Simulation of Short Crack Propagation in a Microstructure Using a Hybrid Boundary Element Technique

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ABSTRACT. *Service life of cyclically loaded components is often determined by stage I-crack propagation, which is highly influenced by microstructural features such as grain boundaries. A 2D-model to simulate the growth of these short fatigue cracks is presented discretising the crack by displacement discontinuity boundary elements. They allow an opening and slide displacement of the crack flanks. The direct boundary element method is used to mesh the grain boundaries which only carry out absolute displacement. A superposition procedure allows to employ these different types of boundary elements in one model. Being enclosed by elements, individual elastic properties of the grains can be considered. Stress intensity factors are determined to verify the elastic model. To simulate short crack propagation the plastic deformation in front of a crack tip is modelled as slip on individual slip planes. Displacement discontinuity boundary elements which only allow a slide displacement mesh the activated slip band. Its length is limited by the distance between crack tip and grain boundary. In the neighbouring grain, stress increases while the crack tip progresses to the grain boundary. If a critical shear stress intensity is reached on a potential slip plane of the adjacent grain, this plane is activated and the plastic zone overcomes the boundary. Varying elastic properties influence the direction of maximum shear stress and therefore the highest loaded slip plane which is activated can differ. Furthermore a change in crack tip slide displacement determining stage I-crack propagation is observed.*

INTRODUCTION

The material of structural components is often cyclically loaded close to its fatigue limit. Service life of such components is determined by the propagation of microstructurally short fatigue cracks. Growth of these stage I-cracks occurs on single slip planes and strongly interacts with microstructural features such as grain boundaries. Therefore, the material cannot be treated as a continuum so that linear elastic fracture mechanics (LEFM) is not applicable to quantify the propagation behaviour of short cracks.

When the crack tip approaches a grain boundary, its propagation rate decreases and when overcoming the boundary, crack progress accelerates significantly resulting in an oscillating crack growth rate. Navarro and de los Rios [1] proposed an analytical yield strip model to describe this behaviour: Plastic slip ahead of the crack tip is blocked by the grain boundary. When a critical stress intensity on a dislocation source in the adjacent grain is exceeded, a slip band is activated and the plastic zone overcomes the grain boundary. This one-dimensional analytical crack growth model is extended in [2, 3] to take arbitrary two-dimensional grain geometries and crystallographic misorientations into account. Plastic anisotropy of the grains is considered as plastic slip only occurs on crystallographic slip planes. The model is solved numerically using dislocation discontinuity boundary elements to discretise the crack which lies in an infinite, homogeneous plate. Individual elastic properties of the grains are not taken into account.

In order to consider these properties each grain has to be enclosed by boundary elements. In contrast to the crack flanks performing relative displacements, the grains are firmly connected resulting in an absolute displacement of their boundaries. Satisfying these conditions, crack and grain boundaries need to be meshed by different types of elements. A superposition method is introduced allowing their use in one model.

SHORT CRACK MODEL

To employ two different types of boundary elements in one model, the problem of a crack in one grain is divided into two sub-problems [4] (Fig. 1). One sub-problem is the crack in an infinite plate (a), which is discretised by displacement discontinuity boundary elements. They are discussed in the following section and allow relative displacements of the crack flanks. The second sub-problem is the crack-free grain (b), whose boundaries are meshed using the direct boundary element method.

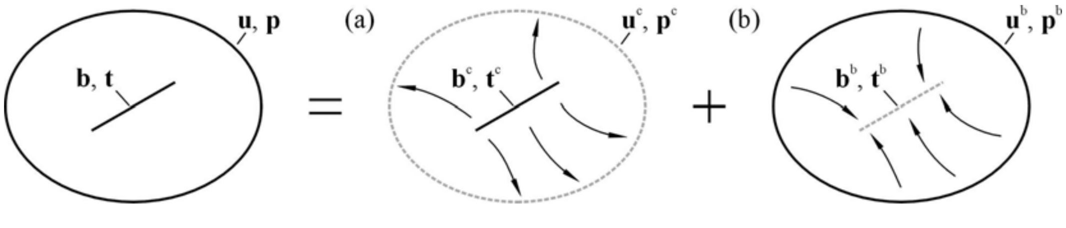


Figure 1. Superposition of a crack in an infinite plate and a crack free grain.

