Influence of low-angle grain boundaries on short fatigue crack growth studied by a discrete dislocation method

C. Bjerkén[1, a] and S. Melin[2,b]

[1]Div. Materials Science, Malmö University, SE-20506 Malmö, SWEDEN

[2]Div. Mechanics, Lund University, SE-21100 Lund, SWEDEN

[a]christina.bjerken@mah.se, [b]solveig.melin@mek.lth.se

Keywords: fatigue, short crack, low-angle grain boundary, crack growth, discrete dislocations

Abstract. The growth of short fatigue cracks in or below the threshold regime are highly influenced by the local microstructure. In the present study, the influence of low-angle boundaries on the growth and arrest of microstructurally short edge cracks in crystalline material is investigated using a discrete dislocation method. The crack is modelled by boundary elements consisting of dislocation dipoles. An external load that is fully reversed during the fatigue cycle is applied to obtain a crack growth rate of a few Burgers vector per cycle. The crack growth and the developing plasticity are given by the emission, and eventual annihilation, of dislocations at the crack tip. The low-angle grain boundary is modelled as an array of aligned dislocations. It is found that the developing local plasticity, is crucial for the growth rates. Different stress ranges are used and both positive and negative low-angle grain boundaries are considered. It is found that depending on sign of the of the grain boundary, different growth behaviour are found. Generally, a positive low-angle grain boundary gives a low, rather stress range independent growth rate. A negative grain boundary results in increasing crack growth when the stress range is increased. The distance between the crack tip and the low-angle boundary is found not to significantly influence the crack growth characteristics, for the geometries and load ranges considered in this study.

Introduction

Short cracks are known to growth fast even below the fatigue limit found for long cracks, cf. Pearson [1], de los Rios *et al.* [2]. Some short cracks can continue to propagate and eventually join the long crack region, where Paris law is assumed to be valid [3]. However, short cracks can also come to an arrest after period of growth. For microstructurally short cracks, the growth rate is strongly dependent on local microstructure, such as grain size, grain boundaries, preferred slip systems for dislocations, the presence and distribution of precipitates, phase transformations, and microcracks. The plastic zone of a very short crack is often several times larger the crack, and the stress state at the crack tip can not be determined using linear elastic fracture mechanics.

Different approaches to model the influence of grain boundaries on the growth of short fatigue cracks are reported in the literature. For example, mesoscale methods based on the cohesive zone model developed by Dugdale [4], such as the so-called N-R model by Navarro and de los Rios , cf [5], can be useful in the threshold regime for long crack growth. However, crack growth rates of the order of a few Burger's vectors demand methods such as dicrete dislocation modelling to be able to catch the discrete events of crack growth, cf. Rice [6], Lin and Thomson [7], Pippan [8], Riemelmoser *et al.* [9], and Deshpande *et al*. [10]. An insight into where plasticity is generated within a crystal can given by molecular dynamics, cf. Zhang and [11] and Hora *et al.* [12].

In this study, a discrete dislocation technique is chosen since the object is to investigate the interaction between low-angle grain boundaries (LAGB) and a growing short crack with a growth rate of a few Burgers vectors. A low-angle grain boundary consisting of an array of dislocations

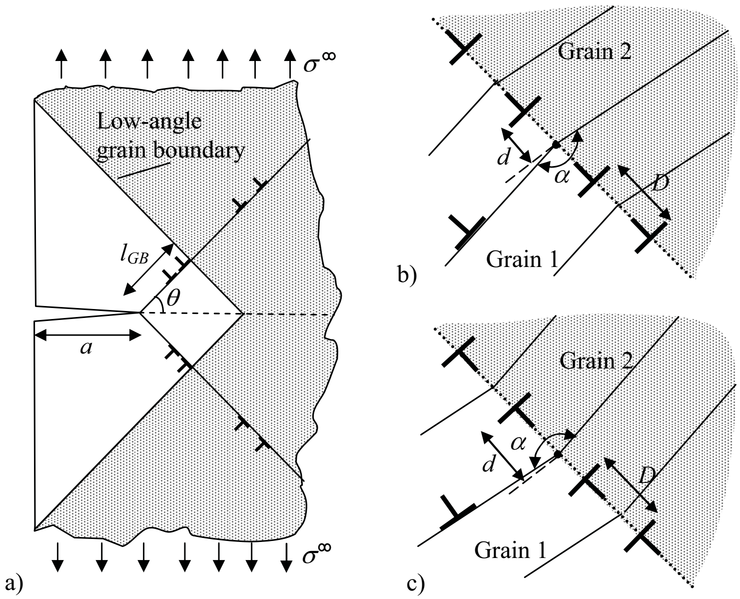

Figure 1. a) Geometry and loading of the edge crack, and the dislocation arrangement in b) a positive and c) a negative low-angle grain boundary, respectively.

