
Understanding the Irradiation Behavior of Zirconium Carbide

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ABSTRACT

Zirconium carbide (ZrC) is being considered for utilization in high-temperature gas-cooled reactor fuels in deep-burn TRISO fuel. Zirconium carbide possesses a cubic B1-type crystal structure with a high melting point, exceptional hardness, and good thermal and electrical conductivities. The use of ZrC as part of the TRISO fuel requires a thorough understanding of its irradiation response. However, the radiation effects on ZrC are still poorly understood. The majority of the existing research is focused on the radiation damage phenomena at higher temperatures ($>450^{\circ}\text{C}$) where many fundamental aspects of defect production and kinetics cannot be easily distinguished. Little is known about basic defect formation, clustering, and evolution of ZrC under irradiation, although some atomistic simulation and phenomenological studies have been performed. Such detailed information is needed to construct a model describing the microstructural evolution in fast-neutron irradiated materials that will be of great technological importance for the development of ZrC-based fuel.

The goal of the proposed project is to gain fundamental understanding of the radiation-induced defect formation in zirconium carbide and irradiation response (ZrC) by using a combination of state-of-the-art experimental methods and atomistic modeling. This project will combine (1) in situ ion irradiation at a specialized facility at a national laboratory, (2) controlled temperature proton irradiation on bulk samples, and (3) atomistic modeling to gain a fundamental understanding of defect formation in ZrC. The proposed project will cover the irradiation temperatures from cryogenic temperature to as high as 800°C , and dose ranges from 0.1 to 100 dpa. The examination of this wide range of temperatures and doses allows us to obtain an experimental data set that can be effectively used to exercise and benchmark the computer calculations of defect properties. Combining the examination of radiation-induced microstructures mapped spatially and temporally, microstructural evolution during post-irradiation annealing, and atomistic modeling of defect formation and transport energetics will provide new, critical understanding about property changes in ZrC.

The behavior of materials under irradiation is determined by the balance between damage production, defect clustering, and lattice response. In order to predict those effects at high temperatures so targeted testing can be expanded and extrapolated beyond the known database, it is necessary to determine the defect energetics and mobilities as these control damage accumulation and annealing. In particular, low-temperature irradiations are invaluable for determining the regions of defect mobility. Computer simulation techniques are particularly useful for identifying basic defect properties, especially if closely coupled with a well-constructed and complete experimental database. The close coupling of calculation and experiment in this project will provide mutual benchmarking and allow us to glean a deeper understanding of the irradiation response of ZrC, which can then be applied to the prediction of its behavior in reactor conditions.