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Influence of heat treatment and high-pressure torsion on phase transformations in TiZrHfMoCr high-entropy alloy

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The study focused on the 21.99 at.%Ti-22.49 at.%Zr-20.35 at.%Hf-17.45 at.%Mo-17.73 at.%Cr high entropy alloy (Fig. 1). The analytical techniques like X-ray diffraction, scanning electron microscopy as well as X-ray absorption spectroscopy were employed to investigate the alloy's structure, phase transformations, and properties. The alloy in the as-cast state contained three phases, namely the body-centered cubic (A2) phase, hexagonal Laves phase (C14) and cubic Laves phase (C15). The alloy has beeen annealed during long time at different temperatures. It led to the disappearance of the hexagonal Laves phase, leaving behind two primary phases, namely the cubic Laves phase (C15) and body-centered cubic phase (A2). At 1200°C the A2 phase almost disappeared, resulting in a practically single-phase sample. After high pressure torsion (HPT) treatment, the hexagonal Laves phase disappeared entirely, while the A2 and C15 phases remained. The grain size of the A2 and C15 phases was refined after HPT and grains were elongated, and their configuration resembled a layered structure. The high hardness of the A2 and C15+C14 phases accounted for this behavior. The lattice parameters in the A2 and C15 phases after HPT treatment approached those observed after prolonged annealing at 1000°C, indicating that the composition of these phases after short-term high pressure torsion at ambient temperature is equivalent to the composition of these phases after long tempering at 1000°C. The rate of diffusion-like mass transfer during severe plastic deformation was estimated to be many orders of magnitude higher than that for conventional bulk diffusion at the HPT treatment temperature and similar to that at elevated temperatures above 1000°C. X-ray absorption spectroscopy results obtained at K-edges of Ti, Cr, Zr, and Mo as well as at L3-edge of Hf indicated that the local environment around metal atoms before HPT is similar to that after HPT (Fig. 2). However, the static disorder increased after HPT, which could be attributed to an increased specific amount of metal atoms in the disordered grain boundary layers after HPT-driven grain refinement (Fig. 3).



Fig. 1. SEM images of the initial microstructure of the TiZrHfMoCr alloy: (a) general view, (b) dots mark the areas of component analysis: light gray (1), dark gray (2), and gray (3) colors. (c) X-ray diffraction pattern of the as-cast TiZrHfMoCr alloy. Reprinted with permission from Ref. [1]. Copyright 2023 MDPI.





Fig. 2. XANES spectra of the original as-cast (AC) TiZrHfMoCr HEA sample and sample after HPT at the Ti, Cr, Zr, and Mo K-edges and Hf L₃-edge. The insets show an enlarged view around the edge. The pre-edge A and the white line WL are indicated. Reprinted with permission from Ref. [1]. Copyright 2023 MDPI.



Fig. 3. Comparison of the Fourier transform of the EXAFS spectra for as-cast (AC) TiZrHfMoCr HEA at the K-edges of Ti, Cr, Zr, and Mo and L₃-edge of Hf. Only the moduli of FTs are shown for clarity. Reprinted with permission from Ref. [1]. Copyright 2023 MDPI.

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