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Novel High-Entropy Ceramic Materials for Extreme Environments

Abstract.

Cutting-edge energy technologies require more rapid discovery of new materials to fulfill the requirements of extreme conditions, such as those in nuclear power plants with high neutron flux, high temperatures, and thermal stress. The **overall goal** of the proposed research is to use a transformative high-entropy concept to develop novel ceramic materials for extreme operating environments in next-generation nuclear energy systems and advanced combustion turbines. The target environment for safe operation with these novel high-entropy ceramic (HEC) materials will be a temperature of over 2000 °C and an irradiation dose of over 50 dpa. Unlike traditional materials, HECs contain more than four metal elements in equal or near-equal concentrations but form a stable single-phase lattice structure due to high configurational entropy. An example of a HEC is $(\text{Hf}_{0.2}\text{Zr}_{0.2}\text{Ta}_{0.2}\text{Nb}_{0.2}\text{Ti}_{0.2})\text{C}$, in which five metal elements, Hf, Zr, Ta, Nb, and Ti are randomly distributed in the cation position. HECs with a large S can be more thermodynamically stable at high temperatures because of the minimization of Gibbs free energy. This proposal is driven by three **scientific hypotheses**: (1) high configurational entropy can enable HEC to be thermally stable at ultra-high temperatures (>2000 °C); (2) chemical disorder and lattice distortion in HECs can slow energy dissipation and suppress formation of irradiation defects, resulting in improved irradiation resistance; and (3) the lattice distortion and sluggish diffusion in HECs can stabilize nanocrystalline grains, resulting in improved mechanical strength and toughness. To fulfil the research goal and test the hypotheses, the following **scientific objectives** will be pursued: (1) discover new high-entropy phases in ceramic material systems; (2) examine the thermal stability of high-entropy phase at elevated temperatures; (3) investigate the high-entropy effect on defect evolution in HECs during irradiation; and (4) synthesize nanocrystalline HECs and determine the high-entropy effect on the thermal stability and mechanical properties.