

A phase-field model for microbiologically influenced corrosion: COMSOL implementation

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Abstract

A phase-field-based reaction-diffusion corrosion model is developed to predict microbially influenced corrosion (MIC) in metal alloys, with a focus on anaerobic conditions and sulfate-reducing bacteria (SRB). The formulation couples microbial sulfate reduction, sulfate transport, electrochemical kinetics, material dissolution, and mechanical effects within a unified framework. Microbial activity is modelled using a Monod-type expression for sulfate consumption, whereas the mechano-chemical coupling is incorporated through an enhanced mobility relationship that captures the influence of mechanical fields on corrosion kinetics. The capability of the formulation to capture both MIC-induced pitting and stress-assisted corrosion across multiple length scales is demonstrated through case studies that include microstructure-sensitive simulations and structural-scale coupling with a cathodic protection model.

The theoretical formulation of the model is provided in the original paper [1] while this document provides instructions for its implementation in the finite element software COMSOL Multiphysics. Input files for pitting and stress-assisted corrosion are provided for demonstration purposes. If the code developed is used for research or industrial purposes, please cite:

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Keywords: Microbiologically influenced corrosion, Sulfate-reducing bacteria, Biocorrosion

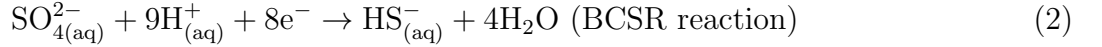
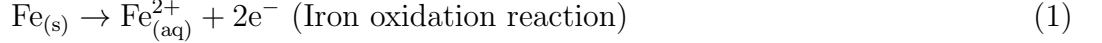
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1. The phase-field model of microbially influenced corrosion

This section briefly introduces the mathematical formulation of the phase-field model for the microbially influenced corrosion in anaerobic conditions. The interested reader is referred to the original paper for more details [1].

The following independent primary variables are introduced to describe the degradation mechanism illustrated in Fig. 1 and the associated bioelectrochemical reactions



Since sulfate availability governs SRB metabolic activity, the normalised sulfate concentration $\bar{c}(\mathbf{x}, t) = c/c_{\text{ref}}$ is introduced in the model to characterise mass transport within the bulk electrolyte. Here, c_{ref} stands for the reference sulfate concentration. The evolution of the corroding interface is tracked by a continuous phase-field variable $\phi(\mathbf{x}, t)$. The variable takes the value $\phi = 1$ in the uncorroded metal and $\phi = 0$ in the corrosive environment. The thin diffuse interface region, representing the metal-environment interface, is described with $0 < \phi < 1$. The mechanical response of the degrading metal is characterised under the assumption of small deformations (linearised kinematics) with the displacement vector $\mathbf{u}(\mathbf{x}, t)$ serving as the primary kinematic variable.

