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A Markov Chain–Monte Carlo model for intergranular stress corrosion crack propagation in polycrystalline materials

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ABSTRACT

A model for intergranular stress corrosion crack propagation in polycrystalline materials has been proposed which overcomes several limitations of the currently available model in the literature for this purpose. Markov Chain theory and Monte Carlo simulations have been combined to predict the maximum crack lengths for different grain boundary character distributions. The effects of grain boundary orientation with respect to the stress axis, frequent and sporadic crack-branching, crack-turn, multiple crack nucleation sites, grain shape, and variable vulnerabilities of the same type of grain boundaries along the depth of the materials on the final crack-length have been investigated.

It has been found that the percolation threshold reported in the literature for honeycomb structure is not valid when the boundary inclination with respect to the stress direction is considered. Incorporation of realistic type crack-turn suggests that, although crack-turning increases the crack length, especially, when the fraction of vulnerable boundaries is relatively high, it is, by no means, as significant as crack-branching or multiple crack initiations in a given microstructure. It has also been observed that infrequent crack-branching, a common occurrence in intergranular stress corrosion cracking of polycrystalline materials, can decrease the crack length to a great extent, indicating that assuming a branching probability of 1 can overestimate the possible intergranular crack length for a given grain boundary character distribution. On the other hand, increased vulnerabilities of different types of grain boundaries with the depth of the material can lead to percolation, which is otherwise unpredictable.

1. Introduction

Susceptibility of polycrystalline materials to intergranular damage has been identified as one of the major obstacles in producing alloys with superior fracture toughness. One classic example of such failure is intergranular stress corrosion cracking (IGSCC) which is the predominant fracture mode in steels used in the pipelines, austenitic stainless steels and nickel based alloys used in the nuclear reactors, etc. (see e.g. [1–6]). Besides IGSCC, several other failures of polycrystalline materials such as, hydrogen induced cracking [7], liquid–metal embrittlement [8], fatigue [9], cold-work embrittlement [10], etc. also tend to choose the weak grain boundary network. In this paper, however, we will focus on the IGSCC of polycrystalline materials which has long been an issue of serious concern in many industrial applications and often regarded as one of the most challenging materials engineering problems [11], although the model that will be presented here can easily be adapted to other types of intergranular cracking as well.

It has been experimentally found by Liu et al. [12] that the local microstructure, in particular, the grain boundary character, plays the most dominant role in the intergranular stress corrosion cracking process. Watanabe [13] introduced the concept of *grain boundary engineering* to improve the fracture toughness of polycrystalline materials based on the experimental evidences that not all the boundaries in a polycrystalline material are alike. Low angle boundaries (*LAB*), defined as boundaries having misorientation angle less or equal 15°, and special coincident site lattice (*CSL*) boundaries, forms when lattice sites coincide between the two neighbouring lattices, are usually fracture resistant due to their low energy configurations while, the random high angle boundaries (*HAB*), classified as boundaries having misorientation angle greater than 15° and do not belong to the special CSL boundaries, have the opposite characteristics (see e.g. [13–20]). It implies that, the more the fractions of *LAB* and special *CSL* boundaries, the less prone the material is to cracking. However, it is virtually impossible to have materials with 100% *LAB* and *CSL* boundaries due to the limitations in the manufacturing technique. Nevertheless, if the crack propagation behaviour is correctly indexed and under-

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stood, it is possible to determine the minimum fraction of such fracture-resistant boundaries required to avoid the failure with reasonable accuracy. It should be pointed out here that, not only the fraction of these boundaries, but also their spatial distribution is important. In addition, boundary inclination with respect to the stress axis determines the vulnerability of different types of grain boundaries, i.e. a particular type of grain boundary may be susceptible to cracking when it is favourably oriented, relative to the loading direction, but, the same boundary could be resistant to cracking when it is unfavourably oriented (see e.g. [21,22]). Some inherent characteristics of IGSCC propagation in a polycrystal, e.g. multiple crack nucleation sites, frequent or sporadic nature of crack-branching, crack-turn, increased vulnerability of the same type of grain boundary with the depth of the material, etc., also pose additional complexities in estimating the crack-length for a given grain boundary character distribution. The complex interplay among the factors that influence the crack propagation process coupled with the large number of possible spatial distributions of grain boundaries make it extremely difficult to experimentally predict the crack-propagation behaviour in a given material that is statistically valid. Computer modeling can overcome this limitation to a large extent. By doing computer experiments, taking into account the characteristics of intergranular cracking and susceptibilities of different types of grain boundaries, it is possible to assess the intergranular crack propagation resistance of a given material for different grain boundary character distributions.

Several models have been proposed in the literature to predict the intergranular damage propagation in polycrystalline materials. Lim and Watanabe [23,24] proposed two- and three-dimensional geometrical models to assess the fracture toughness of polycrystalline materials by taking into consideration the grain shape, grain boundary character, and the orientation of grain boundary plane with respect to the stress axis. Fracture toughness was found to have significantly increased when the fraction of special boundaries was higher and, when the grains were mainly elongated towards the stress direction. They also studied the non-random spatial distribution of grain boundaries and showed that toughness increases noticeably when higher fraction of low energy boundaries are aligned towards the direction perpendicular to the loading axis.

