A 2D mesoscale model for intergranular stress corrosion crack propagation

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Abstract

A mechanical model for simulating intergranular stress corrosion cracking is presented. The model has been developed to address the limitations of percolation-like models, which do not account for the mechanical crack driving force and cannot capture experimentally observed phenomena such as the formation of ductile bridging ligaments by resistant boundaries. The model is based on a regular representation of the material's microstructure and a categorisation of grain boundaries as susceptible and resistant to corrosion. Crack propagation in 2D microstructures with several fractions of experimentally observed susceptible boundaries is studied. Monte-Carlo type simulations with random distributions of boundaries and a range of susceptible and resistant boundaries failure strengths are performed. The effects of crack bridging and crack branching are quantified. It is concluded that together with the fraction of susceptible boundaries, the resistant boundaries failure strength is the significant parameter controlling the shielding effect of bridges on crack propagation.

Keywords: *Grain boundaries; Fracture; Finite element analysis; Stainless steels; Stress Corrosion Cracking.*

1. Introduction

It has increasingly been realised during the last two decades, that the grain size is not the only meso-scale factor influencing the strength of polycrystalline materials. Two other factors have been brought to wider attention. The first is the grain boundary character distribution (GBCD) which describes the fractions of boundaries with different energies, with “special” or low-energy boundaries having higher resistance to intergranular degradation mechanisms and “random” or high-energy boundaries having lower resistance. The second factor is the topological connectivity of “random” boundaries. In connection to these findings, the concept of grain boundary engineering has been introduced by Watanabe [1]. The primary purpose of grain boundary engineering has been to improve the bulk mechanical properties of polycrystalline materials by increasing the number of “special” or low energy boundaries. Together with applications to enhance general fracture toughness [2, 3], it has been shown that the “special” grain boundaries can be much less susceptible to intergranular corrosion and stress corrosion cracking (SCC) [4, 5].

Predictive stress corrosion cracking models aim to determine the probability of crack arrest and distribution of arrested crack lengths for given grain boundary network characteristics. Previously proposed models [6-8] used a percolation-type process to determine the probable extent of crack growth. These are binary models, i.e. a grain boundary is assumed to be either entirely resistant or entirely susceptible to SCC. In the early models [6], the probability of crack advance at a junction is based on the GBCD and orientation of the grain boundary with respect to the applied stress. Later models [7,

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8], additionally account for the network connectivity via the distribution of triple junctions. All these models, however, lack a way to describe the effects of the applied stress magnitude or stress redistribution during crack evolution. Hence, they stand close to a pure geometrical percolation model, giving the critical share of “random” boundaries above which a continuous crack path across a given microstructure is always possible. Previous models also cannot account for the experimentally observed crack bridging behaviour, see Fig. 1. Bridging is created by the yielding of ductile ligaments, formed by resistant boundaries left behind the advancing crack front in the real 3D geometry. A recently proposed analytical model [9], has attempted to take into account the effects of crack bridging on the local crack tip stress intensity factor, thus mimicking 3D crack behaviour.

All the percolation type works mentioned above use a regular representation of the material microstructure. Regular 2D models must choose either a square or hexagonal cell structure. The higher coordination number in hexagonal meshes is more representative of material microstructure, so this has been the standard unit cell in the previous percolation-like models. For the hexagonal cell structure, the critical share of susceptible boundaries, i.e. the percolation threshold, is found mathematically to be around 0.65 [7]. Below this value, a crack will not necessarily percolate through the structure. The fraction of susceptible boundaries can be reduced by grain boundary engineering, through thermo-mechanical processing. Adopting the most widely used regular representations of microstructure in 2D, the principle aim of this work was to develop two-dimensional mechanical models for intergranular crack propagation in thermo-mechanically processed microstructures under the influence of applied stresses. The idea was to establish a finite element model of the microstructure chosen, and use it for calculations of the stress after each change in geometry due to crack advance. This approach allows for a more accurate simulation of crack evolution, as the probability of crack advance depends upon the actual mechanical conditions at the crack tip. These conditions are affected by the crack propagation history, i.e. the effects of crack branching, crack bridging and redistribution of the initial stress state could be accounted for in a natural manner. This is viewed to be a necessary precursor to the development of three-dimensional modelling, which is the ultimate goal of this work [10]. At present the model is relevant only to fully sensitised materials and the kinetics of crack propagation are not taken into account. Therefore, the proposed model should be viewed as an advance to the percolation-like models by including mechanical effects. In this sense, in the same manner as the percolation-like models, it is a tool for assessing the relative microstructure resistance to intergranular fracture that is applicable to intergranular stress corrosion cracking, rather than a model for SCC. 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 model of intergranular crack propagation in a material microstructure used in this work has two levels of abstraction – physical and computational. These are described briefly in the following two subsections. A third subsection is devoted to the computational strategy of crack advance adopted.

