NEUP Nuclear Energy University Programs

U.S. Department of Energy

Project Title: Radiation Behavior of High-Entropy Alloys for Advanced Reactors

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Program: Blue Sky – Reactor Materials (MS-NT1)

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ABSTRACT

The proposed work aims to gain critical knowledge of high-entropy alloys (HEAs) with potential applications in nuclear reactors and related elevated-temperature and high-pressure systems by integrating both theoretical-modeling and focused-experimental efforts. HEAs are composed of five or more elements, typically of similar size and mixed in an equimolar ratio. HEAs, therefore, have high configurational entropy, and they tend to form substitutionally disordered solid solutions with simple crystal structures, such as face-centered-cubic features. Many alloys in this exciting new class of materials show excellent high-temperature strengths and corrosion resistance, making them favorable candidates for advanced reactors, which require operating temperatures in excess of 750 - 850 °C. Preliminary studies of HEAs based upon 4d-refractory elements have exhibited superior strengths, even at temperatures greater than 1,100 °C. There are also indications that HEAs are resistant to radiation damage. Unlike conventional materials, which develop a large number of crystal defects in a radiation environment, HEAs may transform locally into a glass as a result of extensive radiation damage, and, hence, re-crystallize into disordered solid solutions. Thus, HEAs are highly disordered throughout the radiation process, and easily return to their initial state, resulting in a “self-healing” effect.

The proposed work will build upon recent HEA studies, and obtain new results to rigorously investigate specific HEAs for applications in advanced nuclear reactors. Promising types of HEAs will be designed, fabricated, tested, and optimized through the combination of modeling and experimental efforts. Initially, HEAs based on 3d-transition metals, such as $Al_xCoCrFeNi$, will be studied. Subsequently, 4d-refractory elements for high-temperature applications will be considered. The proposed work path includes four integrated tasks, with each team member leading a task well-suited to his/her expertise. Task 1 is to conduct first-principles calculations and molecular-dynamics simulations to determine localized atomic-level stresses and model radiation damage in HEAs. Task 2 is to perform radiation-behavior experiments using ion irradiation with *in-situ* transmission-electron microscopy and three-dimensional atom-probe tomography, which can be compared with first-principles and molecular-dynamics modeling results in Task 1. Task 3 is to carry out thermodynamic calculations to examine phase stability and refine alloy compositions. Task 4 is to complete mechanical and microstructural characterization using *in-situ* synchrotron X-ray and neutron diffraction experiments to verify thermodynamic predictions in Task 3.

HEAs are an exciting new class of materials, which have shown great promise for applications in extreme conditions. The results of the proposed research will provide fundamental understanding of the behavior of HEAs in extreme environments with an ultimate goal of optimizing the composition and properties for use in nuclear reactors and related elevated-temperature and high-pressure systems.