



New phase field model for simulating galvanic and pitting corrosion processes



Weijie Mai^a, Soheil Soghrati^{a, b, *}

^a Department of Materials Science and Engineering, The Ohio State University, USA

^b Department of Mechanical and Aerospace Engineering, The Ohio State University, USA

ARTICLE INFO

Article history:

Received 5 August 2017

Received in revised form

3 December 2017

Accepted 11 December 2017

Available online 14 December 2017

Keywords:

Phase field

Pitting corrosion

Galvanic corrosion

Finite element

Aluminum

ABSTRACT

This manuscript presents a new phase field model for simulating galvanic and pitting corrosion phenomena in metallic materials. The Laplace equation is employed to approximate the electric potential distribution, which determines the phase evolution by relating the anodic current density to the interface kinetics parameter. While the anode is assumed to be nonpolarizable, the nonlinear polarization behavior including the diffusion-limited kinetics is considered as boundary condition on the cathode. Several numerical examples are presented to verify the accuracy of the proposed model. We also demonstrate the application of this model for simulating coupled galvanic-pitting corrosion processes in a hybrid joint and an aluminum composite material under varying environmental conditions. The last example simulates the corrosion of a steel wire, which shows the feasibility of incorporating homogeneous chemical reactions and polarization behavior on the anode into the proposed model.

© 2017 Elsevier Ltd. All rights reserved.

1. Introduction

Electrochemically distinct materials are often joined together to achieve an improved thermal or mechanical performance. For example, dissimilar materials such as steel, aluminum, and composites are joined together to build high-strength structural components for lightweighting applications in the automotive and aerospace industry. However, the improvement in the mechanical performance could come at the risk of accelerated environmental degradation due to the galvanic corrosion, which is caused by electric and ionic contact between two dissimilar metals [1]. In such situations, the more electrochemically active material (anode) will corrode at a higher rate due to the additional cathodic current supplied by the more noble material (cathode). Localized corrosion phenomena, such as pitting, can be viewed as a localized galvanic corrosion in which the actively corroding region serves as the anode and the passive region as the cathode [2]. Such an accelerated metal dissolution, which could either be localized or occur over a large region, can significantly deteriorate mechanical properties and lead to failure (fracture, fatigue, etc.) or loss of

functionality (leakage, perforation, etc.) [3,4]. Therefore, reliable prediction of the possibility and more importantly rates of galvanic and localized corrosion processes are essential for the reliable design and maintenance of metallic structures.

Several analytical models have been developed for evaluating the electric potential and current distributions in different electrochemical systems [5–8]. However, such models are restricted to simple geometrical configurations of electrodes with linear polarization behaviors, which could prohibit their practical application for predicting the corrosion evolution in geometrically complex case scenarios [9]. Such deficiencies can be overcome by approximating the current and potential distributions using numerical techniques such as the Finite Difference Method (FDM). In such simulations, the Laplace equation is often employed as the governing equation to evaluate the electric potential distribution, with the Ohm's law relating the current density to the potential gradient [10–12]. More generic boundary conditions, such as the non-linear Butler-Volmer or Tafel kinetics, as well as the diffusion-controlled polarization, have also been implemented in these models [13–15]. Time dependent evolution of the chemical environment in the electrolyte can also be incorporated by considering the mass transfer processes for species of interest [16]. While such numerical models are highly successful in estimating the instantaneous corrosion rate and its distribution, they are not capable of providing an accurate long-term prediction due to ignoring the evolving

* Corresponding author. Mechanical and Aerospace Engineering & Materials Science and Engineering, The Ohio State University, 201 W 19th Avenue, Columbus, OH 43210, USA.

E-mail address: soghrati.1@osu.edu (S. Soghrati).

Nomenclature

ϕ	phase field variable	f_{int}	free energy density of the interface
c	molar concentration of the metal ion	\mathcal{F}	free energy functional of the system
c	normalized molar concentration of the metal ion	l	thickness of the diffuse interface
c_{solid}	molar concentration of the metal ion in the solid	w	height of the double well potential
c_{sat}	saturation concentration of the metal ion in the solution	A	curvature of the free energy density function
$c'_{\text{Se}}/c'_{\text{Le}}$	normalized equilibrium concentration in the solid/liquid	L	interface kinetics parameter
ψ	electric potential	v	interface velocity
E	electrode potential	M	diffusion mobility
b_c	cathodic Tafel slope	D	diffusion coefficient
κ_s/κ_l	solid metal/electrolyte conductivity	γ	interface energy
\mathbf{i}	current density vector	ξ	velocity proportionality constant
i_0	exchange current density	c_{oxy}	oxygen concentration
i_{corr}	corrosion current density	D_{oxy}	diffusion coefficient of oxygen
E_{corr}	corrosion potential	T	ambient temperature
α	gradient energy coefficient	c_i	concentration of species i
f	local free energy density	n_i	average charge number of ion i
f_s/f_l	free energy density of the solid/liquid phase	F	Faraday's constant
		i_p	passive current density
		μ	water viscosity

shapes of corroding electrodes, which has a significant impact on the IR potential drop and mass transfer processes.

