Available online at www.sciencedirect.com
ScienceDirect
Computational Materials Science 38 (2006) 442–453
COMPUTATIONAL MATERIALS SCIENCE
www.elsevier.com/locate/commatsci

A three-dimensional computational model for intergranular cracking

A.P. Jivkov *, N.P.C. Stevens, T.J. Marrow

School of Materials, The University of Manchester, Grosvenor Street, Manchester M1 7HS, UK

Received 19 December 2005; received in revised form 13 February 2006; accepted 21 March 2006

Abstract

A three-dimensional mechanical model for intergranular crack propagation is presented. The model follows the spirit of existing percolation-like models but offers the inclusion of mechanical effects. This is necessary in order to account more accurately for the crack driving force and the effect of crack bridging ligaments, observed experimentally to be formed by fracture resistant boundaries. The model uses a regular representation of the material's microstructure and a categorisation of grain boundaries as beneficial and detrimental to fracture. This categorisation makes the model applicable to assessing material's resistance to intergranular stress corrosion cracking. The model mechanical behaviour is consistent with experimental observations and demonstrates its capability of simulating the development of bridges in the crack wake as well as crack coalescence. Results show that increasing the fraction of resistant boundaries increases the degree of crack tip shielding developed. This is expected to increase the resistance to stress corrosion crack propagation. The model offers a significant reduction of the computational resources usually needed to simulate intergranular propagation.

Keywords: Stress corrosion cracking; Microstructure; Grain boundaries; Fracture; Crack bridging; Finite element analysis; Stainless steels

1. Introduction

Intergranular stress corrosion cracking (IGSCC) is a mode of crack propagation in susceptible stainless alloys, such as nickel-based alloys and austenitic stainless steels used in structural components in the power generation industry. Uncertainties in short crack behaviour contribute substantially to the hazard in assessing the lifetime of such components. One source of uncertainty is the material's microstructure, which determines the resistance to IGSCC to a large extent. For the materials mentioned, a great deal of experimental evidence is now available which shows that the random grain boundaries form paths of low resistance for intergranular corrosion cracks to follow, while the special grain boundaries, such as twin boundaries, have improved resistance to corrosion and cracking. One of the first reported results in this respect, due to Palumbo and Aust [1], was for pure nickel. Later, Lin et al. [2], Pan et al. [3] and Alexandreanu et al. [4] provided evidence for the nickel-based alloys 600 and X-750. In addition to nickel-based alloys, Bruemmer and Was [5], and Gertsman and Bruemmer [6] demonstrated these properties of the grain boundaries for type 304 and type 316 stainless steels. These findings justify to a great extent a classification of the grain boundaries in a microstructure into two categories – "resistant" and "susceptible" to intergranular corrosion and cracking. This is a useful assumption for fully sensitised stainless steels, in which the grain boundary structure controls the degree of carbide precipitation. This locally reduces the grain boundary chromium content, and thus lowers its corrosion resistance. In other intergranular corrosion systems, and partial sensitisation of stainless steels, a spectrum of boundary properties develops. The concept of grain boundary engineering, introduced by Watanabe [7], had a primary goal to improve the microstructure resistance to intergranular failure by increasing the fraction of special boundaries. As a consequence, the resistance to IGSCC is also expected to improve. The binary classification of the grain boundaries allows for a percolation approach in

* Corresponding author. Tel.: +44 1613063556; fax: +44 1613063586.
E-mail address: andrey.jivkov@manchester.ac.uk (A.P. Jivkov).

0927-0256/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.commatsci.2006.03.012

studying the overall resistance of a microstructure to IGSCC and estimating the impact of grain boundary engineering. For example, by percolation simulations the size of the susceptible boundary paths for a given microstructure and the threshold fraction of resistant boundaries required to interrupt the percolating network can be determined [8]. Palumbo et al. [9] proposed a geometric model for assessing IGSCC susceptibility that was based on the probability of assembling a critical length of susceptible boundary path. This model used a two-dimensional (2D) hexagonal representation of the microstructure and a binary classification of the grain boundaries. Since then, a number of improved 2D hexagonal percolation-like models have been proposed (e.g. [10–12]). The improvements reflect the increase in understanding of grain boundary character distribution and the classification of the boundaries in a microstructure (e.g. [13,14]), as well as the role of topological constraints on the grain boundary networks (e.g. [15,16]).