having the same Burgers vector. The change of slip direction between neighbouring grains is less than 10^o, cf. Hull [13]. For longer cracks this would not affect the growth rate significantly, since plasticity will easily continue into the next grain. However, for very low growth rates it is shown that even a LAGB can contribute to change of growth rate, i.e. by Hansson and Melin [14]. Earlier studies by the authors investigated the influence on short crack growth for high-angle grain boundaries, cf. [15-17]. The method used in these studies is in the present study extended to include LAGB.

Problem formulation

Geometry, loading and material parameters. The influence of LAGB on crack growth rates is studied, a short edge crack close a low-angle grain boundary (LAGB) in a semi-infinite media, see Fig. 1.a. The material is assumed to be linear elastic and the developing local plasticity consists of discrete dislocations. The initial crack has a length $a=a_0$. At the beginning of the simulations, the material is assumed to be free of dislocations, except for those forming the LAGB,. The growth of the crack is due to the emission of edge dislocations (⊥) from the crack tip. Emission of dislocations is assumed to take place if the local stress intensity factor, k_{local}, reaches at critical value k_e. As the crack grows, the emitted dislocations form a plastic zone, and this plasticity shields the crack tip. Thus, k_{local} that differs from the global stress intensity factor K_{I} is needed to characterize the stress state at the crack tip. The emitted dislocations can slip on preferred slip planes as the critical resolved shear stress τ_{rss} overcomes the lattice friction, τ_{crit}. In the present study, only slip planes oriented an angle $\pm\theta$ versus the crack line are considered. The LAGB is oriented perpendicular to the slip planes, and the distance between the crack tip and this grain boundary is denoted l_{GB}. The crack is assumed to grow in mode I driven by an external load, σ^∞, applied vertically versus the crack line, i.e. parallel to the free edge. Thus the geometry is chosen as a system symmetric about the crack line, and only the upper part will be considered in the following. Crack growth during fatigue loading is investigated. The remote stress, σ^{∞}, is varied with a load ratio $R = \sigma_{min}^{\infty} / \sigma_{max}^{\infty} = -1$, i.e. fully reversed. The applied stress needed to initiate crack growth is σ_0^{∞}.

LAGB. A low-angle grain boundary can be described by the means of an array of aligned dislocations having the same Burgers vector, c.f. [3], and forms a symmetry line between two grains with a tilting of crystallographic directions. In Fig. b) and c), two different arrangements of LAGB dislocations considered in this study are shown. A positive LAGB is here defined as a boundary consisting of dislocations oriented in approximately the same direction as the dislocations gliding on the slip planes, and vice versa. The distance between dislocations is denoted D, and d is the offset between a LAGB dislocation and the slip plane. The angle, α, between the coinciding slip planes in the two grains is also defined in the figures. The tilting angle $\phi = \pi - \alpha$ is approximately equal to b/D [13], where b is the length of Burgers vector. In the present study, D=1000b, and thus the change of slip direction is very small and will not hinder the movement of dislocations through the LAGB. Instead, the stress field induced by the LAGB dislocations will influence the spreading of a local plasticity.

Numerical method. The problem is solved numerically using a dislocation technique developed by the authors, cf. [18]. The crack is modelled by a distribution of dislocations dipoles. The stress field is computed using the same influence functions (Hills *et al.* [19]) for all dislocations in the system, where the size of Burgers vector of the emitted discrete dislocations and those in the LAGB equal b. The free edge is included in the model through the influence functions that apply for dislocations located in a semi-infinite body. Geometrically necessary dislocation dipoles are superimposed on the crack dipoles to compensate for the influence from the LAGB on the crack opening. This prevents premature opening of the crack (or overlap of the crack flanks) of the unloaded initial crack. The crack is traction free, and neither re-welding nor overlap is allowed. The dislocations can glide along their slip planes, but climb is not considered.

Results and discussion

In the present investigation, the influence from the sign of the LAGB for different applied stress ranges is investigated. The influence of doubling of the distance between LAGB and crack tip is also studied. The distance between dislocations in the LAGB is kept fixt at D=1000b. Two values of the offset d are used; d=0 or D/2. The sign of the LAGB is either positive or negative, as defined in Fig.1.b and c. The stress range is varied by varying σ_{max}^{∞} between $1.1\sigma_0^{\infty}$ and $1.2\sigma_0^{\infty}$. In the first part, $l_{GB}=a_0/8$, and the influence of doubling l_{GB} is then considered.