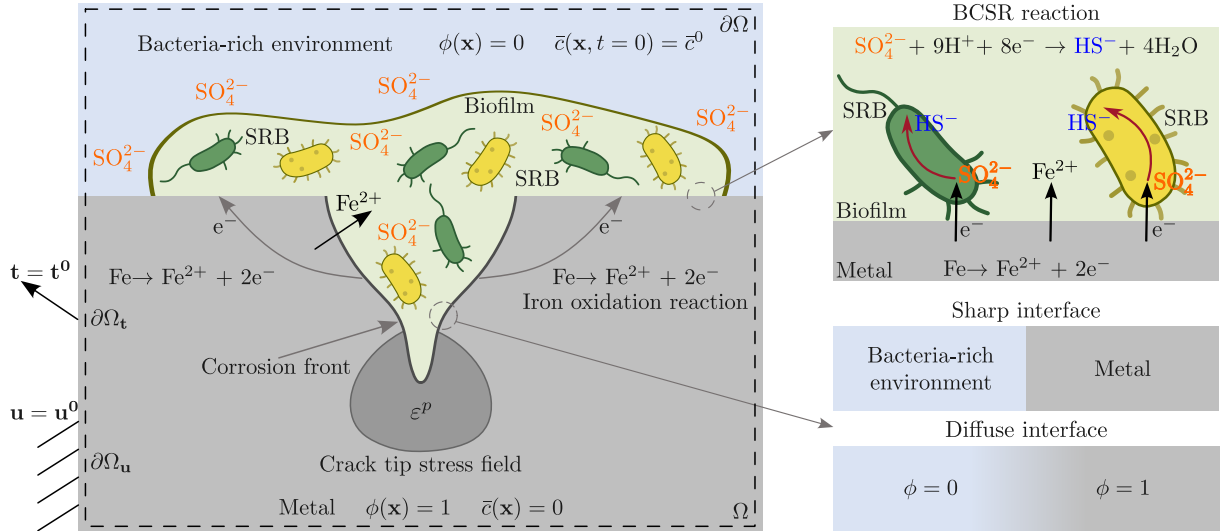


Figure 1: Microbially influenced corrosion mechanism and diffuse interface representation of the corrosive environment (bacteria-rich environment with biofilm $\phi = 0$) and metal ($\phi = 1$) phases.

The free energy functional for the heterogeneous system in Fig. 1 can be written as

$$\mathcal{F} = \int_{\Omega} \left[\mathcal{F}^{\text{chem}}(\bar{c}, \phi) + \frac{1}{2} \kappa |\nabla \phi|^2 + \mathcal{F}^{\text{mech}}(\nabla \mathbf{u}, \phi) \right] d\Omega, \quad (3)$$

where $\mathcal{F}^{\text{chem}}$ is the chemical free energy density, $\mathcal{F}^{\text{mech}}$ the mechanical free energy density, κ the gradient energy coefficient, and Ω the system domain, which includes the corroding metal and the corrosive environment consisting of sulfate ions and SRB. The chemical free energy density of the system can be written as

$$\mathcal{F}^{\text{chem}}(\bar{c}, \phi) = \frac{1}{2} N \Psi \left[\bar{c} - \bar{S}_{\min} (1 - h(\phi)) \right]^2 + \omega g(\phi), \quad (4)$$

where N is the effective SRB cell density, Ψ the effective stored energy in the body of a cell, $g(\phi) = 16\phi^2(1-\phi)^2$ the double-well free energy function, ω the constant that determines the energy barrier at $\phi = 1/2$ between the two minima, and $h(\phi) = \phi^3(6\phi^2 - 15\phi + 10)$ is a monotonically increasing function that interpolates between the chemical free energies of the two phases. $\bar{S}_{\min} = S_{\min}/c_{\text{ref}}$ designates the normalised minimum (limiting) sulfate concentration required for microbial activity, i.e., at or below this sulfate concentration, SRB metabolic activity and growth become negligible, leading to suppression of corrosion. The expression is defined following a Monod-type relation for describing microbial growth: $S_{\min} = K_m b / (Yq - b)$. Here, K_m stands for the Monod half-velocity coefficient for SRB (mol/m³), Y is the true yield of bacterial mass per unit of metal substrate utilised (kg/mol), b denotes the specific decay or maintenance-respiration coefficient (1/s), and q corresponds to the maximum specific rate of metal substrate utilisation by SRB (mol/(kg·s)).

The total mechanical free energy density $\mathcal{F}^{\text{mech}}$ is expressed using linearised kinematics and following an isotropic power law hardening response within von Mises plasticity theory

$$\mathcal{F}^{\text{mech}}(\nabla \mathbf{u}, \phi) = \frac{1}{2} (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) : \mathbb{C}(\phi) : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) + \frac{\sigma_y \varepsilon_y}{n+1} \left[\left(1 + \frac{\varepsilon^p}{\varepsilon_y} \right)^{n+1} - 1 \right], \quad (5)$$

