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Paper Title: Remarkably high fracture toughness of HfNbTaTiZr refractory high-entropy alloy

Content :

1. Introduction

The design strategy of traditional alloy is based on one major element, adding appropriate amounts of other elements to adjust the properties of the alloy. In 2004, Yeh's group [1] and Cantor et al. [2] proposed the concept of high-entropy alloys (HEAs) for the first time. HEAs generally consist of equimolar or nearly equimolar mixtures of multiple elements (usually more than 4) [3]. The invention of HEAs broke the traditional alloy composition space and expanded the possibility of discovering high-property alloys [4,5]. The multi-principal element strategy renders HEAs structural characteristics different from traditional single-principal element alloys [3,[6], [7], [8], [9], [10], [11], [12]]. For instance, the high configuration entropy plays an important role in simplifying the microstructure of HEAs to be simple phases with face-centered cubic (FCC), body-centered cubic (BCC) or hexagonal close-packed (HCP) structure.

Like most other structural materials, HEAs which possess high fracture resistance are of great importance for engineering applications. In the past few years, researchers have studied the fracture resistance of multiple HEAs with different compositions. Some FCC single-phase HEAs show excellent fracture resistance, and their fracture toughness can reach more than 200 MPa $m_{1/2}$ (such as CoCrFeMnNi [6], CoCrNi [13], $V_{10}Cr_{10}Fe_{45}Co_{20}Ni_{15}$ [14] and $V_{10}Cr_{10}Fe_{45}Co_{30}Ni_{5}$ [15]). However, there are only few studies on the fracture toughness of BCC single-phase HEAs and nearly no standard samples have been used for testing, to the best of our knowledge. For example, Zou et al. [16] and Xiao et al. [17] used some micro-cantilever beam samples to study the fracture toughness of single-crystal/dual-crystal and nanocrystalline $Nb_{25}Mo_{25}Ta_{25}W_{25}$, respectively. The measured toughness for these BCC HEAs, however, are quite low due to probably the very confined volume that limits the fracture energy consumption. Wang et al. [18], on the other hand, studied the toughness of BCC $(TiZrNbTa)_{100-x}Mo_{x}$ (x = 0, 5, 10, 20) alloy using specimens without pre-fatigue crack. The results well demonstrate a transition for fracture mechanism as varying the composition, but the data cannot be compared with others because of the non-standard sample and notch geometries. Since the lack of fracture toughness testing using standard test methods so far, it remains unknown that where the BCC single-phase HEAs should be placed among various metals and alloys as considering the fracture properties.

The HfNbTaTiZr refractory high-entropy alloy (RHEA) with BCC phase exhibits great application potential, because it is one of the few BCC single-phase HEAs with good tensile ductility at room temperature, as well as high strength and good high-temperature performance [19], [20], [21], as shown in Fig. 1. The yield strength of the HfNbTaTiZr RHEA at 1000 °C is 295 MPa [20], significantly higher than many other alloys. Although the tensile properties have been well studied, the fracture toughness of HfNbTaTiZr RHEA has not yet been investigated. In this work, we performed single-edge notched bending (SENB) tests with the "single specimen" compliance method according to the ASTM E1820–17 standard to measure the ability of the alloy to resist crack propagation. The fracture toughness value of the BCC phase HfNbTaTiZr RHEA was given, and the deformation and fracture mechanisms of the crack tip area were observed.

Results and discussion

The microstructure and element distribution of the HfNbTaTiZr RHEA were characterized by XRD, EBSD and EDS, and the results are shown in Fig. 3. The XRD pattern displays a single-phase BCC structure, which is consistent with the previous result by Senkov et al. [33]. The EBSD inverse pole figure (IPF) reveals that the alloy has equiaxed grains with grain size ~167 μm. The element maps of the five principal elements by EDS reveal good chemical homogeneity (see Fig. 3(c)), which implies that the segregation among grains is not obvious. The results of impulse excitation of vibration give that for this alloy, the Young's modulus E = 97.7 GPa, and the Poisson's ratio υ = 0.39.

