Numerical Modeling of Pit Growth in Microstructure

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Abstract

Pitting corrosion is a complex phenomenon where rates of: i) chemical reactions, ii) diffusion of various species involve in those reactions, and iii) species dissolution at the metal-electrolyte interface are fully dependent on each other, except under special conditions or assumptions. One set of such conditions is that: a) there are no species concentration gradients due to the rapid mixing of the electrolyte; b) the solvent is incompressible; and c) the electrolyte solution is electro-neutral. Under these assumption, the balance of species reduces down to the well known Laplace equation: where is the electric potential? In a nutshell, these assumptions mean that dissolution (corrosion) of a given species at the interface occur independent of the convective and diffusive modes of transport, and represent an upper bound on corrosion rate for a given set of boundary conditions. In this work, we present numerical modeling of two-dimensional corrosion pit growth at the microstructural scale by solving the Laplace equation. The actual microstructure of a 316 stainless steel provides the matrix in which the stable pit grows. The objective is to determine the influence the of steel concentration distribution on the shape of the pit at a given time. The high-resolution microstructure is obtained through orientation image microscopy (OIM) techniques and is imported in the finite element model through image-processing methods. The steel-electrolyte front movement is simulated with the help of the arbitrary Lagrangian-Eulerian (ALE) meshing technique provided as part of the commercial partial-differential equation solver software, COMSOL. The front speed, or the material dissolution rate, is approximated with a Butler-Volmer relationship that relates the dissolution current density to the electrode potential (fixed) and electrolyte potential, (evolving). The results will show that fluctuations in steel concentration distributions can explain part of the reason why corrosion pits appear to take different shapes despite growing under the same environmental conditions.