HIGH-ENTROPY METAL DIBORIDES: A NEW CLASS OF ULTRAHIGH TEMPERATURE CERAMICS

Jian Luo, University of California, San Diego
jluo@ucsd.edu
Joshua Gild, University of California, San Diego
Tyler Harrington, University of California, San Diego
Cormac Toher, Duke University
Pranab Sarker, Duke University
Jeff Braun, University of Virginia
Lavina Backman, University of Virginia
Samuel Daigle, North Carolina State University
Yuanyao Zhang, University of California, San Diego (currently at Lam Research)
Tao Hu, University of California, San Diego (currently at Central South University)
Elizabeth Opila, University of Virginia
Patrick Hopkins, University of Virginia
Jon-Paul Maria, North Carolina State University
Stefano Curtarolo, Duke University
Kenneth Vecchio, University of California, San Diego
Donald Brenner, North Carolina State University

Key Words: High-entropy ceramics; metal diborides

Several equimolar, five-component, metal diborides were fabricated via high-energy ball milling and spark plasma sintering [*Scientific Reports* 6:37946 (2016)] or conventional pressure-less sintering. Most compositions synthesized, *e.g.*, $(Hf_{0.2}Zr_{0.2}Ta_{0.2}Nb_{0.2}Ti_{0.2})B_2$, $(Hf_{0.2}Zr_{0.2}Ta_{0.2}Mo_{0.2}Ti_{0.2})B_2$ and several others, processed single solid-solution phases of the hexagonal AlB_2 structure, while a few other compositions yielded two or more boride phases. These materials represent a new type of ultra-high temperature ceramic (UHTC) as well as a new class of high-entropy materials that possess a non-cubic (hexagonal) and layered (quasi-2D) crystal structure (Fig. 1).

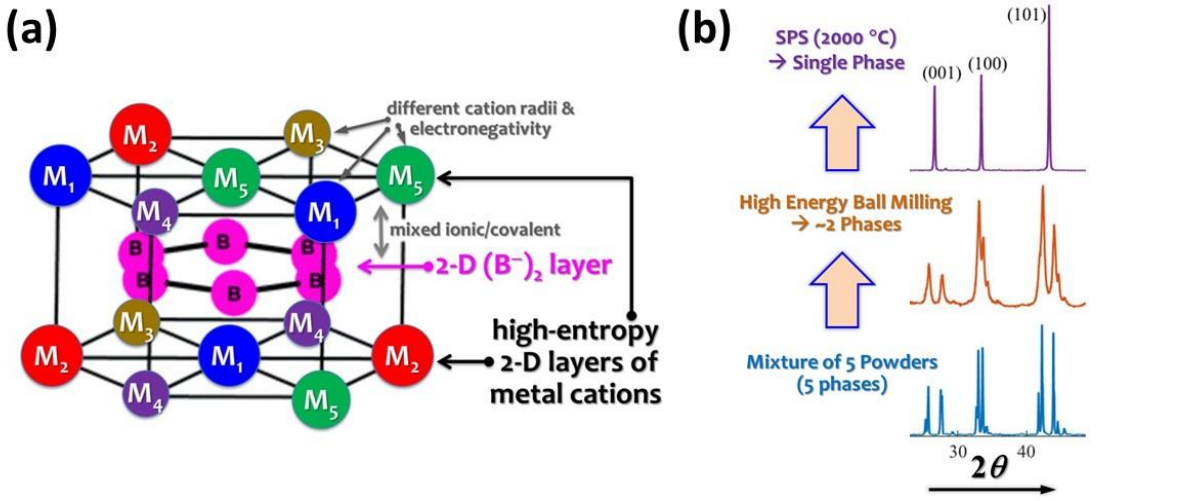

Fig. 1: (a) Schematic illustration of the crystal structures of a high-entropy metal diboride. (b) X-ray diffraction patterns showing the phase evolution during the fabrication of a $(Hf_{0.2}Zr_{0.2}Ta_{0.2}Mo_{0.2}Ti_{0.2})B_2$ high-entropy metal diboride.

A density functional theory (DFT) based partial occupation method was implemented within the AFLOW to calculate energy distributions that were used to construct a descriptor to predict the formation and stability of these high-entropy materials. DFT based modeling of charge disorder and lattice distortions have also been conducted. Results from the most recent on-going studies of processing optimization, mechanical testing, and oxidation measurements of these high-entropy metal diborides will also be presented and discussed