2.1. Physical level

At the physical level, the microstructure geometry is represented as a regular tessellation of space into identical cells, where each cell corresponds to one material grain. The assumptions concerning grain geometry, grain boundaries character and properties and material's failure are as follows:

- Grain geometry
Grains are assumed to be identical in shape and represented by regular hexagons. With the grain geometry assumption, a region of a polycrystalline solid is approximated by an assembly of identical cells. A major geometrical parameter is the unit cell diameter, D .
- Grain boundary characters
Grain boundaries (the common faces in the assembly of cells) are assumed to belong to either of two classes. The first class is formed of the special (i.e. low-angle, low-energy) grain boundaries, which are generally accepted as resistant to corrosion. The second class includes the random (i.e. randomly oriented high-angle, high-energy) grain boundaries, which are accepted as susceptible to corrosion. The fraction of susceptible boundaries (the number of susceptible over the total number of boundaries), f , is a major parameter in the current studies. The distribution of susceptible boundaries is randomly assigned for given f .
- Material failure and grain boundaries properties
Material is assumed to fail via the crack propagating along grain boundaries only. In the present model, the kinetics of the stress corrosion mechanism are not accounted for, so the real time dimension of crack propagation is not determined and crack velocities are not calculated. In principle, the model could be developed to include kinetic factors, however. Experimental observations of intergranular stress corrosion show that susceptible boundaries fail at crack opening displacements of the order of several nano-meters with insignificant inelastic deformations [11]. This suggests that the failure strain of the susceptible boundaries, denoted by ε_{sf} , is around or below the apparent material yield strain, ε_y . The failure strain ε_{sf} is a second model parameter. Resistant boundaries, in contrast to the susceptible boundaries, can yield and rupture well into the inelastic region, as demonstrated by in-situ high resolution tomographic and fractographic observations of intergranular stress corrosion cracking [12]. Therefore, resistant boundaries in the model are allowed to fail after a significant amount of accumulated inelastic strain, denoted by ε_{rf} and defining a third model parameter. This failure strain is assumed to be a fraction of the material ultimate tensile strain, ε_u .

2.2. Computational level

A direct approach to model an assembly of cells in a finite element environment would be based on continuum mechanics. Each cell would have to be tessellated into available shapes of continuum elements and connected to the neighbouring cells with some interface elements, representing the grain boundaries. Such a direct modelling

strategy has so far only been used for an assembly with limited number of grains (for example, up to 50 grains in [13]) as it requires an enormous amount of computer resources especially for 3D models. Therefore, at the computational level of modelling a discrete representation of the assembly was suggested. This is viewed as a good first approximation, while the continuum approach is left for the future as more computational power becomes available.

In the discrete model, each cell is represented as a geometrical point and its connections to the neighbouring cells, which are the grain boundaries in reality, are represented by structural members of linear extension. The idea is illustrated in Fig. 2, where a portion of a plane hexagonal mesh and its corresponding structure are shown. The finite element model consists of nodes, placed in the centres of the grains, and beam-type finite elements for structural members. Thus, the grains deformability is transferred to the deformability of the adjacent beam elements. The discrete representation leads to a significant reduction of the nodes and elements in a model and hence of the computational effort. Essential to the discrete model is the question of how well it represents the solid behaviour. This question is connected to the selection of elements cross sections and elastic properties. Since the regular geometry introduces preferential directions in the assembly, it is generally impossible to make a selection so that the discrete assembly behaves as a continuum solid for all modes of deformation simultaneously. It is possible, however, to make such a selection for every particular deformation mode. In the present work, selections of beam cross sections are made so that the assembly in question, when subject to tensile deformation in the elastic range, behaves like a solid under the same deformation. All elements have identical modulus of elasticity and Poisson's ratio.

