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Multilayer Interface Tracking Model of Zirconium Clad Oxidation

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Abstract

We present a numerical model to predict oxide scale growth and failure in zirconium clad exposed to water in out-of-pile conditions. The model includes the formation of two oxide sublayers on top of the metal clad, whose interfaces are tracked using a Stefan model coupled to diffusion kinetics. The kinetics is coupled to a thermal model that accounts for temperature gradient effects via thermo-migration inside the clad. The model also includes a mechanical failure criterion based on the accumulation of compressive stresses in the oxide near the interface with the metal. We present results of oxygen diffusion into the clad, oxide formation as a function of time, and oxide fragmentation by mechanical failure. We find that the growth of the oxide scale as the cubic root of time is recovered for a special charge distribution near the oxide interface. This charge distribution can be suppressed via alloying, which explains the square root scaling for certain Zr alloys. A sensitivity study has been conducted, showing that variations of ±15% in selected model parameters result in approximately ±5% changes in model predictions.

Keywords: Zirconium oxide, Zircalloy clad, Zircalloy corrosion, Oxidation, Nuclear reactor

1. Introduction

Corrosion of metallic structural materials is an extraordinarily broad phenomenon with implications in many areas of engineering [1–3]. In nuclear reactors cores, understanding the kinetics of corrosion of metallic components is particularly challenging, due to the compounded effects of high temperature, mechanical stresses, complex coolant and fuel chemistry, and irradiation [4, 5]. In light-water nuclear reactors (LWR) zirconium alloys are used as cladding materials in fuel elements to provide a mechanical barrier with a low impact on neutron economy between the coolant (water) and the fuel [6–8]. In principle, Zr clad is subjected to corrosion from the coolant (water) and fuel sides, both by way of oxygen and hydrogen penetration. The oxidation and hydriding performance of zirconium fuel components in LWRs may limit the maximum fuel discharge burn-up, which makes corrosion a critical aspect of Zr materials response in nuclear environments [9–14].

Corrosion in LWR is typically studied in autoclave experiments, subjecting components to temperatures and pressures representative of reactor operation [15–17]. These tests can be performed *in-pile*, with the autoclave directly experiencing conditions in the reactor core, or *out-of-pile*, with experiments done under controllable laboratory conditions. For obvious reasons, in-pile experiments are considered more scientifically relevant, but they are costly and slow to perform, and the different contributing factors are difficult to separate [18, 19]. For their part, although out-of-pile autoclave corrosion tests developed over the years can predict some aspects of in-pile corrosion performance of zirconium alloys, these autoclave tests normally underestimate corrosion rates and do not account for irradiation effects [9, 19–21]. To help bridge the gap between autoclave measurements and in-reactor Zr corrosion, several models of zirconium alloy corrosion

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