NUCLEAR ENERGY RESEARCH INITIATIVE

Radiation-Induced Segregation and Phase Stability in Candidate Alloys for the Advanced Burner Reactor

PI: Gary Was, University of Michigan

Collaborators: University of California-Berkeley; Los Alamos National Laboratory; Oak Ridge National Laboratory

Project Number: 07-015

Program Area: AFC R&D

Project Description

The objective of this project is to investigate the effect of irradiation on the segregation and phase stability in candidate alloys that may be used as structural materials for transmutation in the advanced burner reactor. This project will focus on ferritic-martensitic (F-M) alloys T91 and HT-9, an experimental oxide dispersion-strengthened (ODS) alloy, and an advanced austenitic alloy, D9, to investigate the electronic–magnetic–elastic interactions between chromium and radiation-induced defects. This project will provide an understanding of radiation-induced segregation (RIS) and phase stability that can be used to develop predictive irradiation performance models.

Experiments will be conduced by proton and heavy ion irradiation over the dose range 3-100 dpa and the temperature range 350-550°C. Analysis of RIS, phase microstructure, dislocation microstructure, and hardening will be conducted on all conditions. Investigators will also develop *ab-initio* models of the electronic structure to investigate the configuration-dependent binding and migration energies of Cr with vacancy and interstitial defects. This will enable development of atomistic-based kinetic Monte Carlo models to investigate the Cr diffusivity by interstitial and vacancy mechanisms.

Workscope

The primary tasks are:

1. Proton irradiation series
   - Perform atomic-scale Monte-Carlo modeling
   - Perform *ab-initio* calculations of vacancy-CR binding energies and compare with experimental microstructure measurements
2. Iron ion (Fe^{++}) irradiation series
   - Perform *ab-initio* calculations of interstitial-Cr binding energies
   - Develop atomic scale Monte-Carlo simulation of Cr diffusion
   - Develop kinetic Monte-Carlo and rate theory models of RIS and dislocation loop evolution; compare models with experimental and reactor data

3. Helium irradiation series
   - Develop atomic-scale Monte-Carlo model to simulate Cr RIS and compare to reactor data
   - Develop kinetic Monte-Carlo and MIK rate theory models of RIS and dislocation loop evolution