**Nanocomposites and nanomaterials**

**Evaluation of the degree of solid solution hardening of multielement metal composite material’s diborides**

D. Zakarian\*, A. Khachatrian, V. Kartuzov

*Frantzevich Institute for Problems of Materials Science, Krzhizhanovsky str., 3, 03142, Kyiv-142, Ukraine*

A method has been developed with the help of which the degree of solid solution hardening of multielement metal composite material’s diborides (HEA’S diborides) having an AlB2 type structure is estimated. The method makes it possible to estimate the hardness of both nanosized structures and bulk materials.

To describe the random distribution of metal atoms over the nodes of the crystal lattice, the concept of a characteristic volume is introduced, as a volume where the distribution of atoms of all metals, included in the composition of the alloy, is realized. In this volume, all possible neighborhoods of atoms in the crystal lattice are taken into account. The characteristic volume is a necessary building element, which can be used to construct the HEA’S structure of diborides by its translation. The volume of the characteristic region depends both on the number of possible pair interactions of atoms and on the type of the crystal lattice of the alloy, which are determined from first principles (pseudopotential method) [1].

One of the fundamental properties of multi-element composite HEA’S materials is that the lattice structure of the solid solution is strongly distorted and this creates an obstacle to the free movement of dislocations. To describe hardening, the main emphasis in research is on taking into account the difference in the radii of the atoms present in the alloy.

The main characteristics of alloys that correlate with mechanical properties are the number of various metal elements, the mismatch parameter, which represents the maximum difference in the atomic radii of the elements in the alloy, and the average crystal lattice parameter of the alloy. The increase in hardness depends on the ratio of the values ​​of the mismatch parameter and the lattice parameter of the alloy. If the first factor is associated with the difference in the atomic radii of the elements (the degree of distortion of the crystal lattice of the alloy), then the second is indirectly related to the potentials of different elements, as well as their interaction.

The calculation was carried out for diborides of multielement metal composite materials (Zr0.5Hf0.5B2; Ti1/3Zr1/3Hf1/3B2; Ti0.25Zr0.25Hf0.25Cr0.25B2; Ti0.2Zr0.2Hf0.2Cr0.2Ta0.2B2). It has been found that an increase in the number of types of metal atoms in a composite material leads to an increase in hardness, even if the difference in atomic radii is small.

1. D. Zakarian, A. Khachatrian. Method for evaluating hardening in highly entropy equiatomic metal alloys. (Abstract, 4(FCM)). International Conference on Advance in Functional Materials, 2021, Los Angeles, USA, 18-20 August, 2021. https://aaafm.org/ucla2021/