Predictive Characterization of Aging and Degradation of Reactor Materials in Extreme Environments

PI: Jianmin Qu- Northwestern University

Collaborators: Rémi Dingreville- Sandia National Laboratories
Khalid Hattar – Sandia National Laboratories

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ABSTRACT:

Understanding of reactor material behavior in extreme environments is vital not only to the development of new materials for the next generation nuclear reactors, but also to the extension of the operating lifetimes of the current fleet of nuclear reactors. To this end, we propose a suite of unique experimental techniques, augmented by a mesoscale computational framework, to understand and predict the long-term effects of irradiation, temperature, and stress on material microstructures and their macroscopic behavior. The experimental techniques and computational tools will be demonstrated on two distinctive types of reactor materials, namely, Zr alloys and high-Cr martensitic steels. These materials are chosen as the testbeds because they are the archetypes of high-performance reactor materials (cladding, wrappers, ducts, pressure vessel, piping, etc.).

To fill the knowledge gaps, and to meet the technology needs, a suite of innovative in situ transmission electron microscopy (TEM) characterization techniques (heating, heavy ion irradiation, He implantation, quantitative small-scale mechanical testing, and various combinations thereof) will be developed and used to elucidate and map the fundamental mechanisms of microstructure evolution in both Zr and Cr alloys for a wide range environmental boundary conditions in the thermal-mechanical-irradiation input space. Knowledge gained from the experimental observations of the active mechanisms and the role of local microstructural defects on the response of the material will be incorporated into a mathematically rigorous and comprehensive three-dimensional mesoscale framework capable of accounting for the compositional variation, microstructural evolution and localized deformation (radiation damage) to predict aging and degradation of key reactor materials operating in extreme environments. Predictions from this mesoscale framework will be compared with the in situ TEM observations to validate the model.

Three unique and innovative ideas are proposed here to advance the state-of-the-art: (i) Innovative in situ TEM microscopy of key reactor materials in extreme environments such as ion irradiation of a TEM sample during real time nanoscale observation of the same sample; (ii) A hybrid kinetic Monte Carlo (kMC)/phase-field/crystal plasticity computational model that captures the robustness of kMC models, preserves the continuum compositional gradients terms of the phase-field model and enables localization of the mechanical behavior provided by crystal plasticity. By combining stochastic mesoscale simulations and continuum modeling, this computational model enables the simulation of fully coupled compositional-microstructural evolution including hydrogen (hydride formation), irradiation and their synergetic irradiation damage recovery. Furthermore, the model will be integrated into a unified framework based on the material point method and a scalable algorithm from which physical and mechanical parameters can be extracted for continuum scale materials modeling, thus can be compared to, and validated by, experimental data; and (iii) Integration of the in situ TEM observations with mesoscale modeling and simulations. Such a combination of unique experimental techniques and efficient numerical methods provides predictive capabilities well beyond any existing technologies for understanding reactor material behavior in extreme environments.