Displacement Discontinuity Boundary Elements

The model presented in this paper considers the crack on a single slip plane and allows a plastic deformation by slip on this plane. Crack and slip plane are assumed to be in an infinite plate and discretised by displacement discontinuity boundary elements allowing an opening and slide displacement of the crack flanks as well as sliding in the activated slip band. $\mathbf{b}^c$ represents the relative displacements, which are constant within one crack element. $\mathbf{t}^c$ is the stress acting on opposite faces of the crack surface. The relation between $\mathbf{b}^c$ and $\mathbf{t}^c$ is determined analytically [5] and stored in the influence matrix **C**.

$$\mathbf{t}^c = \mathbf{C} \cdot \mathbf{b}^c \tag{1}$$

Relative displacement of the crack surfaces causes a stress and displacement field in the infinite plate. The influences **D** and **F** from $\mathbf{b}^c$ on the stress $\mathbf{p}^c$ and the absolute displacement $\mathbf{u}^c$ along the imaginary grain boundaries are also obtained analytically [5].

$$\mathbf{p}^c = \mathbf{D} \cdot \mathbf{b}^c, \qquad \mathbf{u}^c = \mathbf{F} \cdot \mathbf{b}^c \tag{2), (3}$$

Dislocation discontinuity boundary elements allow an efficient modelling of cracks and activated slip bands but they are inappropriate to mesh grain boundaries. Enclosing the grains by boundary elements in order to consider the individual elastic properties of the grains, a different boundary element method is used and discussed as follows.

Direct Boundary Element Method

The grains of a microstructure are firmly connected. In the presented model, this is ensured by using direct boundary element method to discretise the grain boundaries. The elements only allow an absolute displacement; no opening or sliding. For an enclosed domain, stress $\mathbf{p}^b$ and displacement $\mathbf{u}^b$ on the boundary are linked by the influence matrices **G** and **H** [6]:

$$\mathbf{H} \cdot \mathbf{u}^b = \mathbf{G} \cdot \mathbf{p}^b \tag{4}$$

Stress along the imaginary crack line inside the enclosed domain is only a function of stresses and displacements on the boundary (Eq. 5).

$$\mathbf{t}^b = \mathbf{A} \cdot \mathbf{u}^b + \mathbf{B} \cdot \mathbf{p}^b \tag{5}$$

A and **B** are influence matrices.

Both sub-problems, the crack in the infinite plate and the crack-free grain, can be solved using the previous equations. Now the two methods are coupled in order to solve the total problem.

Superposition Procedure

In order to couple the boundary element methods discussed above a superposition procedure is used: Stress **t** along the crack as well as stress **p** and absolute displacement **u** on the grain boundaries of the total problem is the sum of the stresses and displacements of the two sub-problems [4].

$$\mathbf{t} = \mathbf{t}^b + \mathbf{t}^c, \qquad \mathbf{p} = \mathbf{p}^b + \mathbf{p}^c, \qquad \mathbf{u} = \mathbf{u}^b + \mathbf{u}^c \tag{6}$$

With the use of these compatibility conditions, Eqs. 1 to 5 are combined yielding Eq. 7 which contains the identity matrix **I** and the null matrix **0**.

$$\begin{bmatrix} \mathbf{H} & \mathbf{GD}-\mathbf{HF} \\ \mathbf{A} & \mathbf{C}-\mathbf{AF}-\mathbf{BD} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{b} \end{bmatrix} = \begin{bmatrix} \mathbf{G} & \mathbf{0} \\ -\mathbf{B} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{p} \\ \mathbf{t} \end{bmatrix} \tag{7}$$

This system of equations can be uniquely solved, if the boundary conditions are known. For an open crack, stress normal to its flanks is zero. Being closed, the crack flanks must not penetrate each other and relative displacement is zero. The crack flanks are assumed to be friction-free so that shear stress along the crack is zero. Domain boundary conditions depend on the external supporting conditions of the domain.

To model the plastic zone, elastic-ideal plastic material behaviour is considered. Due to this non-linear constitutive law, the previously described superposition principle does not seem to be applicable. But the following approach allows its use in a stepwise iteration: The activated slip band in front of a crack tip is discretised by dislocation discontinuity boundary elements. In a first calculation step sliding is suppressed in the slip band and shear stress is calculated for linear material behaviour. New boundary conditions are assigned to elements on which plastic shear stress is exceeded. Sliding is no longer suppressed but shear stress is set to the shear strength. The system of equations (Eq. 7) is resolved iteratively until plastic shear stress is no longer exceeded on any element. In each iteration step linear elastic material behaviour is considered so that the superposition procedure remains applicable.

