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High Temperature Stability and Atomic Segregation in Compositionally Complex RE Zirconates Defect-Fluorites

Compositionally complex oxides (CCOs) are promising candidates for thermal barrier coatings (TBCs) due to their low thermal conductivities, which arise from enhanced phonon scattering caused by cation disorder[1]. Compositionally complex rare-earth (RE) zirconate defect-fluorites ($RE_2Zr_2O_7$) combine low thermal conductivity with high melting temperatures, making them attractive for high-temperature applications. Several $RE_2Zr_2O_7$ compositions were synthesized via solid-state reaction, and preliminary laboratory X-ray diffraction (XRD) confirmed the formation of single-phase defect-fluorite structures. The room-temperature thermal conductivities of equiatomic compositions were measured using the transient plane source (TPS) method. Notably, $(GdDyErYb)_2Zr_2O_7$ exhibited an ultralow thermal conductivity of ~0.9 W/m·K. To investigate the influence of processing on cation ordering, compositions $(TbYb)_2Zr_2O_7$ and $(TbHoYb)_2Zr_2O7$ were synthesized utilizing two milling methods, traditional ball milling and speed-mixing. To better understand the temperature-dependent structural evolution and persistence of atomic segregation, we conducted high-temperature neutron scattering and pair distribution function (PDF) measurements. Using aerodynamic levitation combined with laser heating, we probed the long- and short-range order at elevated temperatures (1200 –~3,000 ℃) relevant to service conditions. The defect-fluorite structure exhibited phase stability above 2,200 ℃ and recrystallization when cooled from a partial melt. These insights into high-temperature structural behavior will inform future efforts to design next-generation TBCs optimized for extreme environments in energy production, storage, and conversion systems.

1. Yang, Z., et al., Thermal and oxygen transport properties of complex pyrochlore RE2InTaO7 for thermal barrier coating applications. Journal of the European Ceramic Society, 2020. 40(15): p. 6229-6235.

Topical Area

Emerging research and multimodal techniques

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