Fatigue crack growth in the vicinity of a grain boundary modelled using a discrete dislocation technique

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Abstract. It is well known that the behaviour of short cracks differs from that of long cracks due to the relatively large plastic zone and strong influence from the surrounding microstructure, and for very low growth rates, it is important to account for discrete dislocations within the material. In this study, a discrete dislocation model is presented for the study of the growth behaviour of a short edge crack, located near a low angle grain boundary. The initial crack is situated within one grain and the developing plasticity in front of the crack is restricted to this grain and the next, adjoining grain. The fatigue crack is assumed to propagate in a single shear mechanism. The model is a combination of a discrete dislocation formulation and a boundary element approach, where the geometry is modelled by dislocation dipole elements and the plasticity by discrete dislocations. The influence from grain boundary character on the development of the plastic zone and, thereby, on the crack growth behaviour is investigated.

Introduction

It is well known that short cracks grow in a different way as compared to long cracks due to the relative large plastic zone and strong influence from the surrounding microstructure. In this paper, by the term short, we mean microstructurally short, of length in the order of the microstructure of the material. A number of experimental studies have shown that short cracks grow through a single shear mechanism, cf. Suresh [1], and that they grow at high rates at load levels well below the threshold value for long cracks. Therefore, such short cracks cannot be treated by the standard methods for long cracks at e.g. life predictions. As examples, studies performed by Uematsu et al. [2], show that short zigzag shaped cracks develop in silicon iron in the low K region, with K denoting the stress intensity factor, and Zhang [3] found that cracks grow along shear bands, created in front of the crack tip in ultra-fine grain sized aluminium.

For very low growth rates, in the order of a few Burgers vectors per cycle only, it is important to account for the generation and movement of discrete dislocations, describing the plasticity within the material. Riemelmoser et al. [4] and Riemelmoser and Pippan [5] developed a discrete dislocation model for a long mode I crack to study the cyclic crack tip plasticity and plasticity induced crack closure. A similar model has been developed by Bjerkén and Melin [6] to study the influence of grain boundaries on short mode I cracks.

In this study a discrete dislocation model, describing both the geometry and the plasticity by discrete dislocations, is used to study the growth of a short fatigue edge crack. The plasticity is in this study, restricted to two grains, separated by a low angle grain boundary, and the change in growth behaviour due to different low angle grain boundary configurations is investigated.

Statement of the problem

In this paper, the growth of a microstructurally short edge crack located within one grain, subjected to a remote fatigue loading, cf. Fig. 1, have been investigated under plane strain and quasi-static conditions.

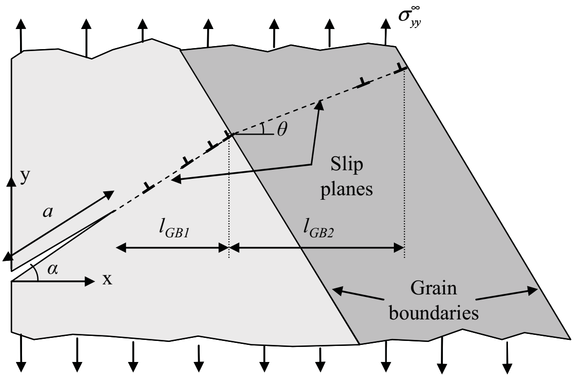


Fig. 1. Initial geometry of the short edge crack with grain configuration and slip planes marked by dotted lines within the two grains.

The crack is assumed to grow in a single shear mechanism as a result from nucleation, glide and annihilation of discrete dislocations from the crack tip along preferred slip planes in the material. The initial crack, of length a and inclined an angle α to the normal of the free edge, is located within a semi-infinite body. The fatigue load is applied parallel to the free edge and is varied between a maximum value, σ_{yymax}^{∞}, and a minimum value, σ_{yymin}^{∞}. Two neighbouring grains are considered, with parallel grain boundaries, perpendicular to the slip plane coinciding with the crack direction, and emanating from the crack tip. In this study, this slip plane is assumed to be the only active slip plane in the first grain. The grain boundary between the two grains is modelled as a low angle grain boundary, consisting of a number of evenly spaced dislocations of same size and direction of their Burgers vectors, placed along a straight line, cf. Fig. 2. Such a dislocation arrangement is stable, cf. Hull and Bacon [7], and the dislocations in the grain boundary are therefore treated as fix. The second grain boundary, at the end of the second grain, is assumed to be a high angle grain boundary consisting of a random dislocation structure, not contributing the overall stress field in the body. This grain boundary is treated as a dislocation barrier, which the dislocations cannot pass and, eventual, as a dislocations reaches this second boundary, it will be trapped in it. However, it will still contribute to the overall stress field in the body.

