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A coupled diffusion–reaction–mechanics framework for grain-boundary oxidation and cracking in IGSCC and IASCC

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Abstract

Intergranular stress corrosion cracking (IGSCC) and irradiation-assisted stress corrosion cracking (IASCC) in structural alloys exposed to pressurized water reactor (PWR) environments are governed by complex, strongly coupled interactions between oxygen transport, oxide formation, mechanical stress, and damage at grain boundaries (GBs). Preferential oxidation along GBs, chemical expansion during metal-to-oxide transformation, and the progressive loss of oxide protectiveness are widely recognized as key contributors to crack initiation and propagation. In this work, a microstructure-resolved numerical framework is developed to improve the mechanistic understanding of oxidation-driven GB degradation relevant to IGSCC and IASCC. Oxygen transport is modeled using a diffusion–reaction formulation implemented in Abaqus through a transient heat-transfer analogy, where a normalized temperature field represents oxygen concentration. Oxide formation is governed by a non-zero sink (reaction) term in the continuity equation, enabling explicit separation between oxygen diffusion and oxide growth. A film boundary condition is applied at free surfaces to represent oxygen exchange with the coolant, while GBs are assigned transport properties up to three orders of magnitude higher than those of the grains to capture fast GB diffusion. Chemical heterogeneity along GBs is explicitly accounted for by distinguishing two oxide families: a Cr-rich oxide and non-Cr oxides (Fe/Ni). The Cr-rich oxide is treated as nearly impermeable to oxygen diffusion and therefore protective, whereas non-Cr oxides remain transparent to oxygen transport and

allow continued oxidation. Separate diffusivity and oxide-formation rate parameters are assigned to grain interiors and GB regions, enabling the framework to capture the preferential formation of non-protective oxides in regions depleted of available chromium, as occurs during sensitization or radiation-induced segregation—key features of IASCC. All simulations are performed on a bicrystal model containing a single grain boundary, allowing systematic investigation of GB-controlled oxidation and cracking mechanisms. The mechanical response is solved using coupled temperature–displacement analyses with a chemical expansion eigenstrain to represent metal-to-oxide transformation. Oxides are modeled as isotropic elastic solids, while the metallic phase exhibits elastoplastic behavior activated through concentration-dependent material properties. A two-way coupling between diffusion and mechanics is introduced by incorporating hydrostatic stress gradients into the oxygen flux, enabling stress-assisted oxidation consistent with SCC conditions. Crack initiation and propagation within the oxide layer are simulated using an effective element-removal strategy driven by a brittle mixed-mode damage criterion, allowing failure under combined tensile–compressive stress states typical of constrained GB oxidation. The numerical framework relies on the development of several Abaqus user subroutines to handle diffusion–reaction kinetics, stress-assisted transport, evolving material behavior, and damage evolution. The proposed approach provides a physically grounded platform for studying the cyclic sequence of GB oxidation, oxide cracking, renewed oxygen ingress, and further oxidation that underlies IGSCC and IASCC, and offers a basis for future extensions incorporating strain localization, GB energetics, and crystal plasticity.

Keywords:

intergranular stress corrosion cracking irradiation-assisted stress corrosion cracking grain-boundary oxidation coupled diffusion–mechanics stress-assisted oxidation chromium depletion oxide cracking finite element modeling