where $\boldsymbol{\varepsilon} = 1/2(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ is the total strain tensor, $\boldsymbol{\varepsilon}^p$ the plastic strain tensor, $\mathbb{C}(\phi) = h(\phi)\mathbb{C}_0$ and $\mathbb{C}_0$ are the effective and intact rank-four elastic stiffness tensors, respectively, σ_y denotes the initial yield strength, ε_y the initial yield strain, n the hardening exponent ($0 < n \leq 1$), and $\varepsilon^p = \sqrt{2/3} \int_0^t |\dot{\boldsymbol{\varepsilon}}^p| dt$ is the von Mises equivalent plastic strain. $h(\phi)$ acts as a degradation function that ensures that mechanical fields are confined to the solid phase and vanish smoothly within

the electrolyte. The rank-four elastic stiffness tensor for the intact solid is described by isotropic linear elasticity: $\mathbb{C}_0 = \lambda \mathbf{I} \otimes \mathbf{I} + 2\mu \mathbb{I}$, where $\mathbf{I}$ is the second-order identity tensor, $\mathbb{I}$ the symmetric fourth-order identity tensor, and λ and μ are the Lamé elastic constants.

Governing equations and mechano-chemical coupling

The evolution of the corroding interface follows the usual Allen-Cahn equation

$$\frac{\partial \phi}{\partial t} = -L \frac{\delta \mathcal{F}}{\delta \phi} = -L \left(\frac{\partial \mathcal{F}^{\text{chem}}}{\partial \phi} - \kappa \nabla^2 \phi \right) \quad \text{in } \Omega, \quad (6)$$

where $L > 0$ is the interfacial mobility that controls the motion of the metal-environment interface. On the boundary $\partial\Omega$: $\kappa \mathbf{n} \cdot \nabla \phi = 0$. The phase-field mobility is multiplicatively decomposed into three contributions

$$L = L_0 \left(\frac{\varepsilon^p}{\varepsilon_y} + 1 \right) \exp \left(\frac{\sigma_h V_m}{RT} \right), \quad (7)$$

where L_0 is the interfacial mobility in the absence of mechanical fields (stress-free corrosion). The last two factors in the previous equation define an amplification factor that depends on the distributions of local plastic strain ε^p and hydrostatic stress σ_h (stress-assisted corrosion). Here, R is the universal gas constant, V_m the molar volume of the metal, and T the absolute temperature. The mechanical fields are obtained by solving the linear momentum balance equation for quasi-static loading

$$\begin{aligned} \nabla \cdot \boldsymbol{\sigma} &= \mathbf{0} \quad \text{in } \Omega \\ \mathbf{t} = \mathbf{n} \cdot \boldsymbol{\sigma} &= \mathbf{t}^0 \quad \text{on } \partial\Omega_{\mathbf{t}} \quad \text{and} \quad \mathbf{u} = \mathbf{u}^0 \quad \text{on } \partial\Omega_{\mathbf{u}}, \end{aligned} \quad (8)$$

complemented by standard boundary conditions with prescribed traction $\mathbf{t}^0$ and displacement $\mathbf{u}^0$ vectors on boundaries $\partial\Omega_{\mathbf{t}}$ and $\partial\Omega_{\mathbf{u}}$. In the previous expression, $\boldsymbol{\sigma} = \partial \mathcal{F}^{\text{mech}} / \partial (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) = h(\phi) \mathbb{C}_0 : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p)$ represents the effective Cauchy stress tensor.

The transport of sulfate ions is governed by the mass balance law

$$\left\{ \begin{aligned} \frac{\partial \bar{c}}{\partial t} &= -\nabla \cdot \mathbf{J} + R; & R &= -\frac{qc_b}{c_{\text{ref}}} \frac{\bar{c}}{(\bar{K}_m + \bar{c})} p(\phi) \\ \mathbf{J} &= -M \nabla \left(\frac{\delta \mathcal{F}}{\delta \bar{c}} \right) = -D \nabla \bar{c} - D \bar{S}_{\min} h'(\phi) \nabla \phi \end{aligned} \right\} \quad \text{in } \Omega. \quad (9)$$