The assumptions for the mechanical properties of the modelled polycrystalline solid and the beam elements of its discrete representation are as follows:

- Solid mechanical properties
The macroscopic mechanical properties are those of grade 304 austenitic stainless steel. The constitutive relationship chosen is elastic-plastic with linear isotropic hardening, which for the purposes of this work describes sufficiently well the stainless steel behaviour. The parameters involved in the constitutive description are Young's modulus, $E = 206$ GPa, Poisson's ratio, $\nu = 0.3$, yield (proof) strength, $\sigma_y = 205$ MPa, yield strain $\varepsilon_y = 0.002$, ultimate tensile strength, $\sigma_u = 515$ MPa and ultimate tensile strain (elongation) $\varepsilon_u = 0.4$.
- Beam elements mechanical properties
Beam elements are ascribed the same mechanical properties as for the solid for the finite element solution. However, in the course of crack propagation, the beams representing susceptible boundaries would fail upon reaching their prescribed failure strain ε_{sf} , which is a fraction of the material yield strain ε_y , while the beams representing resistant boundaries would fail upon reaching their prescribed failure strain ε_{rf} , which is a fraction of the material ultimate tensile strain ε_u . This behaviour of the beam elements is shown schematically in Fig. 3. The average strain, i.e. the strain in the centre of the cross section in beam elements is used in the calculations.

2.3. Crack advance strategy

The strategy for crack advance in the computational model relies on a series of finite element solutions for equilibrium of the (evolving) assembly with the applied loads. Each solution provides the stresses and strains at the grain boundaries (midpoints of the beam elements), necessary to decide upon further crack propagation. If the failure strain of a grain boundary, being either resistant or susceptible, is reached, that boundary is a candidate for failure. In general only one boundary, the most critical, is allowed to fail at a time, i.e. one beam element is deleted from the discrete structure. As every failure event leads to redistribution of stresses and strains that cannot be judged in advance, the single-failure strategy ensures that the recalculated equilibrium will deliver the correct stresses and strains for the subsequent event. Strictly speaking, while the crack is advancing the mechanical equilibrium found by finite elements is physically unstable, and turns into physical equilibrium only at crack arrest.

The search for boundaries that are candidates for failure incorporates the possibility for bridge formation in the 2D settings. This is explained below, assuming a crack has grown to a certain stage and an equilibrium solution has been found for the corresponding discrete model. The approach to determine crack advance is illustrated in Fig. 4, where the current crack is shown with thick light grey lines, denoted by c , and all the boundaries that are in contact with the crack surface are shown in grey and are denoted by s . These surface boundaries are in direct contact with the corrosive environment, and are thus candidates for failure. In addition the subsurface boundaries, i.e. those in contact with surface boundaries, are shown in dark grey and are denoted by s' . The search for candidates for failure is performed first amongst the surface boundaries. For each of these boundaries, the difference between its calculated strain, ε , and its failure strain is obtained. Thus for susceptible boundaries this difference is $\delta = (\varepsilon - \varepsilon_{sf})$, while for resistant boundaries the difference is $\delta = (\varepsilon - \varepsilon_{rf})$. All boundaries with $\delta > 0$ are candidates for failure at the current solution step. If there are any such boundaries, the boundary with largest δ is accepted as being critical and the corresponding beam element is removed from the structure. The simulation then continues. If there are no surface boundaries with $\delta > 0$, the subsurface boundaries are considered. The reason to consider subsurface boundaries is to mimic the real 3D behaviour. For example, consider the boundary between point A and B in Fig. 3. If this was resistant, this would prevent it from failing at the current simulation step. In the real 3D situation the crack could pass from point A to point B via an out-of-plane path along susceptible boundaries. This places the subsurface boundaries adjacent to point B in contact with the environment, i.e. they become surface boundaries. The same possibility for by-passing the current surface boundaries exist for all of the sub-surface boundaries. Depending on the total crack geometry (not only the portion shown in the figure) the critical subsurface boundary could be either adjacent to point B, or adjacent to point C, or somewhere else. Therefore if the surface boundaries cannot fail at a given simulation step, all subsurface boundaries are reconsidered as surface boundaries and the same strategy for failing holds. If there are no candidates for failure among subsurface boundaries, the crack is assumed arrested and simulations are terminated.