The previously described method is only valid for a crack in one grain, however, a microstructure consists of many grains. Thus, a method to couple grains on their common boundaries is described as follows.

Coupling of Individual Grains

Once the superposition procedure has been carried out on each grain containing a crack all grains of a microstructure need to be assembled. As the grains are firmly connected the absolute displacement along a common boundary of two grains is equal for both of them. The stress state along this boundary also needs to be the same for the two coupled grains. Using this additional information for all boundaries of the grains under consideration allows to combine them to a microstructure.

Below, the presented boundary element method is applied to simple fracture mechanics problems. The results are compared to reference solutions for verification.

VERIFICATION

To verify the boundary element method discussed in this paper a tensile specimen with a horizontal crack is studied (Fig. 2). Stress intensity factors K_I are calculated and compared to a reference solution [7]. The modelled specimen is five times longer than wide. In this case the length has negligible influence on the stress field at the crack tip. Therefore the result can be compared to the reference in which the specimen length is infinite. The crack length 2a is half the specimen width 2w. Specimen boundaries and crack are discretised by varying numbers of boundary elements N. The influence of the mesh on

K_I compared to the reference solution is shown in Fig. 2. Here the relative error in K_I is plotted against the ratio of the number of crack elements N_{crack} (80, 120, …, 280 equally sized elements) by the number of elements along the specimen boundary $N_{boundary}$ (96, 120, 144 equally sized elements).

Figure 2 shows a decrease in error with an increasing ratio $N_{crack}/N_{boundary}$ which is mainly met by the meshing of the crack. Tending to zero, the curves prove convergence of the method.

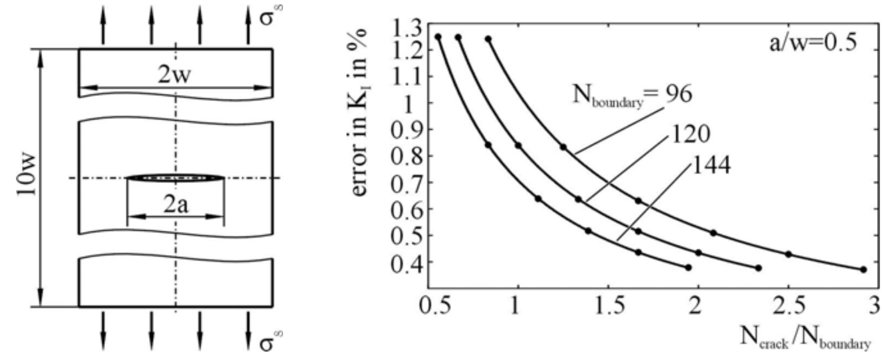


Figure 2. Tensile specimen with horizontal crack and verification results.

A second verification is carried out on a crack going through the interface of two bounded half planes of dissimilar media (Fig. 3). The ratio between Young's modulus E_1 and E_2 is given by Γ. As infinite half planes cannot be considered by this BE-approach, two domains are connected, which are large compared to the crack length. The crack is discretised by 200 elements and stress intensity factors are determined at crack tip B for different ratios of Young's modulus Γ. In Figure 3 the result is plotted against Γ and compared to a reference solution given in [7] showing good accordance. The errors are less than 0.35%.

The presented hybrid boundary element method is capable to solve fracture mechanics problems. In the following it is applied to simulate short crack propagation in a microstructure.

