal gas constant; T – is the absolute temperature.

Slowing down the diffusion process in some systems can provide the following advantages: improved microstructural stability at high temperatures; slowing down some phase transformations; and maintaining material properties over long-term use.

However, diffusion retardation is not characteristic of all high-entropy materials to the same extent. Its manifestation depends on the elemental composition, crystal structure, temperature, and direction of diffusion.

Cocktail effect

The complex effect refers to the formation of overall material properties that differ from the properties of the individual components as a result of the interaction of several elements. For example, different elements in one material:

In increasing mechanical strength;

Ensuring corrosion resistance;

In improving heat resistance;

In controlling electrical and magnetic properties;

They may have a complementary effect in building resistance to erosion.

This effect opens up great possibilities for designing high-entropy materials. Therefore, choosing the optimal composition of elements is one of the important tasks of modern materials science.

When assessing the prospects of high-entropy materials in the military field, there are also their advantages and problems associated with industrial-scale production [5].

of high-entropy materials:

1. Compositional flexibility. Material properties can be controlled by combining several basic elements in different proportions.

2. High mechanical properties. Some compositions exhibit high strength, hardness, and wear resistance.

3. Thermal stability. Materials with special compositions are considered promising for use in high temperature conditions.

4. Corrosion resistance. Resistance to aggressive environments can be improved by optimizing the composition.

5.Variety of functional features. It is possible to control magnetic, electrical and other functional features.

The problems that prevent the widespread industrial implementation of high-entropy materials include: the difficulty of accurately predicting the thermodynamic state of multi -component systems; the relative cost of materials production technologies; the high cost and limited resources of some elements; the sensitivity of the phase composition to production conditions; the difficulty of ensuring a uniform microstructure in large volumes

of materials. The effectiveness of each material should be assessed based on the specific conditions of use and the technical requirements imposed.

THEORETICAL AND PRACTICAL METHODS OF RESEARCH.

Modern theoretical methods for studying high-entropy materials. To deeply study the properties of high-entropy materials, theoretical calculations, computer modeling and experimental studies must be combined [6-7].

CALPHAD method. CALPHAD (Calculation of Phase Diagrams) method allows calculating thermodynamic properties of multicomponent materials and predicting phase diagrams. This method is used to study thermodynamic stability of phases, temperature-dependent phase changes, interaction of components, phase composition in equilibrium.

Density Functional Theory Calculations. Density Functional Theory **(**DFT) is a method that allows us to study the properties of materials at the atomic and electronic levels. It is used to calculate the energetic stability of the crystal lattice, the electronic structure, the interatomic bonds and some physical properties of the material.

Molecular dynamics method. Molecular dynamics is based on modeling the motion of a material at the atomic level. This method can theoretically study the thermal motion of atoms, defects in the crystal lattice, deformation processes, interatomic interactions, and microstructural changes under the influence of temperature.

Applied research methods.

The following methods are used to confirm the results of theoretical calculations [8-9]:

Research method	A defining characteristic
X-ray diffraction (XRD)	Crystal structure and phase composition
Scanning Electron Microscope (SEM)	Microstructure and surface morphology
Electrophoretic Deposition (EDS)	Chemical composition and distribution of elements
Transmission electron microscopy (TEM)	Nanoscale structure and defects
Vickers hardness measurement	Material hardness
Differential Scanning Calorimetry (DSC)	Thermal changes
Corrosion tests	Electrochemical stability

The combined application of these methods helps to reveal the relationship between the composition, structure, and properties of high-entropy materials.

DISCUSSION

Physico-mechanical properties of high-entropy materials. The practical importance of high-entropy materials is determined by their physical, mechanical, and chemical properties [10].

Mechanical strength and hardness. The mechanical properties of high-entropy materials depend on the crystal structure, chemical composition and phase ratio. The following mechanical properties are particularly important: yield strength; tensile strength; hardness; and plastic deformation.
Has attracted scientific interest especially due to its high plasticity and mechanical strength at low temperatures.

Heat resistance. In materials operating at high temperatures, processes such as oxidation, phase transformations, and deformation are observed. Some types of high-entropy materials are able to maintain microstructural stability at high temperatures. In particular, refractory high-entropy materials are developed based on tungsten, molybdenum, niobium, and other elements with high melting points. Their promising areas of application: mechanisms operating at high temperatures; gas turbine elements; promising materials for aircraft engines; heat-protective coatings; some components of power plants.
Factors such as density, oxidation resistance, and production costs must also be evaluated separately.

Corrosion resistance. The corrosion resistance properties of high-entropy materials can be controlled by changing their chemical composition. In particular, chromium, aluminum, and other elements that form a protective layer in oxidizing environments can contribute to the formation of a passive layer on the surface of the material. Such a layer limits the direct interaction of the metal with the external environment.
These properties are important for marine equipment, military vessels, special vehicles, and mechanisms operating in various environments.

Radiation resistance. High-entropy materials are also a promising research object for nuclear energy and mechanisms operating in radiation environments. The arrangement of atoms in different chemical environments in a multicomponent crystal lattice can affect the formation and migration of defects. Therefore, some high-entropy materials are being studied from the point of view of resistance to radiation defects. However, radiation resistance cannot be explained only by high entropy. The phase state of the material composition is important.

SUGGESTIONS

The above theoretical analyses show that high-entropy materials create new opportunities in modern materials science. Their most important feature is the possibility of targeted control of physical and mechanical properties through multi- component composition. The requirements for materials in the military sector are multifaceted, and they must simultaneously provide mechanical strength, thermal stability, corrosion resistance and reliability in use. From this point of view, it is advisable to develop high-entropy materials in the following scientific directions:

1. Creation of corrosion-resistant materials for military transport and special equipment;
2. Research into high-temperature alloys for aviation technology;
3. Study of high-entropy ceramic materials for special mechanisms;
4. Development of multifunctional protective coatings for metal mechanisms;
5. Evaluation of the stability of materials operating in radiation and extreme environments.

It is also necessary to take into account the cost-effectiveness of materials, production technology, environmental safety and recyclability. These approaches can help to find optimal compositions for multi -component systems and reduce the cost of experimentation.

CONCLUSION

Based on the theoretical analyses conducted, the following scientific conclusions were reached:

are composed of a few basic elements, and their properties are determined by configurational entropy and interatomic interactions.

High entropy, lattice deformation, diffusion retardation, and complex interaction effects are important theoretical properties of these materials. However, these effects are not manifested to the same extent in every material.

The mechanical strength, hardness, corrosion resistance, and thermal stability properties of high-entropy materials can be optimized by controlling the composition and microstructure.

To determine the practical effectiveness of materials, it is necessary to combine theoretical calculations with experimental studies. In particular, it is important to use CALPHAD, DFT, molecular dynamics, and modern microstructural analysis methods.

In general, high-entropy materials are a promising class of materials that have the potential to improve the performance of future military and special equipment. Their development is closely related to the integration of materials science, metallurgy, physical chemistry and modern computing technologies.

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