
Atomistically Informed and Experimentally Validated Model for Helium Bubble Growth in Welded Irradiated Metals

PI: Douglas Spearot,
University of Florida

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Collaborators: Simon Phillpot, University of Florida
Mitra Taheri, Drexel University
Michael Tonks, University of Florida
Jon Tatman and Greg Frederick, EPRI
Khalid Hattar, Sandia National Laboratories

ABSTRACT:

High-intensity neutron flux during reactor operation can produce atomic displacement cascades and nuclear reactions that lead to the production of transmuted He within reactor structural components. When welding is used to repair these structural components, heat from the welding process can modify the He distribution within the heat affected zone, leading to He coalescence and bubble growth on grain boundaries (GBs), and potentially intergranular fracture. These phenomena are known to be sensitive to the microstructure of the alloy, the He concentration and welding conditions. However, a fundamental understanding of correlations among these factors is not well known. This has slowed the development of tools or metrics necessary to guide industry towards safe welding conditions for irradiated structural components.

The objective of this NEUP project is to construct a validated computational model for He bubble growth on GBs in irradiated Fe-Ni-Cr microstructures, including intergranular fracture, as a function of material conditions and welding heat input. This model will be based on the phase-field methodology, leveraging numerical solvers in the MOOSE simulation platform, with critical inputs and validation provided by both atomic-level simulations and experiments. Major deliverables include:

- (i) A fundamental thermomechanical understanding of diffusion of He to GBs and the coalescence of He into bubbles on GBs in Fe-Ni-Cr alloys via atomistic simulations.
- (ii) Experimental measurement of key features of alloy microstructures including He bubble distribution and residual stresses in the welding heat affected zone, via quantitative electron microscopy.
- (iii) A validated phase-field model that accounts for He distribution evolution and GB cracking due to He bubble formation and growth during a thermal input representative of welding.
- (iv) A graphical tool for industry to assess safe welding conditions for different techniques, based on the collective results of phase-field simulations of GB cracking for different heating protocols.

This proposal is directly responsive to the Nuclear Reactor Technologies Program RC-10.2. Specifically, a fundamental understanding of the effect of heat input due to welding on the diffusion and coalescence of He on GBs will be provided. This understanding will drive the development of a comprehensive phase-field model of He bubble growth on GBs during welding of irradiated alloys, which accounts for stresses generated during bubble growth and grain boundary decohesion. The phase-field model is supported by atomistic simulations and validated by experiments. For example, microstructures of 304 stainless steel before and after welding will be analyzed experimentally via quantitative transmission electron microscopy, in partnership with the Electric Power Research Institute. In situ welding experiments within the electron microscope, on samples with and without implanted He, will be conducted in partnership with Sandia National Laboratories to establish links between welding parameters and He bubble distribution.