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Paper Title: Preparation of a novel high-entropy alloy AlNbTiVZr with excellent strength and ductility: The effect of Zr composition on microstructure and properties

Content :

Density and hardness

The density and hardness of the $\text{Al}_{0.8}\text{Nb}_{0.5}\text{Ti}_2\text{V}_2\text{Zr}_x$ alloys are shown in Table 4. The density increases with increasing x .

The variation curves of hardness and secondary-phase content of the $\text{Al}_{0.8}\text{Nb}_{0.5}\text{Ti}_2\text{V}_2\text{Zr}_x$ alloys with respect to x are shown in Fig. 6. The hardness and areal fraction of the secondary phase increase significantly with increasing x . Furthermore, $\text{Zr}_{0.9}$ exhibits the highest hardness, which is 73 % higher than that of Zr_0 . Therefore, the hardness of the $\text{Al}_{0.8}\text{Nb}_{0.5}\text{Ti}_2\text{V}_2\text{Zr}_x$ alloys is dependent on the areal fraction of the secondary phase. The following equation was established to predict the hardness (

H_{Valloy}

) of the $\text{Al}_{0.8}\text{Nb}_{0.5}\text{Ti}_2\text{V}_2\text{Zr}_x$ alloys as a function of x .

The corresponding kernel average misorientation (KAM) maps of the $\text{Al}_{0.8}\text{Nb}_{0.5}\text{Ti}_2\text{V}_2\text{Zr}_x$ alloys are shown in Fig. 7. The KAM is used as an index to describe the degree of internal mismatch in crystals. The geometrically necessary dislocation (GND) density was estimated using the following empirical equation [22,23].

$$GND = k \cdot KAM^n$$

where k and n (fixed values) are the empirical constant and the fitting index, respectively. The value of KAM changed from 0.207 to 1.643 with increasing x , as shown in Fig. 7 (b, d, f, and h). The value of GND also increases with increasing x . Furthermore, the GND values are higher at the grain boundaries and secondary-phase precipitates. The value of GND increases with increasing x due to grain refinement (increase in the grain-boundary volume) and areal fraction of the C14-Laves phase. Therefore, the hardness of the $\text{Al}_{0.8}\text{Nb}_{0.5}\text{Ti}_2\text{V}_2\text{Zr}_x$ alloys increases with increasing x .

Compressive properties

The engineering stress–strain curves and SYS of the $\text{Al}_{0.8}\text{Nb}_{0.5}\text{Ti}_2\text{V}_2\text{Zr}_x$ alloys are compared with those of other reported HEAs in Fig. 8. At RT, the ultimate compressive strength (UCS) values of Zr_0 , $\text{Zr}_{0.3}$, $\text{Zr}_{0.6}$, and $\text{Zr}_{0.9}$ specimens are 1936, 2387, 1749, and 1869 MPa, respectively, while their yield strength (YS) values are 971, 1216, 1483, and 1714 MPa, respectively. Fig. 8(a, b) show that the compressive properties of the $\text{Al}_{0.8}\text{Nb}_{0.5}\text{Ti}_2\text{V}_2\text{Zr}_x$ alloys depend significantly on x . The YS of the alloys increases from

974 to 1713 MPa, while the compressive ductility increases from 49.73 % to 55.26 % and then decreases to 12.18 % with increasing x . A previous study showed that the matrix divided by the second-phase could not exert its deformability [16]. Therefore, the Zr_{0.6} and Zr_{0.9} alloys exhibit poor ductility.

The engineering stress–strain curves of the Al_{0.8}Nb_{0.5}Ti₂V₂Zr _{x} alloys at 873 K are shown in Fig. 8(b). The high-temperature UCS values of Zr₀, Zr_{0.3}, Zr_{0.6}, and Zr_{0.9} are 946, 1287, 1319, and 1469 MPa, respectively, while their YS values are 594, 1013, 1273, and 1433 MPa, respectively. The effect of solid-solution strengthening is weakened at high-temperatures [24]. Therefore, the compressive YS and UCS at 873 K are lower than those at RT. Furthermore, the compressive ductility values of the specimens at 873 K (57.93 %, 64.53 %, 26.27 %, and 21.18 %) for Zr₀, Zr_{0.3}, Zr_{0.6}, and Zr_{0.9}, respectively) are higher than those at RT.

