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Paper Title: A single-phase Ti3Zr1.5NbVAl0.25 refractory high entropy alloy with excellent combination of strength and toughness

Content :

Results and discussion

Fig. 1a shows the Tri-color EBSD grain orientation map of recrystallized $Ti_3Zr_{1.5}NbVAl_{0.25}$ alloy. After annealing, the average grain size is measured to be 265 µm. The XRD pattern of the annealed sample as shown in Fig. 1b exhibits a single-phase BCC structure. This is attributed to the high concentration of Nb and V (a total of 30 at.%) elements that stabilized the β phase [9]. In addition, a single BCC solid solution was also predicted by the commonly suggested criteria: the enthalpy of mixing – 15 ≤

ΔHmix

≤ 5 kJ/mol, the atomic size difference

δ

≤ 6.6% and

Ω

≥ 1.1 [10], the valence electron concentration

VEC

< 6.87 [11]. Calculated empirical parameters of the $Ti_3Zr_{1.5}NbVAl_{0.25}$ alloy are summarized in Table S1 in Appendix A of Supplementary data. The TEM bright-field micrograph and the inserted selected-area electron diffraction (SAED) pattern corresponding to the grain boundary region as shown in Fig. 1c further confirm the single-phase structure without any precipitation. This indicates that Al element completely dissolved into the matrix, and no segregation to form B2 phase. As shown in Fig. 2d, TEM-EDS mapping also demonstrates that the components are uniformly distributed in the annealed $Ti_3Zr_{1.5}NbVAl_{0.25}$ alloy. The atomic percentage of the individual element is given in Table S2 in Appendix A of Supplementary data. Moreover, the density of $Ti_3Zr_{1.5}NbVAl_{0.25}$ alloy is ~ 5.76 g/cm3, which is lighter than that of most RHEAs.

The tensile stress–strain curve of $Ti_3Zr_{1.5}NbVAl_{0.25}$ alloy is shown in Fig. 2a. It should be noticed that the annealed alloy exhibits the yield strength of ~ 899 MPa, and the fracture elongation of ~ 24.5%, respectively. The high yield strength of the single-phase $Ti_3Zr_{1.5}NbVAl_{0.25}$ alloy may attribute to the remarkable solution strengthening effect of the whole-solute matrix. Moreover, the solid solution strengthening contribution is evaluated in Appendix B of Supplementary data and reached ~ 709 MPa, suggesting that solid solution strengthening is the dominant strengthening mechanism in the $Ti_3Zr_{1.5}NbVAl_{0.25}$ alloy. Meanwhile, the Charpy V-notch impact toughness of the alloy was measured to be 119.5 J/cm^2, while U-notch impact toughness even reached 131.3 J/cm^2, which has been never found for BCC type of RHEAs. Fig. 2b provides the yield strength as a function of the Charpy V-Notch impact toughness of the presented alloy and other common metallic materials and HEAs, such as 3d-transition HEA [12], [13], metastable β-titanium alloy [14], Ti-5321 alloy [15], Ti-6Al-4V [16], TC21 alloy [17], twin induced plastic (TWIP) steels [18] and transformation induced plasticity (TRIP) steels [19]. It can be derived that the $Ti_3Zr_{1.5}NbVAl_{0.25}$ alloy stands out, with the best synergy of strength and toughness. This can be ascribed to hot forging and subsequent annealing process, which improves the microstructure homogeneity and eliminated casting defects, thereby increasing the toughness.

The fractography of the Charpy impact specimen is shown in Fig. 3. The corresponding fracture surface is covered by overwhelming dimples, typical of the ductile fracture mode. Magnified images of crack initiation and propagation regions exhibit cleavage facets, voids and secondary cracks, demonstrating that quasi-cleavage fracture occurs occasionally during crack initiation and propagation. Fig. 3d shows three-dimensional (3D) fracture surface morphologies of the $Ti_3Zr_{1.5}NbVAl_{0.25}$ alloy. The ductile vein-like patterns observed by using an LSCM also indicate a tendency for ductile fracture, which is typically correlated with the relatively high impact toughness.

With the aim of deciphering plastic mechanisms of the $Ti_3Zr_{1.5}NbVAl_{0.25}$ alloy, detailed TEM observations have been made to monitor the dislocation behavior at different strains. Fig. 4a shows the TEM image after 1.5% strain. Coplanar slip of dislocations dominates plastic deformation in this early stage with occasional cross-slipped dislocations. At middle strain (10%), the massive straight planar slip bands (PSBs) were observed (see Fig. 4b), and around them, the dislocations are arranged in loops and bundles, as shown in Fig. 4c, indicating the frequent dislocation cross-slip, which often prevails in BCC metals due to the close-packed {1 1 0} and {1 1 2} slip planes [20]. With further straining to fracture, wavy slip dominates the plastic flow, and the abundant cross-slip results in the formation of high dense dislocation walls (HDDWs), as shown in Fig. 4d, which effectively contribute to the durability of plastic deformation. Additionally, deformation twins have not been detected after tension to a high strain, analogues to previously reported RHEAs [2], [4]. Based on the above results, the plastic deformation in current RHEA appears to be accommodated mainly by dislocation activity, and the multiple dislocation interactions via dislocation multiplication are considered to be the dominant mechanism for the large plasticity of this RHEA.

4. Conclusions

In this work, a forged $Ti_3Zr_{1.5}NbVAl_{0.25}$ RHEA with a single BCC phase has been prepared. The hot forging followed by annealing at elevated temperature leads to a homogeneous microstructure with coarse equiaxed grain. Owing to the solution strengthening effect and intense dislocation activity, the obtained alloy exhibits an excellent combination of high yield strength (899 MPa), large plasticity (24.50%), and high impact toughness (119.5 J/cm^2), which is far superior to most traditional alloys and HEAs.