NUCLEAR ENERGY UNIVERSITY PROGRAMS

Understanding Creep Mechanisms in Graphite with Experiments, Multiscale Simulations, and Modeling

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Abstract

A limited set of creep data available for grade H-451 graphite and lack of microstructural analyses have precluded a mechanistic understanding of graphitic creep thus far. This research project will address the gap through extensive irradiation and thermal creep tests, state-of-the-art microstructure evaluations, and multiscale simulations. The key emphasis is to characterize the microstructure and to develop mechanistic creep models aided by molecular and multiscale simulations.

Three grades of graphite will be tested: H-451, NBG-17, and highly ordered pyrolytic graphite (HOPG) over a temperature range of 300°C to 900°C and stresses from 5 MPa to 20 MPa. The peak neutron dose is of the order of 1022 n/cm^2 (3-4 dpa), although some irradiation experiments will be performed at 0.5 – 1 dpa. Researchers will perform *ex-situ* tensile, compressive, and impression tests on irradiated and unirradiated samples. These tests will differentiate and quantify the possible effects of thermal creep in the different forms of graphite.

The team will employ several methods to characterize the microstructure: high-resolution transmission electron microscopy (HRTEM) for mapping atomic defects, inelastic neutron scattering for structure functions, and positron annihilation spectroscopy (PAS) for characterizing voids that are generated during irradiation. Several material properties (such as coefficient of thermal expansion and elastic constants) are needed for analytical modeling of creep behavior in graphite. This project will measure the pertinent mechanical and thermal properties. In parallel, radiation cascade simulations using molecular dynamics (MD) and long-time simulations with kinetic Monte Carlo (kMC) and/or accelerated molecular dynamics (AMD) will be employed to aid in building realistic creep models. The simulations are intended to compute the relative change in graphitic properties and to analyze the changes in molecular structure during irradiation. Benchmarking will be pursued through the comparisons with measured properties and microstructural data.