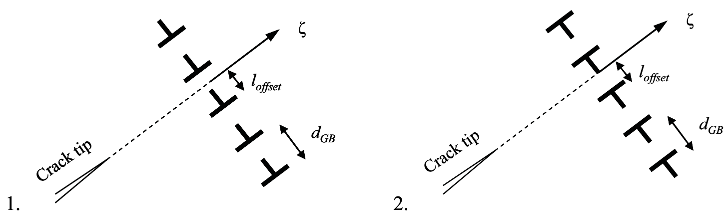


Fig. 2. Low angle grain boundary. 1. consisting of positive dislocations, 2. consisting of negative dislocations.

Initial conditions

The material in this study is pure iron, with a bcc crystal structure, assumed linear elastic. The material parameters are shown in Table 1, cf. Askeland [8], together with the geometrical data for the initial short edge crack seen in Fig. 1.

Table 1. Material data and geometrical data cf. Fig. 1.

Shear modulus, μ	80 GPa	Initial crack length, a	20000b
Poisson's ratio, ν	0.3	Crack angle , α	45°
Burgers vector, b	0.25 nm	Distance to grain boundary , l_{GB1}	5000b
Lattice resistance, τ_{crit}	40 MPa	l_{GB2}	5000b
Load range, σ^{∞}_{yymax} - σ^{∞}_{yymin}	200-40 MPa		

Discrete dislocation technique

The model used in this study rests on a discrete dislocation formulation, were both the geometry and the plasticity is described by discrete dislocations, as developed by Hansson and Melin [9]. Only plane problems are addresses and, therefore, only edge dislocations are used in the formulation. The external boundary, here defined as the free edge together with the crack itself, is modelled by dislocation dipole elements. Such an element consists of two glide dislocations and two climb dislocations, with pair wise equal size but opposite direction. Using both climb and glide dislocations makes it possible to model both the opening and the shearing between the crack surfaces as well as the shape of the external boundary. The dislocations of a dipole element are situated at the end points of the element, and the stresses in the element are calculated at the element collocation point, at the centre of the element, marked CP in Fig. 3.

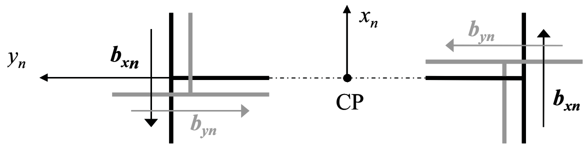


Fig. 3. Dislocation dipole element consisting of four edge dislocations. The climb dislocations are black and the glide dislocations grey. CP denotes the collocation point at which the stresses are calculated.

The stresses at an arbitrary point within the material are calculated as the sum of the stress contributions from the dislocations describing the plasticity, the dislocations forming the dipole elements, the dislocations describing the low angle grain boundary and the applied external load. The magnitudes of the dipole dislocations are determined from an equilibrium equation, Eq. (1), describing the normal and shear stresses along the external boundary. The normal and shear stresses must equal zero along the free edge and the crack, assuming the crack to be open. This assumption makes it possible to calculate the magnitudes of the dipole dislocations.

$$\mathbf{G}\mathbf{b}_{\mathbf{boundary}} + b\mathbf{G}_{\mathbf{internal}} + b\mathbf{G}_{\mathbf{gb}} + \boldsymbol{\sigma} = 0 \qquad (1)$$

In Eq. (1) $\mathbf{G}$ is a matrix containing influence functions from the dipole dislocations, cf. Hills et al [10], giving the stress field from a dislocation, $\mathbf{b}_{\mathbf{boundary}}$ is a vector holding the magnitudes of the dislocations in the dipole elements, b is the Burgers vector of the material, $\mathbf{G}_{\mathbf{internal}}$ is a vector containing the influence functions for the dislocations describing the plasticity, $\mathbf{G}_{\mathbf{gb}}$ is a vector containing the influence functions for the dislocations constituting the low angle grain boundary and **σ** is a vector containing the contribution from the applied external load.

Dislocation nucleation and crack growth

In this paper, the only source for nucleation of new dislocations is the crack tip. Nucleation of a new dislocation pair is assumed to occur if the resolved shear stress in front of the crack tip exceeds the nucleation stress. A dislocation pair consists of two dislocations of equal size but opposite sign, separated a small distance. The dislocations in a dislocation pair are termed positive and negative depending on their direction of their Burgers vector, where the positive dislocation is defined as the one with its Burgers vector pointing inwards, into the material. The nucleation stress is defined as the lowest stress at the nucleation point for which the positive dislocation in the nucleated dislocation pair travels inwards into the material immediately after nucleation. The negative dislocation is assumed to remain at the crack tip causing shearing between the crack surfaces.

It is assumed that no dislocations exist within the material prior to the first load cycle, except the ones constituting the low angle grain boundary. When the applied load gets sufficiently high, dislocation pairs will nucleate from the crack tip, where after the positive dislocations glides inwards in the material along the slip plane as long as the resolved shear stress at its position exceeds the lattice resistance of the material. These dislocations, forming the plasticity, have a shielding effect on the crack tip, and the load must, therefore, be increased before more dislocations can nucleate. A number of positive dislocations will pile up at the low angle grain boundary before, eventually, they can glide pass it into the second grain. Also in this grain a pile up of dislocations will, eventually, be created at the second grain boundary.

