Theoretical predictions and synthesis of (Ti-Zr-Hf-Nb-Ta)B_2 structures with non-equimolar compositions.

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Highly pure High-Entropy Boride ceramics (HEB) were produced by two-step spark plasma sintering, consisting of boro/carbothermal reduction of oxides mixtures and pressure-assisted sintering. This work was focused on the HEB materials with non-equimolar compositions of transition metals (Ti-Zr-Hf-Nb-Ta), which demonstrated a reliable and cost-effective processing way for producing high-entropy diboride ceramics with a single phase solid-solution. High-entropy borides may have a wide composition range, but $(Ti_{0.2}Zr_{0.2}Hf_{0.2}Nb_{0.2}Ta_{0.2})B_2$ is one of the most investigated compositions. Based on the $(Ti_{0.2}Zr_{0.2}Hf_{0.2}Nb_{0.2}Ta_{0.2})B_2$ structure, a group of high-entropy boride ceramics with non-equal transition metal atom ratios were theoretically predicted and experimentally investigated. The theoretical predictions were performed using the Density Function Theory implemented in the VASP program. The Special Quasirandom Structures were used to disorder materials. All structures with non-equimolar ratios had a single phase according to XRD analysis. Nanoindentation was performed to measure both hardness and Young's modulus of the sintered materials. This study investigated the effect of different concentrations of metal elements on the processing and mechanical properties of high-entropy diboride ceramics.