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Finite element implementation of a peridynamic pitting corrosion damage model

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ABSTRACT

Despite the significant improvements in the understanding of pitting corrosion, many aspects of this phenomenon remain unclear and corrosion rate prediction based on experimental data remains difficult. Experimental measurements of corrosion rates under different electrochemical conditions can be complex and time consuming, and the conclusions are limited to the timescale and the conditions in which experiments have been carried out. In order to overcome these limitations, numerical approaches can be a valuable complement. Hence, in this study a new numerical model based on peridynamics to predict pitting corrosion damage is developed. The developed model is implemented in a commercial finite element software and it allows for the reproduction of realistic pitting morphologies, modelling of microstructural effects such as the presence of intermetallic particles and the reduction of the computational cost of the simulations. In conclusion, the results of this study shows that the peridynamic models can be helpful in failure analysis and design of new corrosion-resistant materials.

1. Introduction

Corrosion is a natural process that can be described as the chemical or electrochemical reaction of an engineering material with the environment, which eventually leads to the deterioration of its mechanical properties. There are various types of corrosion mechanisms including stress corrosion cracking (SCC) and pitting corrosion.

Pitting is a localised form of corrosion that leads to the formation of corrosion cavities or pits due to the breakage of the material's passive film. Pitting typically occurs in materials such as stainless steel, aluminium, titanium, copper, magnesium and nickel alloys. Pitting corrosion is the most common, dangerous and destructive type of corrosion in marine and offshore structures (Bhandari et al., 2015).

Despite the significant improvements in the understanding of pitting corrosion, many aspects of this phenomenon remain unclear and corrosion rate prediction based on experimental data remains difficult (Onishi et al., 2012). Experimental measurements of corrosion rates under different electrochemical conditions can be complex and time consuming, and the conclusions are limited to the timescale and the conditions in which experiments have been carried out (Van der Weeën et al., 2014). Moreover, distinguishing the effect of each individual variable becomes extremely difficult (Xiao and Chaudhuri, 2011). In order to overcome these limitations, numerical approaches can be a valuable complement.

Several numerical approaches are available in the literature for the modelling of corrosion damage, and many of them are based on finite element method (Sharland et al., 1989; Walton, 1990; Laycock and White, 2001; Scheiner and Hellmich, 2009). However, the modelling of pit propagation by using finite element method (FEM) is not an easy task since special procedures of moving mesh and remeshing are often needed (Duddu, 2014). Moreover, if remeshing techniques are used, the finite element matrices have to be recalculated for every time step (Vagbharathi and Gopalakrishnan, 2014). In order to overcome these difficulties, an alternative numerical approach to the FEM can be the use of extended Finite Element Method (XFEM). Vagbharathi and Gopalakrishnan (2014) and Duddu (2014) describe numerical models of corrosion pit propagation in stainless steel based on the XFEM framework and Fick's law of diffusion. An extension to the latter work was done by Duddu et al. (2015), where the Fick's law of diffusion was replaced by the Nernst-Planck equation and crevice corrosion in Al-Mg alloy microstructures was investigated.

Although all the aforementioned models have been quite effective in predicting the corrosion rates reported in the experimental literature, none of these models have been able to predict corrosion subsurface damage, which is a phenomenon documented in the experimental literature (Song et al., 2014). With the aim of filling this gap, a new continuum mechanics formulation, peridynamics (PD), has been recently used to create a model of pitting corrosion (Chen and

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Bobaru, 2015) based on a modified Nernst-Planck equation. This work was extended in (Chen et al., 2015), where the influence of the pit cover on the pit morphology was investigated.

In this study, a new numerical model based on PD theory for the investigation of pitting corrosion is introduced. This work is based on the PD model of pitting corrosion developed by Chen and Bobaru (2015). However, the numerical approach used in the present study is different and offers the advantage of a reduced computational time by performing the numerical implementation in a commercial finite element software and utilizing implicit time integration. Moreover, the capabilities of the numerical framework have been extended to the modelling of realistic pit morphologies and determining the influence of microstructural features of the material, e.g. intermetallic particles. The ultimate goal of this study is to produce a non-conventional and more effective numerical framework that can be helpful in failure analysis and design of new corrosion-resistant materials.

2. Peridynamics

The governing equations of classical continuum mechanics (CCM) are based on partial differential equations (PDEs) and its mathematical formulation breaks down in the presence of discontinuities such as cracks. This limitation is partially overcome with the adoption of external crack growth criteria based on fracture mechanics. However, this approach presents its own limitations. In light of the limiting assumptions and difficulties of the current approaches, a new mathematical formulation of continuum mechanics was developed by Silling (2000), which is called “peridynamics”.

The governing equations of PD are integro-differential. The PD equations of motion of a generic material point $\mathbf{x}$ can be written as (Silling, 2000)

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x}, t) = \int_{H_{\mathbf{x}}} \mathbf{f}\left(\mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t), \mathbf{x}' - \mathbf{x}\right) \, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t) \tag{1}$$

where $\rho(\mathbf{x})$ and $\ddot{\mathbf{u}}(\mathbf{x}, t)$ denote the density and acceleration of the material point $\mathbf{x}$ at time t, respectively. In Eq. (1), $\mathbf{f}\left(\mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t), \mathbf{x}' - \mathbf{x}\right)$ represents the PD force between material points $\mathbf{x}$ and $\mathbf{x}'$ (also called mechanical response function) and the term $\mathbf{b}(\mathbf{x}, t)$is the body force acting on material point $\mathbf{x}$ at time t. $dV_{\mathbf{x}'}$ is the volume associated with material point $\mathbf{x}'$. According to this new formulation, a material point can interact with other material points not only within its nearest neighbourhood, but also with material points in a larger neighbourhood (Fig. 1).