On the boundary $\partial\Omega$: $\mathbf{n} \cdot \mathbf{J} = 0$. $\mathbf{J}$ stands for the diffusional flux, M is the mobility parameter ($M = D / (\partial^2 \mathcal{F}^{\text{chem}} / \partial \bar{c}^2)$), D denotes the effective diffusion coefficient, and $h'(\phi) = \partial h(\phi) / \partial \phi$. The

effective diffusion coefficient is interpolated with the phase-field variable: $D = D^s h(\phi) + (1 - h(\phi)) D^l$, where D^l and D^s stand for the diffusion coefficients of sulfate ions in the liquid and solid phases. R in the previous equation is the reaction rate that accounts for sulfate consumption by SRB cells. Here, $\bar{K}_m = K_m / c_{\text{ref}}$ is the normalised Monod half-velocity coefficient for SRB, c_b the bacterial density in the biofilm in units of kg/m^3 , and $p(\phi) = 4\phi(1 - \phi)$ the function introduced to limit annihilation of sulfate ions to a limited area close to the metal-electrolyte interface (i.e., the reaction zone).

Elements of dimensional analysis

The analysis of the phase-field and diffusion equation yields the characteristic time for interface movement, mass transport (diffusion) within the bulk electrolyte, and the reaction rate for the consumption of sulfate ions [1]

$$\tau_\phi = \frac{1}{L\omega} \quad \tau_d = \frac{\ell^2}{D^l} \quad \tau_r = \frac{S_{\min}}{qc_b}. \quad (10)$$

Denoting the nondimensional quantities with a bar, e.g., $\bar{t} = t/\tau_d$ and $\bar{\nabla} = \ell\nabla$, the set of the nondimensional governing equations is written as

$$\left\{ \begin{array}{l} \frac{\partial \phi}{\partial \bar{t}} = -\frac{\tau_d}{\tau_\phi} \left[\frac{N\Psi}{\omega} (\bar{c} - 1 + h(\phi)) h'(\phi) + g'(\phi) - 2\bar{\nabla}^2 \phi \right] \\ \frac{\partial \bar{c}}{\partial \bar{t}} = \bar{\nabla} \cdot \left(\bar{D} \bar{\nabla} \bar{c} + \bar{D} h'(\phi) \bar{\nabla} \phi \right) - \frac{\tau_d}{\tau_r} \frac{\bar{c}}{\bar{K}_m + \bar{c}} p(\phi) \\ \bar{\nabla} \cdot \bar{\sigma} = 0 \end{array} \right\} \quad \text{in } \bar{\Omega}. \quad (11)$$

2. COMSOL implementation

The resulting governing equations and accompanying boundary conditions are solved using the finite element software COMSOL Multiphysics [2]. To demonstrate the model implementation in COMSOL Multiphysics, two case studies are considered: MIC-induced corrosion in the absence of mechanical loading (the model calibration and sensitivity studies from the original manuscript) and a microstructure with an average grain size of 40 μm subjected to tensile deformation (stress-assisted corrosion). The corresponding COMSOL Multiphysics input files, labelled as `Model calibration.mph` and `Stress-assisted corrosion.mph`, are provided along with this documentation. The first file reproduces the results given in Section 3. The second returns

microstructure-sensitive simulations with mechanical loading, given in Section 4.3 of the original paper [1]. The remaining data presented in the original publication can be reproduced following the implementation demonstrated in these two case studies.

2.1. Stress-free MIC-induced corrosion

A schematic illustration of the computational domain for the first case study is shown in Fig. 2. Since only pit depths were measured in the experiment, the simulation is simplified and considers a one-dimensional computational domain. The metal used in the simulation is 1 mm long. The size of the liquid phase is significantly larger than that of the metal phase to mimic the experimental setup. The initial sulfate ion concentrations are set to 0 mM in the metal phase and 0.5 mM in the liquid phase to match the experimental conditions. The boundary conditions for the phase-field and diffusion equations ($\mathbf{n} \cdot \bar{\nabla} \phi = 0$ and $\mathbf{n} \cdot \bar{\mathbf{J}} = 0$) are prescribed on both edges of the computational domain. The role of mechanical fields in influencing corrosion kinetics is not accounted for in this simulation, and hence, the mechanical equilibrium equation is not considered.