During a load cycle, the crack grows if $k_{local}=k_e$, and the emitted dislocation can glide along its slip band. The presence of an LAGB changes τ_{rss} along a slip plane, making the dislocation glide further or hinder its slip. The dislocations may pile-up at the LAGB, get stuck in it or pass through. During unloading slip is reversed, and some dislocations may return to the crack tip and are annihilated their. The emitted dislocations remaining in the material after unloading is said to constitute the static plastic zone, while the cyclic plasticity is represented by the dislocations that are emitted and then annihilated during the same load cycle. In the very first load cycle, often several dislocations are emitted, but during the following cycles a lower but stable crack growth rate is obtained.

Negative LAGB. In this case, dislocations in the LAGB are oriented opposite to the emitted dislocations. Fig. X, the crack growth rate versus different maximum remote stresses in a load cycle is shown. The growth rate is given as the number of dislocations emitted during the cycle. The maximum stress is normalized with the remote stress needed for start crack growth in the system, σ_0^{∞}, which is a constant in all simulations. It is seen that the growth rate increases quite

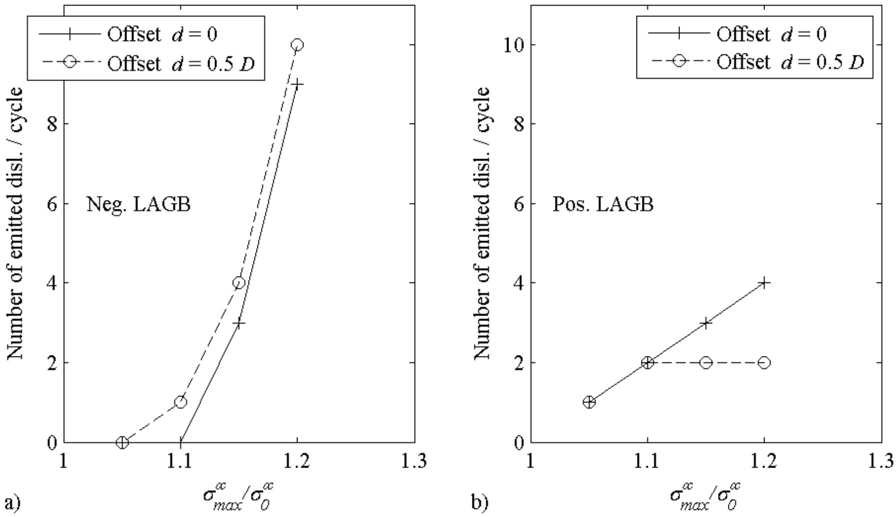

Figure 2. Crack growth rates vs maximum load in a cycle for l_{GB}=a_0/8 with a) a negative and b) a positive low-angle grain boundary, respectively. Results for two offset distances d are shown.

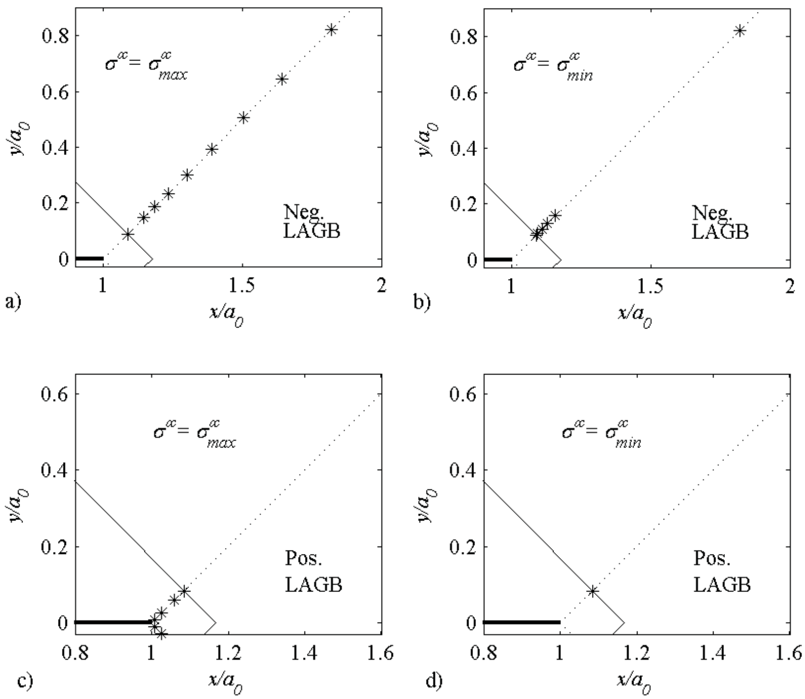

Figure 3. Dislocation distribution at a) maximum load and b) minimum load, for a negative LAGB, and c) maximum load and d) minimum load, for a positive LAGB. For all cases $\sigma_{max}{}^{\infty}$=1.15$\sigma_0{}^{\infty}$, l_{GB}=a_0/8, and d=0.