While the improved percolation-like models address important features of the microstructure, a common drawback for all of them is that they do not account for the mechanical component of IGSCC, namely the crack driving force, which can vary during crack evolution. It should be mentioned that some of the percolation-like models consider the grain boundary orientation with respect to the applied load in the decision for further percolation, but the account for the mechanical component is limited to this. The true development of the crack driving force is clearly of importance. For example, crack branching, observed experimentally [1–6] and in model simulations [9–12], would reduce the driving force for the main crack. In microstructures with certain fractions of susceptible boundaries this may even lead to crack arrest when a percolation path would be still available. Another factor for crack driving force reduction is found in experimental observations by Marrow et al. [17] and Engelberg et al. [18] showing that the non-sensitised special boundaries encourage crack bridging ligament formation. The non-sensitised boundaries responsible for bridging are associated with twin growth [19]. These bridging ligaments are expected to retard crack propagation and, together with the effect of branching, possibly lead to crack arrest. This cannot be assessed on the basis of the percolation-like models. Jivkov et al. [20] proposed a mechanical, finite element based, model for studies of IGSCC in 2D hexagonal microstructures, capable of simulating bridging ligament formation and thus mimicking the real three-dimensional behaviour. The model results demonstrated the significant impact of the mechanical load, branching and bridging on the developed crack lengths and critical thresholds of resistant boundary fractions when compared to percolation-like models predictions. Essential to the mechanical model are the failure properties of the susceptible and the resistant boundaries. Experiments have shown that susceptible boundaries fail by stress corrosion at crack opening displacements of the order of several nanometres without noticeable development of inelastic deformation (e.g. [21,6]), and the bridges formed by resistant boundaries develop significant plasticity prior to rupture [17,18]. These observations set limits to the model parameters representing the failure properties of the resistant and susceptible boundaries. Parametric studies reported by Jivkov et al. [22] can be used for experimental identification of these parameters by comparing fractured and bridged areas, as well as crack opening displacements and bridge elongations.

Cracks are three-dimensional (3D) features however, and although the proposed mechanical model for 2D simulations is found to be consistent in terms of mechanics, and can qualitatively reproduce experimentally observed behaviour, its results cannot be directly translated to three dimensions [22]. A few 3D percolation models have been discussed in the past, such as Lim and Watanabe [23], Lehockey et al. [24], and Frary and Schuh [25]. All these use a regular representation of the microstructure with a unit cell, called truncated octahedron. With six squares and eight regular hexagons for boundaries, the truncated octahedron offers the closest to reality coordination with the neighbouring grains and allows regular tessellation of the 3D space. A computational mechanical model for 3D IGSCC propagation is proposed in this work, based on the regular representation of the microstructure with truncated octahedra. Unlike the percolation-like models, this mechanical model allows assessment of the influence of branching and bridging on the crack driving force. Using finite element calculations of the stress after each change in geometry due to crack advance, the model offers a more accurate simulation of crack evolution, because the crack advance depends upon the actual mechanical conditions at the crack tip. Selected simulation results for crack propagation and cracks coalescence are presented. These are obtained for fractions of resistant boundaries that have been experimentally determined in an as-received and grain boundary engineered austenitic stainless steel [18]. In the range of the fractions allowed and for the boundary conditions considered, crack arrest is found to be improbable in the model, but the effect of crack bridging on the crack driving force demonstrated is expected to reduce the kinetics of crack propagation.

At present the model does not account for the kinetics of crack propagation and should be viewed as an advance from the percolation-like models by including mechanical effects. In this sense it is a tool for assessing the relative microstructure resistance to intergranular fracture. Applied to IGSCC the model is relevant only to fully sensitised materials, similarly to percolation-like models. It should be appreciated, however, that the proposed model allows for the incorporation of the dependence of propagation kinetics on the local mechanical fields and this is a topic of ongoing work.

2. Model description

The computational framework for simulating intergranular stress corrosion crack propagation proposed in this