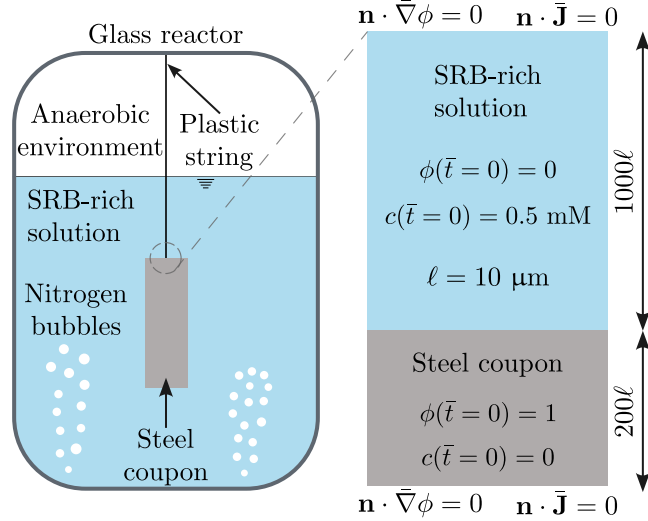


Figure 2: Schematic illustration of the one-dimensional computational domain.

The primal kinematic variables are the normalised sulfate concentration $\bar{c}$ and the phase-field variable ϕ . The **Mathematics** module with the **General Form PDE** interface is used to describe both equations [3]

$$e_a \frac{\partial^2 \bar{c}}{\partial t^2} + d_a \frac{\partial \bar{c}}{\partial t} + \nabla \cdot \Gamma = f \quad e_a \frac{\partial^2 \phi}{\partial t^2} + d_a \frac{\partial \phi}{\partial t} + \nabla \cdot \Gamma = f \quad (12)$$

where the coefficients are chosen as $d_a = 1$ and $e_a = 0$ to represent the diffusion equation. For the

phase-field equation, they are set to $d_a = \tau_\phi/\tau_d$ and $e_a = 0$. The vector Γ and the source term f for the diffusion equation are given as

$$\Gamma = -\bar{D}\bar{\nabla}\bar{c} - \bar{D}h'(\phi)\bar{\nabla}\phi \quad f = -\frac{\tau_d}{\tau_r} \frac{\bar{c}}{\bar{K}_m + \bar{c}} p(\phi). \quad (13)$$

This resembles the diffusion equation in Eq. (11). Similarly, the vector Γ and the source term f for the phase-field equation are set to

$$\Gamma = -2\bar{\nabla}\phi \quad f = -\frac{N\Psi}{\omega} \left(\bar{c} - 1 + h(\phi) \right) h'(\phi) - g'(\phi), \quad (14)$$

which resembles the phase-field equation in Eq. (11).

2.2. Microstructure sensitive stress-assisted corrosion simulations

In addition to the above two equations for the phase-field variable ϕ and sulfate concentration $\bar{c}$, the built-in **Solid Mechanics** interface is used to implement the governing equation for mechanical equilibrium in Eq. (11). A microstructure with an average grain size of 40 μm subjected to tensile deformation ε^∞ is used for demonstration purposes. The corresponding computational domain, along with initial and boundary conditions for the phase-field and diffusion equations, is illustrated in Fig. 3. Additional boundary conditions are imposed for the mechanical equilibrium equation (8). The normal component of the displacement vector $\bar{\mathbf{u}}$ is constrained along the vertical and horizontal edges ($\mathbf{n} \cdot \bar{\mathbf{u}} = 0$) while the remote tensile deformation ε^∞ is enforced on the top surface.