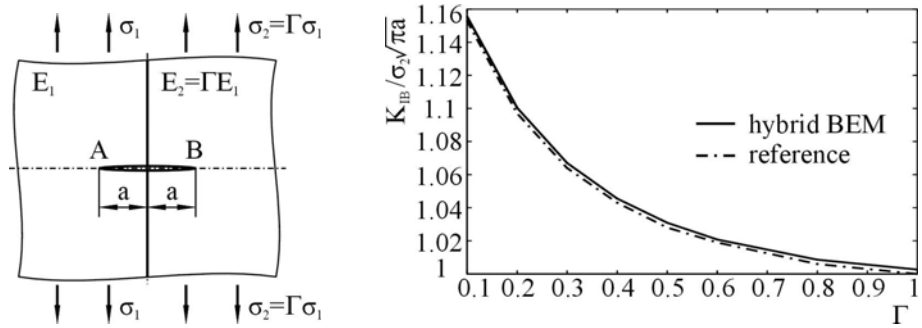
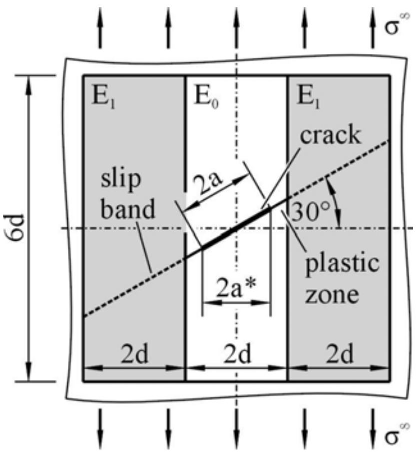


Figure 3. Crack going through the interface of two bounded half planes of dissimilar media and K_I results.

SHORT CRACK PROPAGATION IN A MICROSTRUCTURE

Simulation of short crack propagation is exemplarily shown in a very simple micro-structure consisting of three rectangular grains (Fig. 4). The Young's modulus E_1 of the grains left and right is equal but can be different from the Young's modulus E_0 of the grain in the middle. Poisson's ratio is the same for all grains being embedded in a large plate with the same elastic properties as the middle grain containing a crack. This crack lies on an activated slip plane of an angle of 30° to a horizontal line. Sliding occurs on this plane where the shear strength is reached. In the neighbouring grains, possible slip planes are present in the extension of the activated slip plane. Different simulations of stage I-crack growth are carried out to take different ratios of E_1 by E_0 into account.

At first the Young's modulus is identical for all grains E_1=E_0 and therefore the crack is in a homogeneous plate. In this case there is no need to discretise the grain boundaries; crack propagation is simulated in a large plate where the number of elements along the boundary of each grain is zero: N_{GB}=0. The range of crack tip slide displacement ΔCTSD between the maximum and minimum loaded state is evaluated as it determines short crack propagation. In Figure 4 results are plotted (in the dotted line) against the half projected crack length normalised by half the grain width.



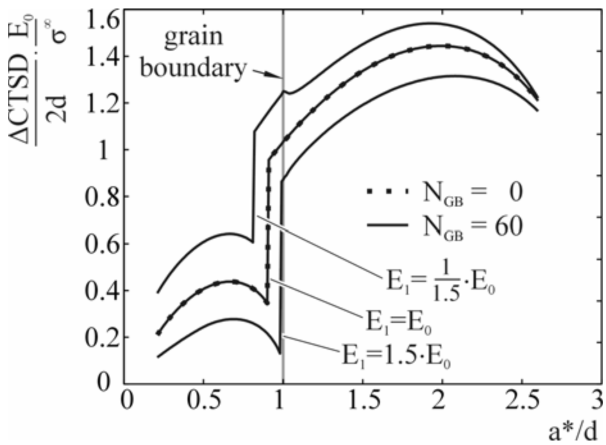


Figure 4. Crack in a microstructure and ΔCTSD results.

Starting from a very short crack length, ΔCTSD increases due to the advancing crack. It decreases when the crack tip approaches the grain boundary, which limits sliding on the slip plane. When overcoming a critical stress intensity the slip planes in the adjacent grains are activated and the plastic zone extends into the neighbouring grains. This causes a jump in ΔCTSD. It increases even more with the growing crack and then decreases due to the influence of the next grain boundary.

In another simulation the grain boundaries are discretised by N_{GB}=60 elements per grain but the Young's modulus is still the same for all grains. ΔCTSD is plotted (as a continuous line) in Fig. 4 showing no difference to the result before. The mesh does not have an influence on the outcome, proving that the superposition procedure can be applied although elastic-plastic material behaviour is considered in the slip plane.