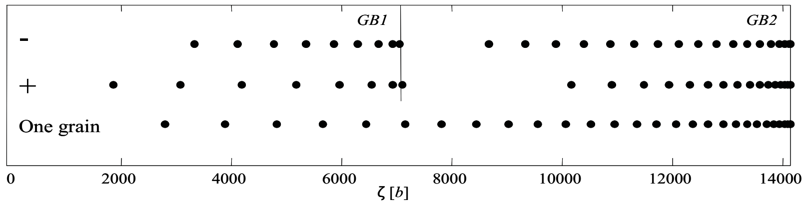
This process of dislocation nucleation and glide continues until the maximum load is reached and the load decreases. When the applied load gets sufficiently low, the dislocations will start to glide back, towards the crack. When a positive dislocation gets sufficiently close to its negative counterpart the two dislocations annihilates, resulting in crack growth in the corresponding direction by one b, under the assumption that no healing between the crack surfaces is allowed. A more detailed description of the crack growth model and the nucleation condition is found in [9].

Results

In the first simulations of the influence on the crack growth behaviour from the configuration of the low angle grain boundary, the distance between the dislocations was set to d_{GB}=100b and l_{offset}=50, cf. Fig. 2. Using this configuration the resulting dislocation distributions at maximum and minimum load are seen in Fig. 4, where + and – describe the signs of the dislocations forming the grain boundary. Also, a dislocation distribution for the case of only one grain of length 10000b, with an impenetrable grain boundary, is included for comparison.

When comparing the resulting pile ups at maximum load, cf. Fig. 4.1, it can be seen that when grain boundary *GB1* is formed by negative dislocations, the emitted dislocations end up closer to *GB1*, as compared to when positive dislocations constitute the grain boundary. This is explained by studying the stress field created by the dislocations constituting *GB1*. Using negative dislocations result in that the boundary attracts the emitted dislocations at long distances, changing to a repelling force at very close distances to the grain boundary. When using positive dislocations constituting *GB1*, the opposite situation occurs.

At minimum load, cf. Fig. 4.2, it is seen that the dislocation spacing is larger than at maximum load and that the dislocations occupy a larger part of the grain in the case of only one grain. The same holds in the case of negative dislocations in *GB1*. However, when the dislocations in *GB1* are positive, *GB1* produces a repelling force on the dislocations in the first grain, forcing them to annihilate thus, leaving the first grain free of dislocations at minimum load.



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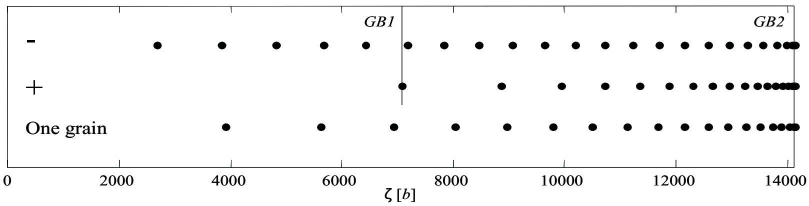

2.

Fig. 4. Dislocation distributions along the slip planes for different grain boundary configurations: 1. at maximum and 2. at minimum load. The + and – signs describes the signs of the Burgers vectors of the dislocations constituting *GB1*.

The crack growth behaviour and plastic zone development for a number of different combinations of d_{GB} and l_{offset} have been performed. It was found by comparing results for different choices of d_{GB} that, when the dislocations in the boundary are closer, more dislocations will pile up against *GB1* before breaking through into the second grain. The value of l_{offset} was also found to have an effect on the growth behaviour. For the case of negative dislocations in *GB1*, the crack growth rate was reduced when the distance from the slip plane and the closest dislocation in *GB1* decreased. This is a result due to the increasing attracting force from *GB1* on nearby dislocations, resulting in a large number of dislocations at minimum load. Consequently, for the case of positive dislocations in *GB1*, the precise opposite was found. It was also found that the number of piled up dislocations, before break through, increases when d_{GB} decreases, resulting in a lower number of dislocations at maximum as well as at minimum load. In a case of, l_{offset}=0, one dislocation in *GB1* lies directly on the slip plane, resulting in that no dislocations were able to penetrated *GB1* into the second grain, resulting in a high growth rate.

Summary

It was found that when modelling the grain boundary as a low angle grain boundary, consisting of discrete dislocations of same size and direction separated a certain distance, different growth behaviour was obtained for different grain boundary configurations. In all cases, it was found that a pile up at the first grain boundary first was created before the plasticity could spread into the second grain. Both the crack growth rate and the size of the pile up before break through was strongly depended on the sign of the dislocations of the grain boundary, the distance between them and the distance between the slip plane and the closest dislocation in the grain boundary. It was found that when positive dislocations forms the grain boundary the boundary repelled dislocations, resulting in higher growth rates than as the case of using negative dislocations, which, in contrary have an attractive force on the dislocations.

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