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Combined modeling and experiments to predict corrosion and embrittlement in dual-phase stainless steels within the MARMOT framework

PI: Dr. Julie Tucker, Oregon State University

Program: NEAMS

Collaborators:
Dr. Líney Árnadóttir - Oregon State University
Dr. Burkan Isgor - Oregon State University
Dr. Yongfeng Zhang - Idaho National Laboratory

ABSTRACT:

Extending service of Light Water Reactors (LWRs) to beyond 60 years will demand a high integrity of materials and components in the reactors. The accurate evaluation and prediction of materials performance under anticipated operation conditions are of particular importance for ensuring the safety of nuclear power plants over their extended lifetime. Stainless steels are extensively used as structural alloys in light water reactor (LWR) systems because of their excellent combination of mechanical properties and corrosion resistance. Austenitic stainless steel welds and cast austenitic stainless steels (CASS) contain significant amounts of ferrite ~5-30%, and are ubiquitous in LWR piping (elbows, pump casings, valves) and internal structural components. During their lifetime, these components are subjected to thermal aging at the temperature range of 288-327°C for a pressurized water reactor (PWR) and 282°C for a boiling water reactors. A phase transformation within the ferrite phase of these materials leads to embrittlement and degradation in corrosion resistance, which undermines the materials selection criteria.

This detrimental phase transformation occurs in the temperature range of 204°C - 538°C in Cr rich ferritic alloys. A miscibility gap in the Fe-Cr system causes α-α' phase separation within the ferrite grains through either spinodal decomposition or nucleation and growth. The resultant Cr-rich (α') and Cr-poor (α) regions produce a material with degraded mechanical properties. Although α-α' phase separation is limited to the ferrite grains, the loss of mechanical properties is observed in the overall dual phase material. The reduction of corrosion resistance can be severe, enhancing the likelihood of leaks or failure in these components. Small changes in alloy composition can alter the rate of the phase separation and property degradation.

This project is proposing an enhancement to MARMOT to predict mechanical and corrosion properties of dual-phase stainless steels as a function of composition, aging time and temperature. The model will be trained and validated by an extensive experimental database of duplex stainless steel alloys, where aging, mechanical properties and atom probe characterization are already complete. Additional corrosion experiments will be performed on aged alloys in PWR water chemistry to provide the corrosion data training set. The phase field capabilities of MARMOT will also be parameterized with Reactive Force Field Molecular Dynamics (ReaxFF-MD) and Density Functional Theory (DFT) simulations to provide kinetic information at the molecular and atomistic levels. This multi-pronged approach will yield several outcomes: 1) relationships between microstructure, property and corrosion resistance of thermally aged materials, 2) fundamental understanding of interactions of ionic species with metal surfaces through first principles (DFT) calculations, and 3) mechanistic understanding of corrosion kinetics and corrosion mitigation strategies of thermally aged materials in representative exposure conditions through ReaxFF-MD studies. These outcomes will be impactful in evaluating components for plant life extension and add to the predictive capabilities of MARMOT.