High-entropy carbides: A novel group of materials for extreme environments

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Abstract

Bulk equiatomic (Hf-Ta-Zr-Nb)C high-entropy ultra-high temperature ceramic (UHTC) carbide was fabricated by ball milling and Spark Plasma Sintering (SPS). It was found that the lattice parameter mismatch of the component monocarbides is a key factor for predicting single phase solid solution formation, revealing a vast new compositional space for the exploration of new UHTCs. The microstructure characteristics were investigated using X-ray diffraction (XRD), scanning electron microscopy (SEM) in combination with electron back scattered diffraction (EBSD) and transmission electron microscopy (TEM). Atomic structure and local chemical disorder was determined by means of scanning transmission electron microscopy (STEM) in conjunction with energy dispersive X-ray spectroscopy (EDS). Optimisation of processing route revealed high purity, dense (99%), single phase and homogeneous high entropy carbide with Fm-3m crystal structure for (Hf-Ta-Zr-Nb)C. The grain size ranged from approximately 5 μm to 25 μm with average grain size of 12 μm. Chemical analyses proved that all grains had the same chemical composition at the micro as well as on the nano/atomic level without any detectable segregation. This optimised material was subjected to nanoindentation testing and directly compared to the constituent mono/binary carbides, revealing a significantly enhanced hardness (36.1±1.6 GPa,) compared to the hardest monocarbide (HfC, 31.5±1.3 GPa) and the binary (Hf-Ta)C (32.9±1.8 GPa). Additional micropillar compression test of grains revealed that (Hf-Ta-Zr-Nb)C had a significantly enhanced yield and failure strength (6.20±0.12 GPa) compared to the corresponding base monocarbides (3.93±0.28 GPa for HfC, 3.03±0.11 GPa for TaC), while maintaining a similar ductility to the least brittle monocarbide (TaC) during the operation of 110 110 slip systems.