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Phase stability, precipitation kinetics, nanoscale elemental distributions and their effect on tensile properties in refractory TiZrNbHfTa BCC high-entropy alloys

Keywords: phase stability, precipitation kinetics, multi-scale characterization, nanoscale elemental distribution, segregation at grain boundaries, mechanical behavior

Refractory high-entropy alloys (RHEAs), consisting of elements with high melting points, are promising candidates for high-temperature applications beyond Ni-based superalloys and other conventional refractory alloys. Among RHEAs, the equiatomic body-centered cubic (BCC) TiZrNbHfTa alloy exhibits an excellent combination of ductility and strength at room temperature. This alloy was initially thought to be stable since its high mixing entropy should inhibit the formation of secondary phases. However, upon aging below 900 °C, a hexagonal close-packed (HCP) phase precipitates, leading to a severe deterioration in ductility. Also, local clustering and/or short-range ordering (SRO) could affect tensile properties. To improve the mechanical performance of BCC RHEAs, one must know how to control the formation of these microstructural features and understand their roles in deformation behaviors. Therefore, the objective of this collaborative study is to provide a better understanding of these fundamental aspects and establish the relationships between microstructure and mechanical properties.

Here, an equiatomic single-phase TiZrNbHfTa RHEA with a recrystallized microstructure will be annealed in the range [300-1200 °C] for various times followed by microstructural and chemical analyses at multiple length scales. 1000-h anneals followed by X-ray diffraction, scanning electron microscopy, and electron backscatter diffraction will be performed to examine thermodynamic equilibria. Additional anneals for shorter times will allow us to establish the first time-temperature-transformation diagram for the TiZrNbHfTa RHEA. To further reveal the corresponding rate-controlling mechanisms, the evolution with time and temperature of the microstructures as well as concentration profiles building up at matrix/precipitate interfaces will be systematically studied. Early-stage HCP precipitation within grains, segregation, and partitioning at high-angle grain boundaries will be investigated in detail by atom probe tomography (APT) and transmission electron microscopy (TEM) to unravel the nucleation mechanisms of HCP precipitates. Furthermore, nanoscale compositional modulations and/or SRO will be assessed by APT and TEM in the BCC matrix at various temperatures and durations. The effects on tensile properties of different microstructures (nanoscale compositional modulation, SRO, different volume fractions and morphologies of HCP phase) resulting from various anneals will be investigated to gain a better understanding of deformation and failure mechanisms in TiZrNbHfTa. Overall, this project will advance our understanding of the elementary processes associated with precipitation kinetics and phase stability but will also uncover unusual microstructural features that potentially lead to outstanding mechanical properties in RHEAs.