



Stochastic reduced order models for uncertainty quantification of intergranular corrosion rates



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ABSTRACT

We present a stochastic reduced order model (SROM) approach for quantifying uncertainty in systems undergoing corrosion. A SROM is a simple random element with a small number of samples that approximates the statistics of another target random element. The parameters of a SROM are selected through an optimization problem. SROMs can be used to propagate uncertainty through a mathematical model of a corroding system in the same way as in Monte Carlo methods. We use SROMs to estimate the statistics of corrosion current density, considering randomness in anode–cathode sizes. We compare the performance of SROMs against the more common Monte-Carlo approach.

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1. Introduction

The rate of corrosion in an alloy–electrolyte system is determined by several parameters like the temperature of the system, the electrolytic conductivity, and the composition of the alloy–electrolyte interface. All of these quantities are inherently uncertain due to variability in manufacturing processes and environment. Therefore, a probabilistic framework is in general needed to adequately model real corroding systems.

In this work, we focus on a particular type of uncertainty that is of paramount importance in corroding systems: the variability in anodic and cathodic locations and sizes along an alloy–electrolyte interface. Randomness in anodic and cathodic locations is evident in the case of intergranular corrosion (IGC), where the material phases at the grain–boundaries of an alloy get depleted due to corrosion [1]. Al 5083 is one of the alloys that suffers damage due to IGC. A sample micrograph of Al 5083 [2] is shown in Fig. 1a, where the grains of various sizes are separated by the dark grain–boundaries. Due to the process of sensitization, deposits of high energy β -phase (Al_3Mg_2) are formed along the grain–boundaries. Fig. 1b shows the β -phase deposits at the grain boundaries etched selectively using phosphoric acid [3]. During intergranular corrosion the grains in Al 5083 act as cathodes and β -phase deposits act as anodes. Hence, the width of grains and β -phase precipitates determine the corrosion current density. It is well

known that the width of grains and β -phase deposits depend on the temperature and duration of annealing [4–6]. Uncertainty in the latter processes translates into uncertainty in the locations and the sizes of anodes and cathodes.

The main goal of this paper is to introduce stochastic reduced-order modeling as a novel and efficient computational approach for propagating uncertainty in corroding systems. For instance, given probabilistic descriptions of cathode/anode sizes and locations, we devise an efficient strategy for approximating the statistics of the average current density. We also investigate the effect of uncertainty in the cathodic and anodic sites on the corrosion rate (described as the average current density).

Existing probabilistic modeling of corroding systems has been almost exclusively carried out using Monte Carlo (MC) methods [7–9]. Although Monte-Carlo methods are simple to implement due to their non-intrusive nature, they can be computationally prohibitive, especially when modeling complex systems. In this work, we propose stochastic reduced order models (SROMs) as a computationally efficient and accurate alternative to MC methods for uncertainty quantification in corroding systems. A SROM \tilde{X} of a random input X is a random element with a finite and small number of samples, which in general are not equally likely. The defining parameters of the SROM, its range and corresponding probabilities, are selected through an optimization problem with an objective function measuring the discrepancy between the statistics of \tilde{X} and X .

The SROM concept was originally introduced by Grigoriu in [10] and was later applied to determine effective conductivity for random microstructures and to calculate statistics of the states of linear dynamic systems in [11,12], respectively. Most recently,

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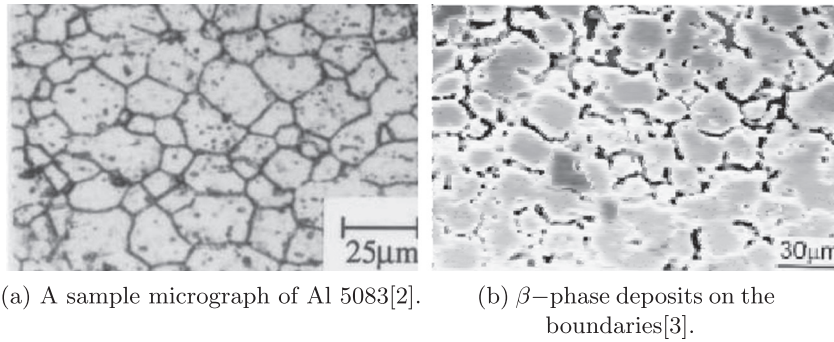


Fig. 1. Sample images of Al 5083 grains, grain-boundaries, and β -phase precipitates.

the algorithm to construct SROMs was improved upon in [13], and the models were then applied to solve random eigenvalue problems that arise in uncertain structural dynamics applications. The main appeal of SROMs is that, as shown in the cited references, the statistics of quantities of interest can be obtained in a fraction of the computational time required by MC methods.