To study the influence of varying elastic properties, Young's modulus of the grains left and right is chosen 1.5 times higher than of the grain in the middle ($E_1=1.5E_0$). Loading in the middle grain decreases as it is softer than the adjacent grains. Therefore ΔCTSD starts at a lower level. The critical stress intensity in the neighbouring grains to activate the slip bands is identical to the homogeneous case but is reached at a larger crack length. When the crack overcomes the grain boundary, the increase in ΔCTSD is less than before as the crack now grows in the stiffer grains. In another case the grain in the middle is 1.5 times stiffer than the adjacent grains. Here the critical stress in the neighbouring grains, which is still unchanged, is achieved at a lower crack length. When the crack - not only the plastic zone - overcomes the grain boundary, ΔCTSD decreases as crack propagation occurs in softer material with less loading.

A further simulation in this microstructure focuses on the stress field in the adjacent grain at the end of the plastic zone. Crack propagation is simulated in the middle grain, but no certain slip plane is considered in the neighbouring grain. The shear stress τ is evaluated in points on a circular arc with a small radius r_e at the end of the plastic zone (Fig. 5a). Here, the absolute value of shear stress is plotted against the angle φ under which the stress has been evaluated. Figure 5 (b) shows the evolution of maximum shear stress $|\tau_{max}|$ when the crack tip advances towards the grain boundary. The influence of varying elastic properties of the grains has been taken into account. At certain crack lengths depending on these properties, $|\tau_{max}|$ reaches a critical shear stress level τ_S. This indicates that the stress intensity is sufficient to activate a slip band which is aligned in the respective direction $\varphi_{(|\tau_{max}|)}$ of the maximum shear stress. Figure 5 (c) illustrates that the crack lengths leading to the activation of a slip band are linked with varying angles of maximum shear stress $\varphi_{(|\tau_{max}|)}$. If activation of differently aligned slip planes is possible in the neighbouring grain, varying elastic properties influence which slip plane is activated. As the crack follows the plastic zone, elastic properties of the grains play an important role determining crack paths.

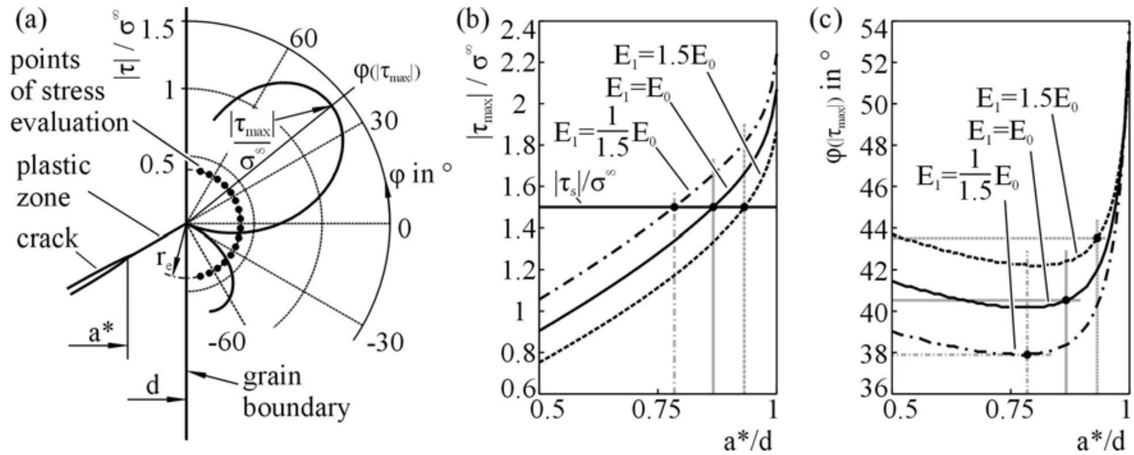


Figure 5. Evaluation of the stress field in the adjacent grain.

CONCLUSIONS

A two-dimensional stage I-crack propagation model has been presented that discretises the crack by dislocation discontinuity boundary elements and uses the direct boundary element method to mesh grain boundaries. A superposition procedure couples these different boundary element methods to employ them in one model. This model is capable to reproduce the oscillating growth rate of short fatigue cracks. Varying elastic properties of the grains are considered and their influence on short crack propagation is studied. A change in crack tip slide displacement determining crack propagation is observed. Furthermore, the shear stress field in a grain adjacent to a crack-containing grain is influenced. This stress field decides which of the diverse possible slip bands becomes activated when the plastic zone overcomes the grain boundary. The crack follows the plastic zone and therefore the crack path can vary. Thus, considering the individual elastic properties of the grains provides additional reliability to the prediction of crack propagation rates and crack paths.

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