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PII: S0955-2219(18)30211-5
DOI: https://doi.org/10.1016/j.jeurceramsoc.2018.04.010
Reference: JECS 11820

To appear in: *Journal of the European Ceramic Society*

Received date: 6-2-2018
Accepted date: 7-4-2018

Please cite this article as: Gild J, Samiee M, Braun JL, Harrington T, Vega H, Hopkins PE, Vecchio K, Luo J, High-Entropy Fluorite Oxides, *Journal of the European Ceramic Society* (2010), https://doi.org/10.1016/j.jeurceramsoc.2018.04.010

High-Entropy Fluorite Oxides

Joshua Gild[a], Mojtaba Samiee[b], Jeffery L. Braun[c], Tyler Harrington[a], Heidy Vega[b], Patrick E. Hopkins[c], Kenneth Vecchio[a, b], Jian Luo[a, b, *]

[a]Program of Materials Science and Engineering; University of California, San Diego, La Jolla, CA 92093-0418, USA;

[b]Department of NanoEngineering, University of California, San Diego, La Jolla, CA 92093-0448, USA;

[c]Department of Mechanical and Aerospace Engineering, University of Virginia, Charlottesville, Virginia 22904, USA

Abstract (<150 words)

Eleven fluorite oxides with five principal cations (in addition to a four-principal-cation $(Hf_{0.25}Zr_{0.25}Ce_{0.25}Y_{0.25})O_{2-\delta}$ as a start point and baseline) were fabricated via high-energy ball milling, spark plasma sintering, and annealing in air. Eight of the compositions, namely $(Hf_{0.25}Zr_{0.25}Ce_{0.25}Y_{0.25})O_{2-\delta}$, $(Hf_{0.25}Zr_{0.25}Ce_{0.25})(Y_{0.125}Yb_{0.125})O_{2-\delta}$, $(Hf_{0.2}Zr_{0.2}Ce_{0.2})(Y_{0.2}Yb_{0.2})O_{2-\delta}$, $(Hf_{0.25}Zr_{0.25}Ce_{0.25})(Y_{0.125}Ca_{0.125})O_{2-\delta}$, $(Hf_{0.25}Zr_{0.25}Ce_{0.25})(Y_{0.125}Gd_{0.125})O_{2-\delta}$, $(Hf_{0.2}Zr_{0.2}Ce_{0.2})(Y_{0.2}Gd_{0.2})O_{2-\delta}$, $(Hf_{0.25}Zr_{0.25}Ce_{0.25})(Yb_{0.125}Gd_{0.125})O_{2-\delta}$, and $(Hf_{0.2}Zr_{0.2}Ce_{0.2})(Yb_{0.2}Gd_{0.2})O_{2-\delta}$, possess single-phase solid solutions of the fluorite crystal structure with high configurational entropies (on the cation sublattices), akin to those high-entropy alloys and ceramics reported in prior studies. Most high-entropy fluorite oxides (HEFOs), except for the two containing both Yb and Gd, can be sintered to high relative densities. These single-phase HEFOs exhibit lower electrical conductivities and comparable hardness (even with higher contents of softer components such as Y_2O_3 and Yb_2O_3), in comparison with 8 mol. % Y_2O_3-stabilized ZrO_2 (8YSZ). Notably, these single-phase HEFOs possess lower thermal conductivities than that of 8YSZ, presumably due to high phonon scattering by multiple cations and strained lattices.

Keywords: high-entropy ceramic; fluorite oxide; thermal conductivity;

hardness; sintering

*Correspondence should be addressed to J.L. (E-mail: jluo@alum.mit.edu)