The crack advance strategy, described above, is implemented by an in-house computer program written in Java. The program is responsible for creating the initial model and consecutively calling external equilibrium solver, ABAQUS [14], deciding upon crack advance from the equilibrium solution and changing the model if required.

3. Problem description

With respect to a fixed coordinate system (X_1, X_2) , the assembly of grains studied fills the solid rectangular region $\{-50D \leq X_1 \leq 50D, 0 \leq X_2 \leq 50D\}$. This region contains 7740 grains, which form 22850 internal grain boundaries, modelled by 7740 nodes and 22850 beam elements in the finite element model. An initial crack, extending along three grain boundaries, is introduced from the surface point at the origin of the coordinate system and running in towards the centre of the element assembly.

The load is symmetric and applied via prescribed displacements: $u_1 = -0.025D$ along the boundary $\{X_1 = -50D, 0 \leq X_2 \leq 50D\}$ and $u_1 = 0.025D$ along the boundary $\{X_1 = 50D, 0 \leq X_2 \leq 50D\}$. Displacements $u_2 = 0$ are prescribed along the boundary $\{-50D \leq X_1 \leq 50D, X_2 = 50D\}$, while zero stresses are prescribed for all other boundary conditions. This boundary conditions introduce a homogeneous strain in the assembly $\varepsilon_\infty = 5 \times 10^{-4}$, equivalent to a homogeneous stress $\sigma_\infty \approx 0.5\sigma_y$.

For comparative purposes the analytical stress intensity factor for a straight edge crack in a finite geometry has been used [15]:

$$K_I = F(\alpha)\sigma_\infty\sqrt{\pi a}, \quad (1)$$

where a is the crack length, σ_∞ is the remote tensile stress and $F(\alpha)$ is given by

$$F(\alpha) = 1.12 - 0.231\alpha + 10.55\alpha^2 - 21.72\alpha^3 + 30.39\alpha^4. \quad (2)$$

for parameter $\alpha = a / W$ with $W = 50D$. Eq. (2) gives an error of $\pm 0.5\%$ for $\alpha \leq 0.6$.

Computationally, the stress intensity factor is calculated in the way illustrated in Fig. 5, where a portion of the solid is shown. The actual crack is shown by a thick white line and a bridge along the crack path is depicted with grey. The corresponding straight, unbridged crack is also shown for comparison. The rectangle ahead of the crack tip shows the region that is accounted for in determining the stress intensity factor of the bridged crack. The possible crack tip plastic zone is dashed, while the rest of the rectangular region is taken to span over ten grains. For any given distance from the crack tip, r , with a step one grain diameter, a stress σ_{11} has been calculated by averaging the stresses in all grains along the line shown in the figure. The approximate relationship $\sigma_{11}(r)$ established by this method is then used to calculate the stress intensity factor via

$$\sigma_{11}(r)\sqrt{2\pi r} \xrightarrow{r \rightarrow 0} K_I^{FEM}. \quad (3)$$

