Informing Macroscale Constitutive Laws through Peridynamic Modeling of Grain-Scale Mechanisms in Plutonium Oxide

David Littlewood, Veena Tikare, and John Bignell
Sandia National Laboratories, Albuquerque, NM

Abstract

The constitutive response of plutonium oxide is largely determined by mechanisms at the grain scale. Of particular interest are material failure along grain boundaries and the subsequent collapse of microstructural voids that correspond to the observed nonlinear yielding behavior at the macroscale. We present a multiscale approach to characterize the response of plutonium oxide by means of a peridynamic model at the grain scale. Microstructure models are created by employing sintering simulations that begin with a powder compact and produce statistically representative, topologically correct grains and pores as a function of fabrication and storage conditions (Tikare, et al., 2010). Representative models are then analyzed using peridynamics, a nonlocal extension of continuum mechanics (Silling, 2000). Results from mesoscale simulations inform a macroscale 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 macroscale significantly improves our ability to predict mechanical failure and to design post-process heat treatments for improved system resilience.

SAND2012-9927C

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.