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PROPERTIES OF CAST MULTICOMPONENT HIGH-ENTROPY BORON-DOPED ALLOYS.

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Abstract

The physical, mechanical and tribological properties of cast multicomponent high-entropy boron-doped alloys obtained by vacuum-arc melting are studied. It was found that cast multicomponent high-entropy alloys doped with boron have a hardness of 20-30 GPa and a modulus of elasticity of 400-600 GPa. Alloying high-entropy alloys with a Borut lab6 mixture increases the hardness to 35-45 GPa and the modulus of elasticity to 700-780 GPa. The possibility of setting the coefficient of conversion of hardness to the yield strength knowing the elastic modulus of the material is shown.

Alloying high-entropy alloys with boron significantly improves their heat resistance. Thus, the high-entropy tihfnbtamo alloy with the addition of 2% boron reduces the hardness from 13.0 GPa at 20 °C to 8.5 GPa at 900 °C.

Keywords: high-entropy alloys, boron, hardness, elastic modulus, elastic deformation, elastic limit, conversion coefficient, friction .

Introduction

The emergence of a new class of materials — multicomponent high-entropy alloys and opened the way for the development of new, higher-strength and thermostable alloys and coatings [1-5] and kermets based on them [6-14]. Recently, doping with silicon carbide and boron has been used to increase the strength of high-entropy materials [15, 16]. According to the literature data, high-entropy alloys based on refractory metals doped with boron increased their hardness to 24-38 GPa[17-19].

The aim of the work is to determine the effect of boron alloying on the physical, mechanical and tribotechnical properties of cast multicomponent high — entropy alloys based on BCC phases obtained by vacuum-arc melting.

Methodology and materials

Multicomponent high-entropy alloys with boron addition were melted in a purified argon medium by an electric arc method with a non-consumable tungsten electrode on a water-cooled copper hemispherical well. The resulting ingots for homogenization of the composition were melted down five times, followed by cooling on a hemisphere at a rate of ~100 °C/s.

Hardness (H) and" effective " elastic modulus (E_r) were determined in accordance with the international standard ISO UNE EN ISO 14577-1: 2016 (Part 1. Test Method. ISO 14577-1: 2015) using automatic microindentation (Micron-gamma device) by the Berkovich pyramid at a load of 3 N. The level of elastic deformation (ε_s) was calculated according to [20]. When calculating the elastic modulus of boron-doped alloys, the Poisson's ratio was 0.18.

The average values of the HEA electron concentration (the number of valence electrons per atom) and the Poisson's ratio were calculated using the mixture rule.

The size discrepancy was estimated by the formula:

$$\delta = \sum c_i \left| (a_i - a_{\text{average}}) / a_{\text{average}} \right|, \quad (1)$$

where c_i the concentration of this element; a_i , a_{average} is the lattice parameter and its average value.

The mixing enthalpy was calculated as a linear combination of the interaction energies between pairs of alloy atoms, using the formula:

$$\Delta H_{\text{mix}} = \sum_{i=1, j\neq i}^{n} 4H_{ij}^{\text{mix}} C_i C_j \quad , \tag{2}$$

where ΔH_{mix} is the enthalpy of mixing two atoms i and j, which is calculated in the Miedema model [21]. Its value for further calculation was taken from the work [22].

Tribotechnical characteristics were studied using a micron-tribo friction machine [23], which is designed to conduct a finger–disk wear test. As a finger, a diamond with a sharpening angle of 30 degrees and a rounding radius of 20 microns is used. The friction load was 0.6 H. The high-temperature hardness was determined by indentation with a four-corner pyramid in vacuum at a load of 10 H.

Results obtained and their discussion

Studies have shown that one of the features of wind farms is the presence of distortion (lattice-distortion), which makes a significant contribution to the strengthening of such alloys [24-27]. However, in [26], it is noted that the distortion level in solid-soluble wind farms based on the BCC phase is not always proportional to the hardness. To determine the effect of boron doping on the properties of wind farms, solid-soluble wind farms based on the BCC phase with different distortion levels were selected. In the table 1 presents the data of cast multicomponent high-entropy alloys based on the BCC phase obtained by indentation and calculations.

