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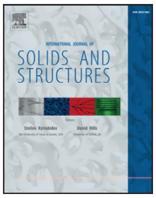

A phase field method for modeling stress corrosion crack propagation in a nickel base alloy

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ABSTRACT

Stress Corrosion Cracking (SCC) is a very common failure mechanism characterized by a slow, environmentally influenced crack propagation in structural components. The mechanisms proposed to explain, at the microscopic scale, the cracking propagation processes are not able to elucidate all aspects of this phenomenon in different metal/environment systems. This work is concerned with the development of a new multiphysics model for understanding the phenomena of crack propagation under the effect of SCC. This new model is based upon: (i) a phase field method, based on a variational formulation of brittle fracture with regularized approximation of discontinuities; (ii) a robust algorithm capable to prescribe the displacements (over the boundary of a small sub-volume) and crack onset obtained by image processing based on digital image correlation in the sample during the numerical simulations; (iii) a coupling with a diffusion model informed with first-principles computations of diffusion coefficient. In this new model, the phenomenon of environmentally assisted cracking phenomena was successfully represented as well the interactions between cracks and the subsequent shielding effects. The analyses, performed on several samples of Inconel 600 alloy containing a crack network, show a remarkable agreement between the crack morphology and history obtained by the model and by the experiments.

1. Introduction

Predicting the strength and durability of engineering components and structures using numerical simulations of fracture phenomena induced by Stress Corrosion Cracking (SCC) is a very challenging problem. SCC can often be regarded as the result of localized oxidation enhanced by stress/strain: a combined action of a sustained mechanical loading and a chemically aggressive environment. The occurrence of SCC in a structure can lead to catastrophic failures, it has thus long been recognized as potentially dangerous. One of the mechanisms responsible for this process noted in the literature is the embrittlement of the material due to local anodic dissolution of fresh metal created by slip band emergence at the crack tip. In this area recent developments and corresponding issues have been reviewed in Newman and Healey (2007), followed by some original contributions related to different aspects of the problem: loading rate effects, harmonization of different formulations of the model, and sensitivity of the model to various parameters. Developing numerical models for the quantitative evaluation of stress corrosion cracking growth rates in terms of key engineering parameters is highly required.

Various experimental methods have been proposed in the literature to study cracks induced by SCC. The measurements of corrosion contribution is usually based on electrochemical methods such as Electrochemical Noise (EN) (Hladky and Dawson, 1981; Kearns, 1996; Kovac et al., 2010). Due to its capacity of distinguishing between different corrosion types, the (EN) method is mostly applied to detect and evaluate SCC activity. Acoustic Emission (AE) (Bellenger et al., 2002; Jomdecha et al., 2007; Shaikh et al., 2007) is also widely used because of its ability to detect material deformation, cracking and fracture. Many microscopy techniques have been applied to characterize SCC at different scales. For example, magnetic force microscopy (MFM) has been used to detect the chromium depleted regions of type 304 stainless steel (Takaya et al., 2004), the early stages of pitting and localized corrosion have been studied by combining *in situ* observations and electromechanical atomic force microscopy (EAFM) (Williford et al., 2000), and scanning electron microscopy (SEM) is used to study the pitting corrosion of Al (Richardson and Wood, 1970). This technique is also used to observe the fracture surface of SCC in high

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strength steel fasteners (Abhay et al., 2010). The Diffraction Contrast Tomography (DCT) is another technique used to characterize SCC, for example the work of King et al. (2008) study the interaction between intergranular stress corrosion cracking and microstructure in a Grain-Mapped Polycrystal. In the work of Babout et al. (2006), the phenomenon of intergranular stress corrosion cracking in a sensitized type 302 stainless steel wire has been observed *in situ* using high resolution X-ray microtomography. An important step after image acquisition by OM/SEM is the processing of microstructural images to obtain a qualitative/quantitative analysis of the sample. Many techniques have been developed in the literature with this aim. Among these techniques, digital image correlation (DIC), or digital volume correlation (DVC) in 3D, is one of the most efficient and versatile tool. This procedure is based on the comparison of images acquired at different stages of a mechanical test and provides quantitative descriptions of local deformation. DIC could be used instead of, or in addition to the prevailing methods to detect defects, by observing the singularity due to the change in the strain distribution, or a step jump in the displacement field across the cracks.