A post-processing computer program has been developed to implement the computational procedure for determining the stress intensity factors. It delivers the stress intensity factor and the current crack geometry, including the number of bridges along the crack surface, after each step of the simulations. The bridges can be in the elastic regime or yielding plastically. In addition, the programme calculates the shielding effect of the bridges via the stress intensity factor that the bridges create with respect to the corresponding crack fronts. The contribution from all bridges, and the

fraction of this that is due to yielding bridges are obtained. The stress intensity due to all bridges is an algebraic sum of the contributions from every bridge, given by the formula:

$$K_{br} = F(\alpha)P \sqrt{\frac{\pi}{2r}}, \quad (4)$$

where P is the force in the bridge parallel to the loading (crack opening) direction, r is the distance to the corresponding crack front and $F(\alpha)$ is given by (2). Eq. (4) is the solution for a crack loaded in Mode I by a couple of symmetric concentrated forces of magnitude P placed on the crack surfaces at distance r from the tip [15]. The programme has been checked with straight cracks without bridges or branches (i.e. zig-zag cracks in the hexagonal microstructure) for the entire range of crack extensions between one grain and 25 grains. Comparison with theoretical values given by (1) and (2) showed identical results for the stress intensity factors to within 0.1%.

4. Results and discussion

One approach to understand the sensitivity of stress corrosion crack propagation to microstructure influences would be to develop a series of simulations with variable strengths of the susceptible and the resistant boundaries, together with a variable fraction of the susceptible boundaries in the assembly, random distributions of the boundaries within the assembly. The aim with such a series would be to answer the following questions:

- Do the observed resistant boundaries control crack growth by dissipating energy in plastic deformation, or are they just energetically unimportant remnants left by crack propagation?
- How does this answer change with the strength and fraction of susceptible and resistant boundaries?

The microstructures of interest are those which have been experimentally studied. These had susceptible boundaries fractions in the range $0.65 \leq f \leq 0.75$ [9][10].

Before commencing full-scale parametric studies in 2D, it was advisable to check if the proposed mechanical model could reproduce the existing results from percolation models. This has been reported in [16], where simulations with 2D geometry have been run for the full series of susceptible boundaries fraction, $0.1 \leq f \leq 0.9$ and for a number of susceptible boundaries failure strains, $\varepsilon_{sf} = 0, 0.1, 0.2 \varepsilon_y$. The resistant boundaries failure strain has been fixed at $\varepsilon_{rf} = 10\varepsilon_y$. For each fraction f , 30 different random distributions of the boundaries have been considered and results have been averaged over these random distributions to give a single value for the given fraction. The parameters that have been monitored are the projected crack length, denoted by a , and the total crack surface, i.e. main crack including branches and kinks, denoted by A . From the results presented in [16] it is evident that the role of mechanical strain is to direct the crack growth by decreasing crack branching and kinking compared to the percolation models. For a given fraction of susceptible boundaries, the crack arrest length determined by the 2D model with bridges is always smaller than the 3D percolation prediction and larger than the 2D percolation prediction. Any decrease of

the susceptible boundaries failure strain, ε_{sf} , leads to an increase of the arrest length, i.e. shift towards the 3D percolation prediction, as expected. Conversely, an increase of ε_{sf} shifts the arrest length towards the lower limit that is given by the 2D percolation prediction. This influence of ε_{sf} , however, is pronounced only for microstructures that are dominated by resistant boundaries, $f < 0.5$, and becomes insignificant for the microstructures of interest, these with $0.65 \leq f \leq 0.75$. In addition, ε_{sf} is a parameter that controls crack branching. This is also most pronounced for $f < 0.5$, and is not significant for microstructures with $0.65 \leq f \leq 0.75$.

Returning therefore to the microstructures of interest, Fig.6 gives an illustration of a crack grown in a 2D hexagonal microstructure with fraction of susceptible boundaries $f = 0.7$. The cracked boundaries are given with thick white lines. The thin and thick black lines show susceptible and resistant boundaries, respectively. The bridges formed in the crack wake by resistant boundaries are clearly identifiable. In the model for crack advance used here, a bridge can always form when a subsurface boundary is in a critical state, i.e. it is assumed that the real 3D microstructure will always allow by-passing of a resistant boundary. Strictly this cannot be always the case, as it depends on the fraction and distribution of susceptible boundaries in 3D. This means that a direct correspondence in the results from the present model and the 3D microstructure for a given f cannot be claimed. It is anticipated that results for given f obtained with the present model will correspond to a 3D microstructure with larger fraction of susceptible boundaries. Therefore a wider region of change has been adopted, namely $0.5 \leq f \leq 0.8$.