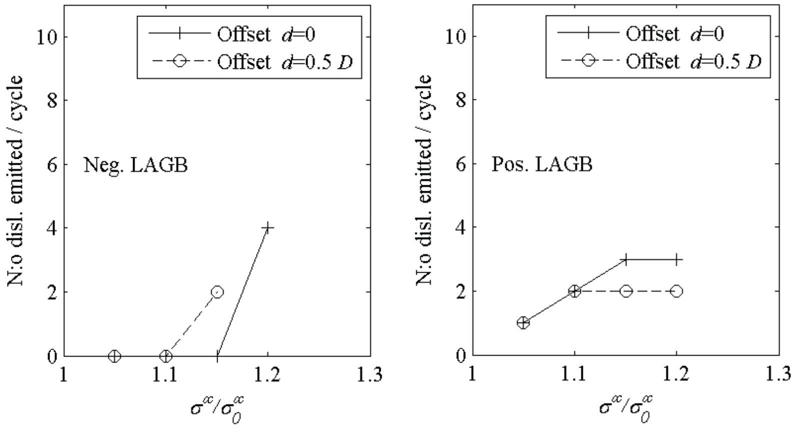

Figure 3. Crack growth rates vs maximum load in a cycle for l_{GB}=a_0/4 with a) a negative and b) a positive low-angle grain boundary. Results for two offset distances d are shown.

dramatically for both offsets d studied here. For example, the number of dislocations increases 10 times, while changing the stress range 10%. In these cases, all dislocations are located in the second grain, due to the attracting forces in the vicinity of the LAGB. The dislocations' contribution to the shielding of crack tip is limited, thus promoting crack growth. In Fig. 2.a and b, the distribution of dislocations at maximum and minimum load, respectively is shown for $\sigma_{max}^{\infty}/\sigma_0^{\infty}$=1.15 with d=0.

Positive LAGB. In this case, the LAGB dislocations have the same Burgers vector as the dislocations gliding along slip planes. At the vicinity of the LAGB, the dislocations are repelled. Thus, the possibility for the dislocations to pass a negative LAGB is much less compared to a positive one. In Fig. 2.b, it can be seen that the growth rates are lower than for positive LAGBs, and only increasing slightly with increasing stress range, or even reaching a constant level, which could be expected. In Fig 3.b, dislocation arrangements at maximum and minimum load are displayed for $\sigma_{max}^{\infty}/\sigma_0^{\infty}$=1.15 with b=0. In this case, the first dislocation emitted during the first load cycle has nearly reached the grain boundary, and is able to remain there. The following emitted dislocations all return to the crack tip during unloading. With a local plasticity confined within the first grain, the pronounced shielding of the crack tip results in a lower crack growth rate, however not necessarily arrest the propagation. Instead, a constant growth rate for increased stress range is expected, due to the limited cyclic plastic zone.

Distance between crack tip and LAGB. Simulations with a doubled distance between the grain boundary and crack tip, i.e. l_{GB}=a_0/4, are also investigated. For positive LAGB, approximately the same growth rates are found as for l_{GB}=a_0/8 (see Fig. 4.b), with the difference that for both offsets a constant level is reached for the larger stress ranges. It can be concluded that with a positive LAGB, the cyclic plastic zone is confined with in the grain holding rendering a limited amount of crack growth. During the positive part of a load cycle, all emitted dislocations, even if only a few, are close to the crack tip and contribute to the shielding. The dislocations are also repelled by the LAGB. The obtained results seem reasonable based on this reasoning.

In the case of a negative LAGB, it is found that larger stress ranges are needed to obtain a cyclic crack growth for the grain boundary located further away from the crack. This is due to that during the first cycle a relatively large plastic zone containing several dislocations is formed in the second grain, and thus the shielding of the crack tip is so large that the crack growth criterion is not reached during the following cycles. However, as a threshold stress range is overcome, the crack growth rate will increase with increasing load range in the same manner as for $l_{GB}=a_0/8$, see Figs 2.a. and 4.a. The shielding of the crack tip is crucial, and as the load increases more dislocations are emitted thus pushing the dislocations in the static plastic zone farther into the second grain. In this study, the largest plastic zone size found is more than 10 times the crack length.

