



## Using a spherical crystallite model with vacancies to relate local atomic structure to irradiation defects in ZrC and ZrN

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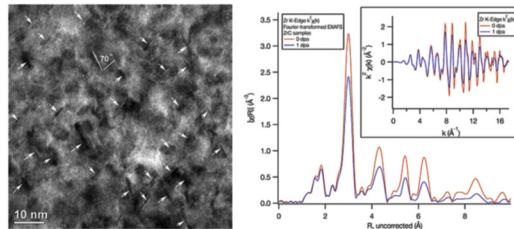
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### HIGHLIGHTS

- ZrC and ZrN were irradiated at the ATR NSUF reactor to 1 dpa at 800 °C.
- Dislocation loop size and density determined with TEM.
- Defects in ZrC are similar to proton irradiated ZrC under similar conditions.
- EXAFS modeling of radiation damage using a spherical crystallite model.

### GRAPHICAL ABSTRACT



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### ABSTRACT

Zirconium carbide and zirconium nitride are candidate materials for new fuel applications due to several favorable physicochemical properties. ZrC and ZrN samples were irradiated at the Advanced Test Reactor National Scientific User Facility with neutrons at 800 °C to a dose of 1 dpa. Structural examinations have been made of the ZrC samples using high resolution transmission electron microscopy, and the findings compared with a previous study of ZrC irradiated with protons at 800 °C. The use of X-ray absorption fine structure spectroscopy (XAFS) to characterize the radiation damage was also explored including a model based on spherical crystallites that can be used to relate EXAFS measurements to microscopy observations. A loss of coordination at more distant coordination shells was observed for both ZrC and ZrN, and a model using small spherical crystallites suggested this technique can be used to study dislocation densities in future studies of irradiated materials.

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### 1. Introduction

Zirconium carbide was one of six ceramics that met melting temperature, neutronic, and irradiation performance requirements for composite fuels in gas-cooled fast reactors (GFR) [1]. Those properties and the ability to retain fission products also make ZrC a possible replacement for SiC in tri-isotropic (TRISO)-coated fuel particles in high temperature applications [2,3]. ZrN has been proposed as a suitable material for fast neutron systems from the

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