Palumbo et al. [25] utilized a simple probabilistic model to assess the intergranular damage resistance by considering the fraction of special grain boundaries and average grain size for equiaxed hexagonal polycrystals. The model was used to predict the distance required in arresting 99% of the cracks. Lehockey et al. [26] formulated a similar probabilistic approach to predict grain dropping due to intergranular corrosion as a function of fraction of special grain boundaries and showed that the depth of grain dropping reduced significantly with the increase of the fraction of low energy boundaries. Gertsman et al. [27,28] also applied the modeling concept proposed in [25] to predict the intergranular crack propagation length, however, they considered, additionally, the misorientation relationship between the adjacent grain boundaries by taking the triple junctions (TJ, defined as the point where three grain boundaries meet) as "unit cell" for calculation instead of treating the grain boundaries separately. The latter approach was based on the idea that certain grain boundary correlations might exist in a microstructure and similar types of grain boundaries tend to link together [29]. The developed model was mainly for fcc materials that exhibit large fraction of twin boundaries but could be extended for other materials as well.

A number of researchers [30–33] used the percolation (or, percolation-like) model, a mathematical model that predicts the pass-through vulnerability of a grain boundary network. The percolation threshold for two-dimensional honeycomb structure is 0.6527 [34], if boundary inclination with respect to the stress direction is not considered, that is, if the fraction of vulnerable boundaries is greater or equal to 0.6527, there exists a path for the crack to reach the other side of the microstructure. Percolation threshold for three-dimensional Kelvin's tetrakaidecahedron, alternatively known as truncated octahedron, was also determined by Wells et al. [30], through Monte Carlo Simulations, and found to be 0.23 ± 0.01, if one-dimensional crack path is considered. The predicted value agreed reasonably well with their experimentally determined percolation threshold of IGSCC in sensitized AISI 304 stainless steels. The percolation-like models were further advanced by Jivkov et al. [31,32] by incorporating the mechanical crack driving force into the model.

Pan et al. [35] pointed out that the Percolation theory has the drawback of generating a crack where the previous grain boundary was not necessarily cracked which is not the case in reality for IGSCC. They proposed Markov Chain model, assuming no crack-turn, to simulate the IGSCC in austenitic alloys. Later, Gertsman and Tangri [11] proposed a Markovian–Percolation model to account for the crack-turn and illustrated that multiple crack nucleation sites and crack-turn can increase the crack length to a great extent. They also demonstrated that certain crystallographic orientation and development of multiple twinning can increase the intergranular crack propagation resistance for the materials that are susceptible to annealing twinning.

Even though extensive modeling efforts were expended in the literature, as evident from the above review, to predict the intergranular crack propagation behaviour in polycrystalline materials, these models have their own limitations. For example, the geometrical models proposed in [23,24] are not capable of allowing crack-branching and multiple crack nucleation sites because crack-movement was restricted to one grain height; models described in [25,27,28] could only predict the crack-length before certain number of cracks get arrested but not all of the cracks; the limitation of the percolation theory has already been mentioned (a comprehensive list of other limitations of the percolation model can be found in [27]); vulnerability variations of grain boundaries due to their alignment with respect to the stress axis and crack-turns, two essential features of IGSCC, was not considered in [35]. The model proposed by Gertsman and Tangri [11] overcame some of the above limitations but the effect of stress direction was not considered in that study which is a major shortcoming. In addition, their model took crack-turn into account but the condition for crack-turning, to our understanding, was rather imposed than real. Crack, in their model, could turn anytime whenever it finds a *HAB*, even when a forward boundary is available for the crack to continue propagating. Crack-turn usually occurs when the forward boundaries are resistant, a *HAB* boundary is available for such turn and, each crack-segment does not continue breaking boundaries more than once in the backward direction before moving forward. Besides, the algorithm of their model suggests that dynamic display of crack-propagation is not possible because accommodating crack-turn can allow the crack propagation through the boundaries that were already cracked. The re-cracking phenomenon will be discussed later in Section 2.2.

In this paper, a new modeling approach, based on Markov Chain theory and Monte Carlo simulations, of intergranular crack propagation in polycrystalline materials is proposed, assuming equiaxed hexagonal shaped grains, which can take into account the characteristic features of intergranular cracking, grain boundary inclination with respect to the stress axis and numerous possible spatial distributions of the grain boundaries for a given grain boundary character distribution. Realistic type crack-turn is incorporated in the model and dynamic display of crack-propagation is made possible by modifying the algorithm for computer modeling. Although equiaxed hexagonal grains are considered, the effect of grain shape was also investigated by suitably manipulating the spatial distribution of different types of grain boundaries and, changing the stress direction. In addition, the model can take the grain boundary character