In Fig. 8(c), many equiaxed dimples were observed at fractured surfaces, which suggests that the HEA alloy was ductile fracture caused by microvoid coalescence. In order to further explore the deformation and fracture behaviors of the HEA alloy, the SEM image of half-sectioned smooth specimen with thickness of 3 mm was observed under the same experimental conditions, as shown in Fig. 8(d). As can be seen on the EBSD image of Fig. 8(e), many parallel band structures which are different from the matrix can be observed in the grains. In the kernel average misorientation (KAM) map of Fig. 8(f), the KAM values at grain boundaries and parallel band structures are higher than those of intragranular. The result indicates that the grain boundaries and parallel band structures act as strong obstacles against the dislocation movement during plastic deformation. Thus, the formation of parallel band structures can significantly contribute to the R-curve behavior. To quantitatively evaluate the difference in crystal orientation between parallel band structures and the matrix, the misorientation profile (Fig. 8(h)) was plotted along the direction of the red arrow in Fig. 8(g). It can be seen that the misorientation angles in the range of 18° to 35° exclude the possibility of twinning. The misorientation differences indicate that the bands are kink bands. This result is consistent with the previous studies of Zherebtsov et al. [39], Chen et al. [40] and Wang et al. [8] on the tensile deformation mechanisms of HfNbTaTiZr at 77 K and in different rolling states. Therefore, the high fracture toughness of HfNbTaTiZr alloy is attributed to the fully-ductile fracture mode. The formation of kink bands can effectively hinder the movement of dislocations and increase the resistance to crack propagation, thereby contributing to the high toughness of the HEA alloy.

Fig. 9(a) plots the relation between fracture toughness and yield strength of various HEAs with different phase structures at room temperature. Only a small number of alloys are tested for toughness according to the ASTM standard, while the toughness tests of most alloys have not been measured using pre-fatigue cracked specimens. In Fig. 9(a), it can be seen that some FCC single-phase HEAs generally exhibit very excellent fracture toughness. However, as the volume fraction of the FCC phase decreases, the fracture toughness of dual-phase HEAs decreases [41], [42], [43], [44]. BCC phase HEAs usually display brittle cleavage or quasi-cleavage fracture at room temperature, and it is difficult to accommodate enough dislocations to cause unsteady crack propagation [42], [43], [44], [45], [46], [47]. Therefore, the fracture toughness of BCC phase HEAs are much lower than that of FCC phase HEAs. In this work, the research of HfNbTaTiZr HEA found that this alloy can exhibit excellent fracture toughness, and its toughness value is almost equivalent to that of FCC phase HEAs. Besides the excellent fracture toughness, its strength is significantly higher than that of the FCC phase HEA. Compared with traditional alloys, as shown in Fig. 9(b), the fracture toughness of HfNbTaTiZr also stands on the top position, which renders this HEA promising application potential.

4. Conclusion

The fracture behaviors of HfNbTaTiZr RHEA were investigated according to the ASTM E1820–17 standard test method in this work. The HfNbTaTiZr alloy exhibits a single-phase BCC structure and a desirable combination of strength (σ_{UTS} = 957 ± 34 MPa) and ductility (ε_f = 16.5% ± 0.2%). The fracture toughness of the alloy was measured by the “single- specimen” compliance method to be a very high value of J_{IC} = 384 kJ/m^2, leading to a remarkably high fracture toughness of K_{JIC} = 210 MPa m$^{1/2}$. Rising R-curve behavior and a wide critical stretch zone width (SZW ~162 μm) can be observed, well consistent with the high fracture toughness. It is found that ductile fracture mechanisms of microvoid nucleation and aggregation dominate the fracture of HfNbTaTiZr RHEA, and dislocation slip mediates the plastic deformation. Besides, kink bands have been also formed, which effectively hinders the movement of dislocations and increases the resistance to crack propagation, thereby contributes to the high toughness of the alloy