In the literature, most of the models proposed to predict SCC rates are based on linear elastic fracture mechanics concepts without deeply considering corrosion kinetics. A numerical simulation scheme of SCC is developed in the work of Choi et al. (2007) for a thermoplastic material based on crack layer theory. SCC is here considered as a superposition of creep, it induces aging and chemical degradation. Then, they use the phenomenological power laws to describe the loss of material toughness due to these two mechanisms. In addition, this work proposed a generic kinetic parameter to represent the rate of chemical corrosion. Both SCC and mechanically driven crack growth were simulated. In the work of Saito and Kuniya (2001), a predictive methodology for SCC crack growth using a mechanochemical model based on a slip formation/dissolution mechanism is presented. The mechanochemical model consists of the combined kinetics of the plastic deformation process as a mechanical factor and the slip dissolution–repassivation process as an environmental factor at the crack tip. The role of the passive film has also been studied in many works, its physical degradation is usually expressed by a unique parameter namely the “crack tip strain rate”. Many works in literature use this concept that is applied to study SCC in many cases, such as those by Vermilyea (1972), Vermilya and Diegle (1976), Parkins (1980, 1987), Ford and Andresen (1987), ... However, the results of these models are rarely compared with experimental ones, especially concerning crack morphology.

With recent advances in numerical simulation methods new studies are now possible, allowing the development of fracture models at microscale, in particular for complex cracks morphology including phenomena of crack initiation, coalescence and propagation. The objective of this proposed paper is to construct a numerical model to simulate the failure of a nickel base alloy under SCC in an acidified tetrathionate environment. The reaction–dissolution process is simulated with a kinetics model, and integrated into a mechanical analysis. The anodic dissolution, that is involved in the decrease of fracture property is considered to be dependent on the extent of corrosion, and such dependence is implemented within a fracture model. For this purpose, we use the phase field method based on the variational formulation of the crack evolution problem due to Francfort and Marigo (1998). The regularized setting of their framework has been considered in Bourdin et al. (2000). Another contribution for the phase field method based on LandauGinzburg type phase-field evolution equations can be found in Karma et al. (2001). The phase field method may be approached both theoretically and practically, providing an excellent framework for taking into account environmental effects on the failure phenomenon. This framework is also extremely suitable for establishing parametric trends besides enabling the assessment of safety margins. This work is concerned with the development of a new multiphysics model for simulating the phenomena of crack propagation under the effect of SCC based on the phase field method and the numerical implementation proposed by Miehe et al. (2010). Direct comparisons between the simulationed crack paths and experimental data are performed. In addition, a strategy is proposed to identify the parameters of the constitutive model by using DIC results.

The overview of the paper is as follows. A brief introduction of experimental methods is described in Section 2. Then, we present a short review about the slip dissolution model for SCC in Section 3. The new model proposed for SCC propagation based on the phase field method is presented in Section 4. The proposed algorithm is described in Section 5. Finally, the method is evaluated and illustrated by damage benchmarks and practical examples involving crack onset and propagation provided by SCC, and then we present the direct comparisons between the model and the experiments in Section 6.

2. Experimental method for observation of crack propagation

2.1. Experimental procedures

This study focuses on Inconel 600 alloy material. Its chemical composition is given in Table 1. The presented experiments were performed on specimens with a gauge dimension of 117 mm length, 8 mm width and 2 mm thickness as depicted in Fig. 1(a). (see Bolivar et al., 2016 for more details of sample preparation)

To use DIC, a specific procedure has been proposed to improve the grey level contrast on the sample surface. Finally, the samples exhibit many random heterogeneities that give local contrast of grey levels in the images, what is promising for DIC. The details of experimental setup has been described in Bolivar et al. (2016)

Constant load tests were performed for this study. First, the samples are immersed in the test solution (10 mM $K_2S_4O_6$, pH = 3) for about 45 min. Then, the specimens are subjected to a constant applied load corresponding to 80% of the yield stress (263 MPa) by using an electromechanical tensile machine (LLOYD LR30K Plus).

The sample surface was observed in-situ through a 2/3” CCD Stingray camera of 5 Mpx with a pixel size of 3.45 μm (see Fig. 1(b)). The camera was coupled with a 1X telecentric lens. The surface was enlighted with a led lamp in order to eliminate the light variation on the surface. Two polarizing filters (linear and circular) were also used in order to avoid light reflection.

The test is stopped when crack colonies are observed and the electric potential is stable (around −195 mv/SCE). Finally, we use either Optical Microscopy (OM) or Scanning Electron Microscopy (SEM) to observe the cracked surfaces, this step will be used to validate the results of crack detection by DIC.

2.2. Detection of crack network by using image processing based on DIC

DIC is a full-field measurement technique, based on the comparison of images acquired at different stages of a mechanical test. DIC provides access the displacement field at the surface of the sample. DIC principles have been introduced in experimental solid mechanics more than 20 years ago by Sutton et al. (1983) and this technique is currently used for many applications.

We refer to Sutton et al. (2009) for a detailed description of this technique. The specific 2D-DIC procedure used in this work is similar to the one used in Besnard et al. (2006).

The DIC analysis is performed using the in-house software. The procedure is based on four main steps:

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