To provide a basis for comparison, the curves for the specimen tested at 1073 K and 1273 K are included, as shown in Fig. 8(c and d). The results demonstrate that the Al_{0.8}Nb_{0.5}Ti₂V₂Zr _{x} alloys displays excellent high-temperature plasticity, exhibiting a compressive strain of over 70 % without fracture (the compression test was manually interrupted to save time) at all testing temperatures. However, the YS gradually decreases as the temperature increases, ranging from 382 to 606 MPa at 1073 K to 135–185 MPa at 1273 K, as shown in Fig. 8(e). Furthermore, the Al_{0.8}Nb_{0.5}Ti₂V₂Zr _{x} alloys exhibited strain softening at 1073 K and 1273 K. This observation underscores the importance of 873 K as a critical temperature threshold. Beyond 873 K, there is a notable decline in the material's performance, which is a crucial characteristic to consider for high-temperature applications.

Compared with other alloys (Zr₀, Zr_{0.6}, and Zr_{0.9}), the Zr_{0.3} alloy exhibits significantly superior compressive properties at RT and 873 K. The strain hardening rate at different temperatures is shown in Fig. 8(f). The Zr_{0.3} alloy demonstrates excellent strain hardening ability, and the strain hardening rate decreases rapidly in the later stage of deformation, suggesting that some special deformation mechanisms are activated at RT and 873 K. The above results demonstrate that the Zr_{0.3} alloy retains excellent mechanical properties at RT and 873 K. In the following sections, we will focus on the microstructural evolution and deformation behaviors of the Zr_{0.3} alloy deformed at RT and 873 K.

The SYS is an important index for evaluating material properties and selecting appropriate materials. Therefore, the compressive SYS and ductility were selected for evaluating the mechanical properties of the alloys developed in this study. The compressive SYS and ductility of Al_{0.8}Nb_{0.5}TiV₂Zr _{x} alloys and related LHEAs and RHEA reported in the literature are shown in Fig. 9. At RT, the compressive SYS of Zr₀, Zr_{0.3}, Zr_{0.6}, and Zr_{0.9} are 184, 227, 275, and 309 MPa cm³ g⁻¹, respectively, as shown in Fig.

9(a). Furthermore, the Zr_{0.3} alloy has a good balance between strength and toughness. The intermetallic compounds precipitated in an LHEA after the addition of Zr resulted in higher strength but lower ductility [16]. Therefore, the Zr_{0.6} and Zr_{0.9} alloys with high x had high SYS and low ductility. The compressive SYS and ductility of Al_{0.8}Nb_{0.5}TiV₂Zr_x alloys at 873 K are shown in Fig. 9(b). At 873 K, the compressive SYS of Zr₀, Zr_{0.3}, Zr_{0.6}, and Zr_{0.9} are 113, 188, 235, and 258 MPa cm³ g⁻¹, respectively. The LHEAs and RHEAs exhibit good compressive ductility at 873 K. However, the Zr_{0.3}, Zr_{0.6}, and Zr_{0.9} alloys exhibit superior specific yield strength and ductility compared to most HEAs.

The fracture morphologies of Al_{0.8}Nb_{0.5}TiV₂Zr_x after compressive tests at RT and 873 K are shown in Fig. 10. The RT fracture surface of Zr₀ and Zr_{0.3} exhibits tearing features and a small amount of river patterns (Fig. 10(a and b)). In contrast, many river patterns are observed on the fracture surface of Zr_{0.6} and Zr_{0.9}. Previous studies showed that the areal fraction of the secondary phase in Zr_{0.6} was low (Table 2), which provided little hindrance to dislocation movement. Therefore, Zr_{0.6} exhibits higher compressive ductility than Zr_{0.9}. Both the Al_{0.8}Nb_{0.5}TiV₂Zr_x alloys exhibit smooth fracture surfaces after compressive testing at 873 K, indicating cleavage fractures (Fig. 10(e–h)). Furthermore, Zr_{0.9} exhibits pronounced river-like features with larger cleavage planes and smaller tearing edges than Zr_{0.6}, indicating poor compressive properties compared with Zr_{0.6}.