The mechanical properties of steel S355 are adopted for the simulations, with Lamé elastic constants of $\lambda = 121.15$ GPa and $\mu = 80.80$ GPa. The metal is modelled as an isotropic elasto-plastic solid. Plastic deformation is described using the J₂ flow theory with nonlinear isotropic hardening, characterised by a yield stress of $\sigma_y = 355$ MPa and a strain hardening exponent of $N = 0.1$. The yield strain $\varepsilon_y = \sigma_y/E$ is defined using a Young's modulus of $E = 210$ GPa. These mechanical properties are assigned uniformly to all grains. The elastic mechanical properties are multiplied by the degradation function $h(\phi)$ to account for the degradation of the material stiffness associated with the evolution of the corrosion front ϕ .

The **Solid Mechanics** interface computes and gives access to the effective plastic strain ε^p and the hydrostatic stress σ_h , which are required to enhance the phase-field mobility in Eq. (7).

The evolution of stress-assisted corrosion for this representative microstructure is presented in

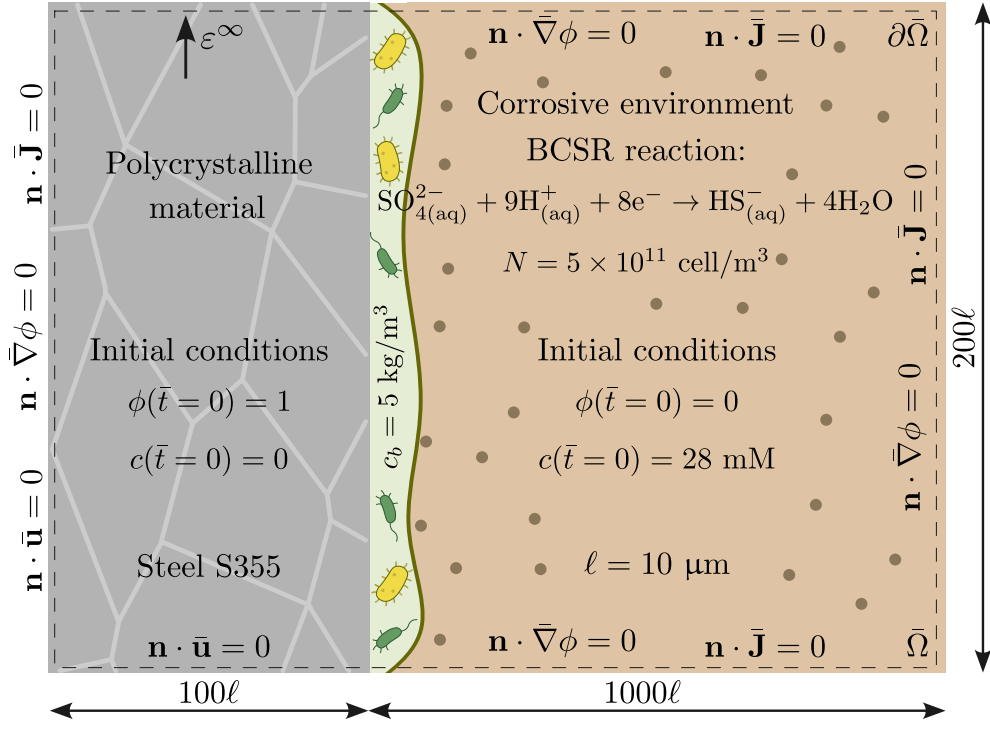


Figure 3: Microstructure-sensitive simulations of corrosion in the buried zone.