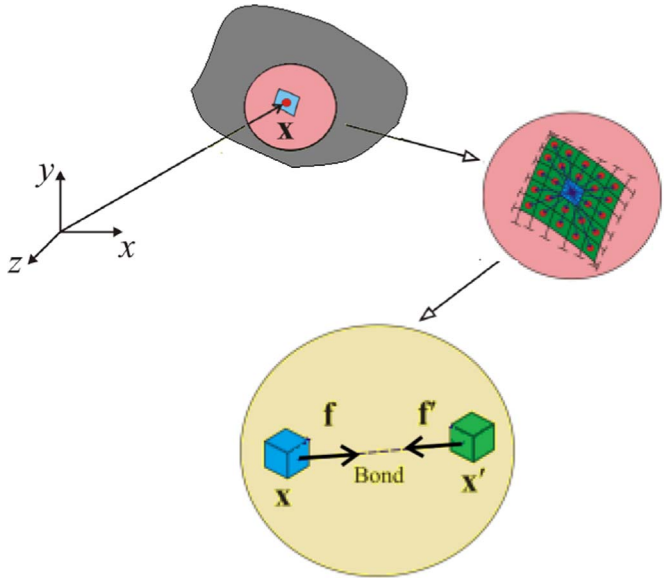

Fig. 1. Peridynamic forces between material points $\mathbf{x}$ and $\mathbf{x}'$.

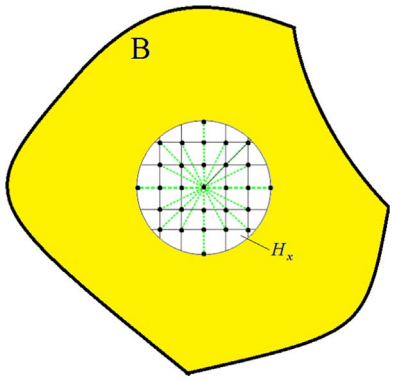

Fig. 2. Peridynamic bonds between material points inside the peridynamic horizon, $H_{\mathbf{x}}$.

It can be assumed that the interaction between material points decreases as the distance between them increases. Therefore, an influence domain, named horizon,$H_{\mathbf{x}}$, can be defined for each material point as shown in Fig. 2.

The material point $\mathbf{x}$ can only interact with material points within this domain, which are called the “family” of $\mathbf{x}$. This interaction is called “bond” and its length is simply the distance between the two material points. In the case of an elastic material, the peridynamic force between material points $\mathbf{x}$ and $\mathbf{x}'$, can be expressed as

$$\mathbf{f} = c\, s\, \frac{\mathbf{y}' - \mathbf{y}}{|\mathbf{y}' - \mathbf{y}|} \tag{2}$$

where $\mathbf{y}$ represents the location of the material point $\mathbf{x}$ in the deformed configuration as shown in Fig. 3, i.e. $\mathbf{y} = \mathbf{x} + \mathbf{u}$, while c is the bond constant which can be related to material constants of CCM as described in Madenci and Oterkus (2014).

In Eq. (2), the stretch parameter, s, is defined as

$$s = \frac{|\mathbf{y}' - \mathbf{y}| - |\mathbf{x}' - \mathbf{x}|}{|\mathbf{x}' - \mathbf{x}|} \tag{3}$$

In the case of a brittle material behaviour, the peridynamic force and the stretch relationship are shown in Fig. 4.

The parameter s_0, in Fig. 4, is called critical stretch and if the stretch of a peridynamic bond exceeds this critical value, the peridynamic interaction (bond) is broken. As a result, the peridynamic force between the two material points reduces to zero and the load is redistributed among the other bonds, leading to unguided material failure. Peridynamics can be applicable for different material systems including metals and composites (Oterkus and Madenci, 2012). Moreover, PD framework can be extended to other fields such as thermal (Gerstle et al., 2008), moisture (Oterkus et al., 2014), etc., so that it can be used as a single platform for multiphysics analysis of

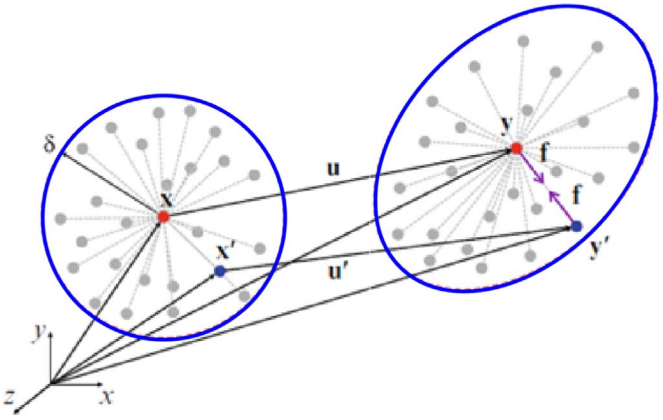

Fig. 3. Peridynamic horizon in the undeformed configuration (left) and the deformed configuration (right).