For the series of fractions $0.5 \leq f \leq 0.8$, with intervals of 0.05, simulations with different values of the variable $\varepsilon_{sf} = 0.1, 0.2, 0.3, 0.4 \varepsilon_y$ and fixed $\varepsilon_{rf} = 10 \varepsilon_y$, as well as simulations for three values of resistant boundaries failure strain, $\varepsilon_{rf} = 5, 10, 50 \varepsilon_y$, and fixed $\varepsilon_{sf} = 0.1 \varepsilon_y$ have been performed. For illustration, Fig. 7 gives the total number of bridges (a) and the number of yielding bridges (b) formed as the crack extends for the base case where $\varepsilon_{sf} = 0.1 \varepsilon_y$ and $\varepsilon_{rf} = 10$ and three selected fractions of susceptible boundaries. The number of bridges is normalised with the projected crack length in terms of number of grains, $L = a / D$, while the crack extension, a , is normalised with the total assembly thickness, W . Values for the total number of bridges (N_{total}/L) in Fig. 7(a) that are larger than 1.0 indicate that there are significant number of bridges formed not only along the main crack, but also along various crack branches. With increasing f , the number of branches decreases and N_{total}/L should become comparable to f . In theory, in the absence of branches, these two values must coincide, but this could be the case only if the crack has straight (zig-zag) geometry. In reality, with increasing f the crack has more opportunities to grow by kinking from the straight geometry and bridges form only when other possibilities are exhausted. This makes the value N_{total}/L smaller than expected on theoretical grounds, and this is visible in the curves for $f = 0.6$ and $f = 0.7$ in Fig. 7(a). Fig. 7(b) shows that the number of yielding bridges is much less dependent on the fraction of susceptible boundaries in the region of interest and is more controlled by the current crack extension. It should be noted that decreases in the number of yielding bridges in Fig. 7(b), reflecting in decreases in the total number of bridges in Fig. 7(a), indicate failures of yielding ligaments. These failures occur earlier, i.e. at shorter crack extensions, for larger fractions of susceptible boundaries, since the total number of bridges that are shielding the crack decreases.

Fig. 8 gives the evolution of the stress intensity factors with crack extension for the base case $\varepsilon_{sf} = 0.1 \varepsilon_y$ and $\varepsilon_{rf} = 10$ and four selected fractions of susceptible boundaries.

Crack extension, a , is normalised with the total assembly thickness, W . Stress intensity factors are normalised as depicted in the figure, where σ_∞ stands for the actual remote stress in the structure. As the load is applied via prescribed displacements, the actual stress depends on the current stiffness of the cracked assembly and is found from the finite element solution. With crack advance the remote stress decreases, by a factor of 8% for the stiffest structure with $f = 0.5$ to 18% for the most compliant structure with $f = 0.8$, in the interval of crack extensions shown in the figure. The stress intensity development is obtained through the stress results from finite element solutions using Eq. (3), while the theoretical value is calculated using Eq. (1). In the figure, K_{sh} , denotes the shielding effect of the microstructure, which includes not only the effect of bridges but also the effect of branches on the crack driving force reduction, as will become clear shortly.

The shielding effect is almost independent of the susceptible boundaries failure strain, ε_{sf} , but depends on the resistant boundaries failure strain, ε_{rf} , in the region of interest. This is demonstrated in Fig. 9, where the shielding stress intensity factor, K_{sh} , is plotted versus the susceptible boundaries fraction, f , for a selected crack extension, $a = 0.3W$, and for the series of failure strains of susceptible boundaries (a) and the series of failure strains of resistant boundaries (b). The stress intensity is normalised as in Fig. 8. The dependence on ε_{rf} comes from the larger contribution of bridges to the total shielding effect, which increases with the resistant boundaries failure strain.