This paper is organized as follows. We first formulate a basic mathematical model for a corroding system and introduce a simple probability model for the sizes of cathodes and anodes. Then, we motivate and describe the method for constructing a stochastic reduced order model (SROM) of a random quantity. Using numerical examples, we establish that SROMs are an efficient alternative to Monte-Carlo method for characterizing uncertainty in corroding systems. Our calculations also show that the randomness in anode–cathode widths induces a noticeable amount of variance in the resultant corrosion current density. Finally, we demonstrate the use of SROMs to determine the joint distribution and correlation between different random variables.

2. Formulation

In this section, we present the governing differential equations along with appropriate boundary conditions for modeling a corroding system. Furthermore, we describe a simple approach to describe cathodic and anodic boundaries as random elements, and explain the theory and construction of SROMs in the context of the corrosion problem. In the sequel, we will use (non-bold) italic fonts for scalars and bold fonts for vectors.

2.1. Mathematical model

In Fig. 2, we show the schematic representation of an alloy–electrolyte system. The electrolytic domain is Ω_E , the alloy domain is Ω_A , the anodic boundary is Γ_a , and the cathodic boundary is Γ_c . We assume the electrolytic domain to have uniform ionic conductivity κ . So, the electric potential field in Ω_E can be described using Laplace's equation as

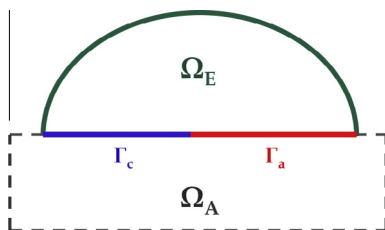


Fig. 2. Schematic sketch of an alloy–electrolyte system.

$$\nabla^2 \varphi = 0 \quad \text{in } \Omega_E \quad (1)$$

and the current density \mathbf{i} is given as

$$\mathbf{i} = -\kappa \nabla \varphi \quad \text{in } \Omega_E \quad (2)$$

The electrodic reaction rates at the anodic and the cathodic boundaries are obtained using the Butler–Volmer model [14,15] as

$$i_a = i_{oa} \left[\exp \left(\frac{\varphi - \varphi_{oa}}{\beta_f^a} \right) - \exp \left(\frac{\varphi - \varphi_{oa}}{\beta_r^a} \right) \right] \quad \text{on } \Gamma_a \quad (3)$$

and

$$i_c = i_{oc} \left[\exp \left(\frac{\varphi - \varphi_{oc}}{\beta_f^c} \right) - \exp \left(\frac{\varphi - \varphi_{oc}}{\beta_r^c} \right) \right] \quad \text{on } \Gamma_c \quad (4)$$

where i_{oa} and i_{oc} are the anodic and cathodic open-circuit current densities, φ_{oa} and φ_{oc} are the open-circuit potentials, and (β_f^a, β_r^a) and (β_f^c, β_r^c) are forward and reverse Tafel constants for the anodic and the cathodic reactions, respectively.

Notice that the current density \mathbf{i} defined in Eq. (2) is a vector field, whereas i_a (3) and i_c (4) are scalars. They are related as

$$i_a = -\mathbf{i} \cdot \mathbf{n} \quad \text{on } \Gamma_a \quad (5)$$

and

$$i_c = \mathbf{i} \cdot \mathbf{n} \quad \text{on } \Gamma_c \quad (6)$$

where \mathbf{n} is the unit outward normal over the boundary of Ω_E .

The variational form of the boundary value problem given in Eqs. (1)–(6) can be stated as find $\varphi \in S$ such that

$$\int_{\Omega_E} \nabla w \cdot \nabla \varphi d\Omega_E = \int_{\Gamma_a} w \left(\frac{i_a}{\kappa} \right) d\Gamma - \int_{\Gamma_c} w \left(\frac{i_c}{\kappa} \right) d\Gamma \quad \forall w \in \mathcal{W} \quad (7)$$

where S and \mathcal{W} are suitable function spaces [16].

A quantity of interest that will be used throughout this paper is the average corrosion current density defined as

$$i_{avg} = \frac{1}{A(\Gamma_a)} \int_{\Gamma_a} i_a d\Gamma \quad (8)$$

where $A(\Gamma_a)$ is the area of the anodic surface. In the current study, we will take Γ_a and Γ_c as random variables, while we assume that the geometry of the electrolyte domain Ω_E , the conductivity of the medium κ , and the electrodic parameters $\{i_{oa}, i_{oc}, \varphi_{oa}, \varphi_{oc}, \beta_{af}, \beta_{ar}, \beta_{cf}, \beta_{cr}\}$ are known with certainty (*i.e.* deterministic). Then, we can abstractly represent the combination of Eqs. 3, 4, 7, and 8 as

$$i_{avg} = \mathcal{M}(\Gamma_a, \Gamma_c) \quad (9)$$

where \mathcal{M} is a mathematical model that maps anodic and cathodic boundaries $\{\Gamma_a, \Gamma_c\}$ to the average corrosion current density.

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