More recently, moving boundary models based on numerical techniques such as the finite element method (FEM) have been proposed to simulate the surface evolution during the metal dissolution process [17,18]. In such sharp interface models, the interface velocity is evaluated based on the Faraday's law and the metal interface is moved explicitly at each time step [19]. A major challenge toward performing such simulations is the requirement for extensive remeshing throughout the simulation to maintain an appropriate mesh that conforms to the evolved geometry of the domain [20]. To alleviate this challenge, one can implement techniques such as the level set method (LSM) [21,22] and the arbitrary Lagrangian-Eulerian (ALE) [23–25] to implicitly track the moving interface location and locally evolve the conforming elements of the mesh. However, even with such treatments and in particular for corrosion problems with intricate evolving morphologies, maintaining a high quality mesh during the simulation could be a challenging, computationally expensive task.

Alternatively, some researchers have successfully employed the finite volume method (FVM) to simulate the pitting corrosion phenomenon [26–28]. This approach obviates the difficulties associated with creating conforming meshes by determining the location of the moving pit interface as an implicit function of the ions concentration in each volume element. Meshfree methods are also viable alternatives for simulating moving boundary problems, including corrosion. For example, a meshfree pitting corrosion model relying on the Green's discrete transformation method (GDTM) is presented in Ref. [29]. In this method, the domain is discretized using a set of discrete nodes, where only the nodes located along the pit interface are updated at each time step. Another approach for the treatment of such problems is to implement mesh-independent methods, including the eXtended/Generalized FEM (X/GFEM) [30,31] and the Hierarchical Interface-enriched FEM (HIFEM) [32,33]. Such techniques allow the use of non-evolving nonconforming meshes for discretizing the domain, where appropriate enrichment functions are employed to capture the discontinuity in the ions concentration along the pit boundary. Another method that is successfully used for simulating localized corrosion and corrosion assisted damage is the peridynamics (PD)

[34,35]. In this approach, the domain can be discretized using a simple structured grid, where, similarly to FVM, the interface location is identified based on the ions concentration associated with each node.

Instead of considering the abrupt jump in the field values (e.g., ions concentration) along the moving boundary, which is used in sharp interface models, diffuse interface models assume an interface with a finite thickness to allow the implicit tracking of its evolution via a phase field variable. The Phase Field (PF) method is one of the most popular diffuse interface models, which has been employed for simulating varying phase transformation problems with evolving geometries, including the solidification [36,37] and dendrite growth [38,39]. A detailed review of this method and its applications are provided in Refs. [40,41]. Recently, PF models have been formulated for simulating corrosion processes in a dual-oxidant [42] and a V_2O_5 hot corrosion environment [43]. Mai et al. [44] have introduced a PF model, relying on the Kim-Kim-Suzuki (KKS) model [45], to simulate the pitting corrosion of stainless steel in an electrolyte solution. More recently, Mai and Soghrati expanded this model to incorporate the effect of mechanical stresses for simulating the stress corrosion cracking (SCC) phenomenon [46].

The current manuscript aims to further expand the PF model presented in Ref. [44] to enable incorporating the effects of electric potential and current distributions. To achieve this goal, we employ the Laplace equation as the governing equation to evaluate the electric potential, which determines the current density distribution using the Ohm's law. While the corroding anode is assumed to be nonpolarizable to avoid introducing the interface double layer on the moving boundary, the negligible corrosion rate on the cathode surface allows assigning boundary conditions that characterize its polarization behavior. To incorporate the potential distribution in the PF model, the interface kinetics parameter is characterized as a linear function of the potential gradient normal to the moving interface. We also take into account the effect of the oxygen diffusion when the rate of the oxygen reduction reaction (ORR) is limited by the accessibility of oxygen. The evolution of the corroding metal interface is then simulated by approximating the coupled governing equations associated with the corrosion electrochemical processes using the FEM, although the PF model

Download English Version:

<https://daneshyari.com/en/article/6604737>

Download Persian Version:

<https://daneshyari.com/article/6604737>

[Daneshyari.com](https://daneshyari.com)