Table 1. data of cast multicomponent high-entropy alloys based on BCC phases obtained by indentation and calculations

Alloys	C_{sd}, el/at	H, GPa	E_r, GPa	H/E_r	E, GPa	ε_s, %	σ_s, GPa	δ, %	H/σ_s exper.	H/σ_s calcul.
TiZrHfVNbTaCrMoW	4,88	7,6	150	0,050	155	1,53	2.30	5,37	3,30	
TiZrHfVNbTaMoW	4,86	6,0	130	0,046	136	1,41	1,83	4,97	3,27	
TiHfNbTaMo	4,60	6,0	150	0,039	155	1,19	1,79	3,93	3,35	
AlTiVCrMoNb	4,83	6,8	165	0,041	178	1,26	2,25	3,75	3,02	3,01

As can be seen from the table 1 all selected cases meet the criteria of hard-soluble Alloys [3] and have a high level of hardness and distortion. Subsequently, these alloys were melted down with the addition of 2% boron or a 2% mixture of B+LaB_6.

In the table 2 shows the physical and mechanical properties of high-entropy alloys additionally doped with boron or a mixture of B+LaB_6.

Table 2. Physical and mechanical properties of high-entropy alloys doped with 2% boron or a mixture of B+LaB6.

Склад	H, ГПа	E_r, ГПа	H/E_r	E, ГПа	ε_s, %	σ_s, ГПа	H/σ_s exper.	H/σ_s calcul.
(TiZrHfVNbTaCrMoW)B	32	257	0,1245	330	3,822	12,61	2,54	2,77
(TiHfNbTaMo)B	18	243	0,0741	306	2,275	6,961	2,58	2,81
(AlTiVCrMoNb)B	16	234	0,0684	292	2,100	6,131	2,61	2,83
(TiZrHfVNbTaMoW)B	31	284	0,1091	378	3,349	12,66	2,44	2,70
(TiZrHfVNbTaMoW)B+LaB6	36	425	0,0847	695	2,600	18,07	1,99	2,22
(TiZrHfNbTaCrMoW)B+LaB6	45	458	0,0982	786	3,015	23,69	1,90	2,04

The addition of 2% boron to the BCC lattice-based wind farm increased the hardness from 6-8 GPa to 16-32 GPA and the elastic modulus from 140-190 to 290-378 GPA. The normalized hardness values of boron-doped C HEA, according to [3], are in the region of the nanostructured state (0.0847-0.1245), which is typical for borides. The presence of boron is confirmed by the spectral analysis shown in Fig. 1. The presence of all elements of both the high-entropy AlTiVCrMoNb alloy and B is recorded.

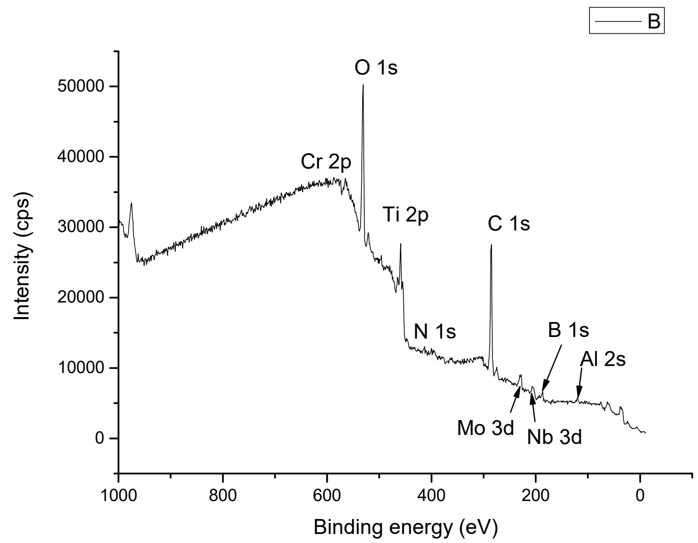

Fig.1. Energy spectrum of the system (AlTiVCrNbMo)B.

Doping of a spring-based BCC lattice with a mixture of B+LaB6 is accompanied by a significant increase in the elastic modulus to 690-780 GPA. Similar values of the elastic modulus are typical for monoborids.

Analysis of Tables 1 and 2 shows that as the elastic modulus increases, the coefficient of conversion of hardness to the yield strength decreases. For materials where the hardness does not exceed the values of 10 GPa, and the modulus of elasticity is below 150, the conversion coefficient at the level of 3.3 can be used to determine the yield strength from indentation data. For materials with an increased level of hardness or elastic modulus, the conversion coefficient decreases with increasing elastic modulus. Therefore, for materials with an elastic modulus above 170 GPA, a formula is proposed for determining the conversion coefficient, which takes into account the influence of the elastic modulus:

$$H/\sigma_s = 3,3-(0,0015\,E+0,004E^{-1/3})\ ГПа \quad (3)$$

In Fig. 2 presents the data of the conversion coefficient of materials determined in the experiment and calculated by Formula (3) as a function of the elastic modulus.