To quantify the relative effects of branching and bridging on the total shielding effect, the crack driving force reduction solely due to bridges has been estimated. This was done by calculating the stress intensity factors using Eq. (4) and the stress results from finite element solutions. As an illustration, Fig. 10 presents the stress intensity factors due to bridges alone for the same grain boundaries properties and fractions as in Fig. 8. The normalising factors for the two axes of the plot are also the same.

Fig. 11 demonstrates the effects of all bridges (a), only the elastic bridges (b), and only the yielding bridges (c) for the particular values of grain boundary properties depicted. Bridging effects are shown as fractions of the total shielding effect. The effect of elastic bridges is a non-linear decreasing function of f , almost independent of ε_{rf} , while the effect of yielding bridges depends on ε_{rf} , and may turn into an increasing function of f , for sufficiently large ε_{rf} . Thus, in the region of interest for f , the yielding bridges provide the larger contribution to the crack shielding and this relative contribution increases with increasing f .

As a general observation from all the 2D simulations, the parameter controlling the effect of bridges is the resistant boundaries failure strain and the parameter controlling branching is the susceptible boundaries fraction. The effect of the susceptible boundaries failure strain is negligible in the region of interest for fractions of susceptible boundaries in the constraints of the model. The initial crack extension (pre-crack) and the applied load set a threshold for the susceptible boundaries failure strain above which the pre-crack cannot start propagating. For any value of the susceptible boundaries failure strain smaller than this threshold the cracks will propagate and will have the behaviour presented by the above results. Conversely, a fixed value of the susceptible boundaries failure strain will set a threshold on the applied load, below which the cracks cannot start propagating. It may therefore be considered to be a material/environment parameter.

5. Conclusions

The proposed discrete structural model has the potential to simulate intergranular crack propagation and crack coalescence in a realistic manner by including the phenomenon of crack bridging by ductile ligaments. It accounts for the effects of external load magnitude and the failure properties of susceptible and resistant boundaries. Crack arrest was not observed in the region of interest for susceptible boundaries fraction, but a significant degree of crack tip shielding was developed, which would be expected to reduce the crack propagation rate. Increasing the fraction of resistant grain boundaries is therefore predicted to increase the resistance of short cracks to intergranular stress corrosion cracking.

Any further refinement of the model requires that it be related to experimental observations of intergranular stress corrosion crack extensions and distributions to tune the model parameters. This is necessary in order to turn the model into a predictive tool. The first step is the identification of the susceptible boundaries failure strain, ε_{sf} , which is essentially a local criterion for stress corrosion crack advance. This could be estimated from experimental results without noticeable bridging. The influence of the bridging ligaments could then be determined, comparing the local crack driving force in the model with the stress intensity predicted theoretically for a non-bridged crack of the same geometry and applied load. Another tuning parameter is the failure strain of the resistant boundaries, ε_{rf} , which may be connected to twin thickness. This parameter could be estimated comparing experimental results showing failed bridging ligaments with model simulations.

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Figure captions

Figure 1. In-situ observation of the failure of a crack bridging ligament. a) and b) are successive images obtained by high resolution X-ray tomography of a propagating stress corrosion crack [9].

Figure 2. The discrete model for the 2D hexagonal structure.

Figure 3. Schematic illustration of the deformation and failure characteristics for susceptible and resistant boundaries.

Figure 4. Illustration of the search for failing boundaries in the model of crack advance for a crack tip located at point A.

Figure 5. Stress intensity factor calculation for the bridged crack in the finite element model, compared to a straight edge crack.

Figure 6. Example of a crack propagated in a microstructure with $f=0.7$.

Figure 7. Average number of bridges with crack extension: (a) all bridges (elastic and yielding) (b) yielding bridges only.

Figure 8. Stress intensity factor evolution with crack extension with variation in f .

Figure 9. Variation of shielding with boundary failure strain with fraction f : (a) The effect of susceptible boundaries failure strain; (b) The effect of resistant boundaries failure strain.

Figure 10. Bridging stress intensity factor evolution with crack extension with variation in f .

Figure 11. The contribution of bridges to the shielding effect: (a) all bridges, (b) elastic bridges only, (c) yielding bridges only.

Figure 1.

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