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Peridynamic Modeling of Void Collapse in Representative Plutonium Oxide Microstructures

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Abstract

Plutonium oxide is the key compound in the radioisotope thermoelectric generators used to power spacecraft such as the Mars rover. It is therefore critical to understand the effects of environmental conditions on the grain structure of plutonium oxide, and to correlate these effects with changes in macro-scale mechanical response. Of specific interest is the observed nonlinear yielding behavior and subsequent fracture patterns under compressive loads. Yielding under compression is a result of void collapse and material failure along grain boundaries, both of which are strongly dependent on microstructure.

We present a multiscale approach to determine macro-scale constitutive properties as a function of grain structure. Microstructure models are created by employing grain-growth simulations that begin with a recrystallized, fresh clad, and produce statistically representative distributions of grains and pores. Representative models are then analyzed using peridynamics, a nonlocal extension of continuum mechanics that facilitates crack initiation and propagation (Silling, 2000). Grain-scale simulations incorporate a constitutive law governing the elastic response of individual grains, a failure model that dictates the breaking of peridynamic bonds, and a contact algorithm to control post-failure interactions of grains and grain fragments. Pores within the grain structure serve as stress concentrators, strongly affecting the formation of intergranular cracks and subsequent void collapse. Results from meso-scale simulations are then homogenized to inform a macro-scale constitutive model, enabling analyses at the system level in which full resolution of the microstructure is computationally intractable. Linking the environmental conditions of fabrication, storage, and deployment to mechanical response at the macro scale significantly improves our ability to predict mechanical failure and to design post-process heat treatments for improved system resilience.

Keywords: Microstructure, peridynamics, void collapse, multiscale, plutonium oxide.

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