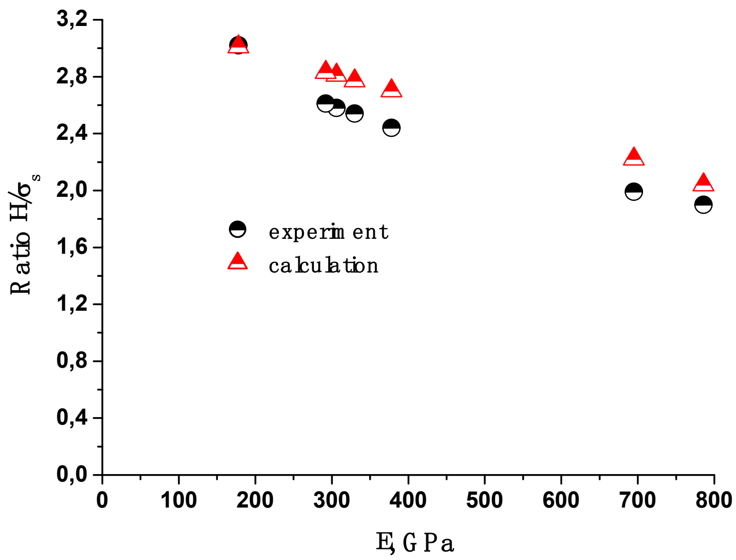

Fig. 2. The values of the conversion coefficient of materials determined in the experiment and calculated by the formula (3) depending on the elastic modulus.

The data is shown in Fig. 1 show the possibility of calculating the coefficient of conversion of hardness to the yield strength knowing the modulus of elasticity of the material.

High-entropy alloys are characterized by a fairly high heat resistance due to their increased entropy. For this purpose, we compared the high-temperature properties of a high-entropy TiHfNbTaMo alloy and after its alloying with 2% boron (fig. 3).

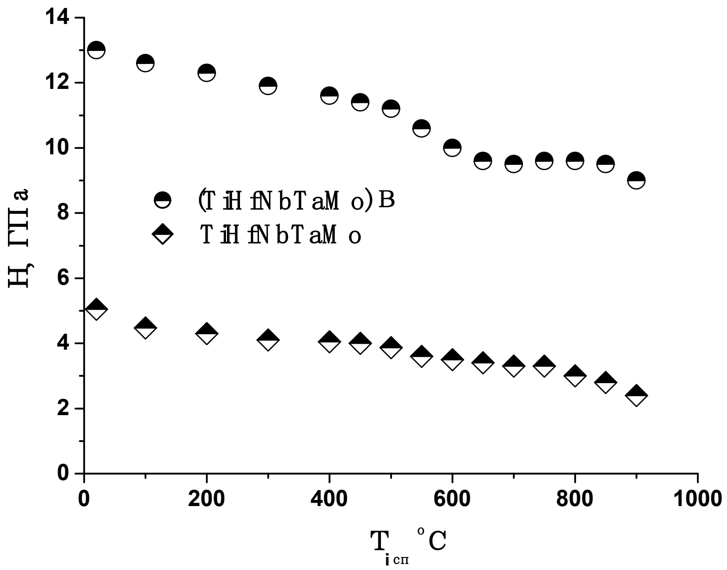

Fig. 3. High temperature hardness characteristics of high-entropy TiHfNbTaMo alloy based on BCC phases, as well as this alloy with the addition of 2% boron depending on the test temperature.

The presented data show that due to the processes of dynamic deformation aging [28, 29] and delayed diffusion [30, 31], a high-temperature plateau is observed in high-entropy alloys. Its presence makes it possible to maintain the hardness of cast alloys at the level of 3 GPa even at a temperature of 900 ° C. The addition of boron significantly improved the high-temperature hardness of such a material while maintaining a high-temperature plateau. The hardness of the high-entropy TiHfNbTaMo alloy with the addition of 2% boron decreased from 13 GPA at room temperature to 8.5 at 900 ° C. Similar alloys can be used for Blade metalworking.

Conclusions

The possibility of creating cast high-entropy rims due to vacuum-arc melting of a high-entropy alloy with boron and LaB6 is determined. The physical and mechanical properties of various mixtures of high-entropy alloys doped with boride are established, which increases their hardness to 31 GPa. Alloying the weight with a mixture of boron and LaB6 increases the hardness to 35-45 GPa and the modulus of elasticity to 700-780 GPa.

It is shown that alloying high-entropy alloys with boron significantly improves their heat resistance. Thus, the high-entropy tihfnbtamo alloy with the addition of 2% boron reduces the hardness from 13.0 GPa at 20 °C to 8.5 GPa at 900 °C.

It is possible to calculate the coefficient of conversion of hardness to the yield strength knowing the elastic modulus of the material.

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