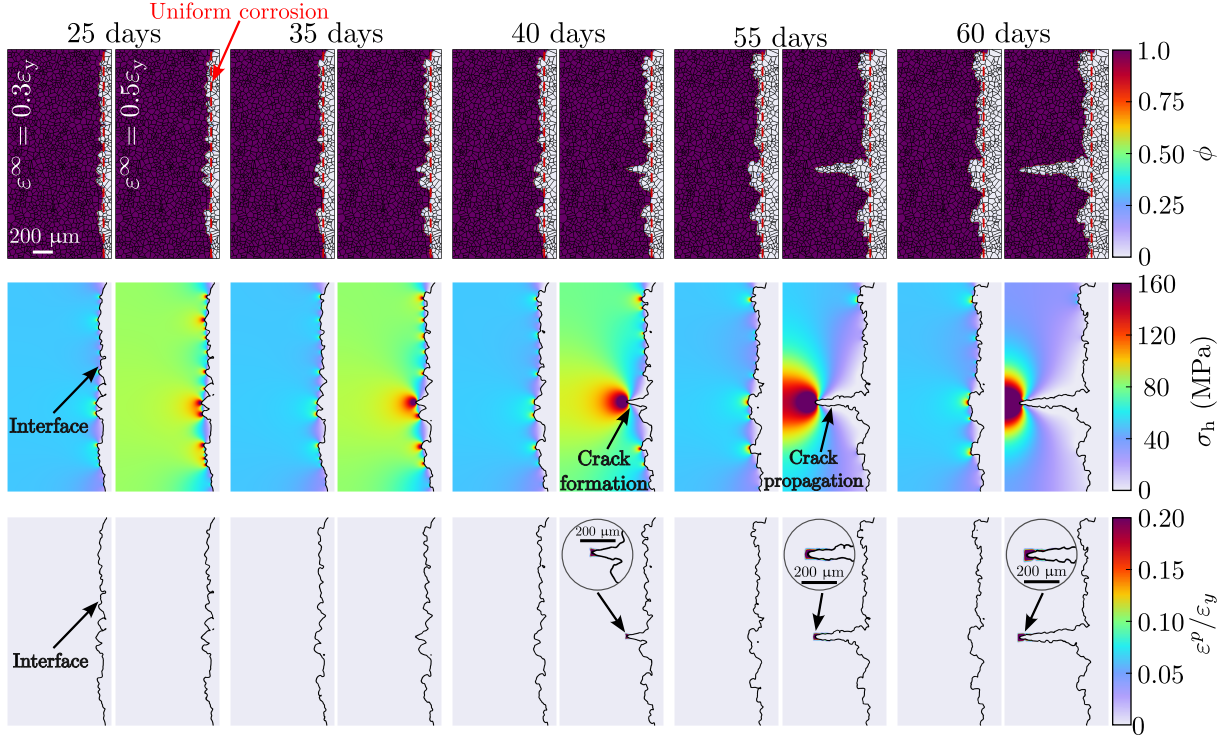


Figure 4: Corrosion evolution for the representative microstructure with an average grain size of 40 μm subjected to remote deformation ε^∞ . The red lines correspond to uniform corrosion. The initial surrounding corrosive environment is not shown in the plots. The scale bar for all plots is 200 μm .

Fig. 4. Pits nucleated at the metal-environment interface act as stress concentrators in the presence of mechanical loading, accelerating dissolution locally in regions where hydrostatic stress σ_h and plastic strains ε^p are high. The distribution of mechanical fields is highly nonuniform and depends on the evolution of the corrosion front. There are multiple small areas with high mechanical fields during early immersion times, which can potentially act as hot spots for crack initiation. The locations of these hot spots with amplified mechanical fields vary over time as the corrosion front changes shape in response to the underlying microstructure. As shown in Fig. 4, the low-load case ($\varepsilon^\infty = 0.3\varepsilon_y$) does not lead to crack formation. This load case produced zero plastic strains and low hydrostatic stresses, which are insufficient to trigger rapid local pit propagation that could serve as a site for crack initiation. On the other hand, increasing the load ($\varepsilon^\infty = 0.5\varepsilon_y$) activates plastic strains and higher hydrostatic stresses, leading to more rapid and severe pitting along the corroding interface. At a certain time, mechanical fields rise in a specific area, setting a precursor for a dominant location of crack initiation. After that time point, a crack forms and propagates due to high mechanical fields at the defect tip.

3. Concluding remarks

A finite element implementation of the phase-field model for simulating the microbially influenced corrosion (MIC) in metal alloys under anaerobic conditions developed in Ref. [1] is presented. The present document provides details of the model implementation in the COMSOL Multiphysics software package. Two case studies, namely stress-free and microstructure-sensitive stress-assisted corrosion, are explained in this documentation. The code developed is freely available at <https://mechmat.web.ox.ac.uk/codes>.

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