Comparisons with earlier studies. Hansson and Melin [14] have recently investigated the influence of a LAGB on crack growth rate for a very short edge crack. In their study, the crack is assumed to grow by single shear through emission and annihilation of dislocations at the crack tip. The dislocation glide along a slip plane that coincides with the crack line. The results from this study also show that the sign of the LAGB influences the spreading of the local plasticity. However in their study, the growth rates were larger and no arrest of the cracks was reported. One explanation may be that a different fatigue load cycle was adopted. The load was not fully reversed (R=0.1), and the maximum stress was relatively large.

In a previous study, the authors have found that the growth rate of a short fatigue crack is highly influenced by the characteristics of a grain boundary in the vicinity [15-17]. In these studies, the interaction between the developing local plasticity and a high-angle grain boundary was considered. As the grain boundary was assumed to be an impenetrable object, crack growth rates were found to be low and independent of distance to the grain boundary during several hundred load cycles, further cycling resulted in both acceleration and retardation, and eventually arrest. Also high-angle grain boundaries, where the plasticity could spread through the boundary, were studied. No dislocations could pass the grain boundary, instead new dislocations were nucleated and then slipping in the neighbouring grain. In this case, the local plasticity was shown to develop differently depending on the distance between the crack tip and the grain boundary, and the crack growth rate was found to increase with the distance. The tilt angle between preferred slip planes was also varied but was found not to influence the growth rate even though the size of local static plasticity decreased with increasing angle.

The different investigations indicate that the size of the plastic zone cannot be used for predicting initial crack growth rates for microstucturally short fatigue cracks. The distribution of dislocations during a load cycle is found to be important, the type of grain boundary regarding degree of tilting and the sign of LAGB. The crack opening, the free edge, the discrete dislocations and dislocations in a LAGB all contribute to the total stress field and this in its turn governs the crack opening and the resolved shear stress experienced by the discrete dislocations.

Concluding remarks. However, since crack growth rates of the order of a Burgers vector is very hard to study in *in-situ* fatigue experiments, the authors find it important use numerical models for simulation of crack growth. The model used here to compute crack growth rates for microstructurally short fatigue cracks is of course a simplification of the conditions in a real material. For example, it is a two dimensional model where dislocations are restricted to move along certain slip planes, the initial material is assumed to be dislocation free, partial dislocations are not considered, climb is not allowed, and a stage II growth mode is modelled. The primary advantage is that the method models the developing plasticity by the emission, slip, and eventual annihilation of discrete dislocations. This allows detailed studies of the interaction between the microstructure, the crack and the local plasticity. Small changes of external load and differences in the local microstructure, may result in acceleration, retardation or even arrest of the crack growth. This behaviour is known to be typical for very short fatigue cracks, cf. Suresh [20].

Summary

A numerical method based on a discrete dislocation formulation, earlier developed by the authors, is here extended to include low-angle grain boundaries. The propagation of a short edge crack subjected to fatigue loading is investigated. The focus is to study the influence on local plasticity

and crack growth from LAGBs located in the vicinity of the crack tip at growth rates of the order of Burgers vector.

- It is found that positive LAGBs hinder the spreading of local plasticity and results in low growth rates. The plastic zone is confined between the LAGB and the crack tip, where the number of dislocations is limited. Despite this, the shielding of the crack tip is considerable, due to the close distance between the dislocations in the plastic zone and the crack..

- For a negative LAGB, the crack growth rate is found to increase with increasing stress range of the fatigue cycles. The discrete dislocations can quite easily pass the grain boundary, thus the size of the plastic zone increases with increasing maximum external stress. For most cases studied, the static plastic zone is located fully in the second grain. For lower stress ranges, when the plastic zone is not very large, the shielding of the crack tip will result in low growth rates. However, as the load range increases the shielding is reduced since the local plasticity is spread over larger distances. Plastic zones reaching more than 10 times crack length from the crack tip is obtained in the present study.

- With a LAGB located farther away from the crack, the characteristic features of crack growth and local plasticity is not changed. Only somewhat lower growth rates are found, and the stress range needed for a cyclic crack growth rate of one dislocation per cycle is a little bit larger.

For short fatigue cracks, the size is of the plastic zone can be several times longer than the crack and linear elastic fracture mechanics are not suitable for predicting the growth rate. Other methods have to be considered, such as molecular dynamics and dislocation techniques, that can account for large scale yielding and discrete events at a microstructural level. With the adopted dislocation technique used in the present study, short fatigue crack growth in the vicinity of a LAGB is found to strongly depend on the cyclic changes of the distribution of discrete dislocations in the plastic zone.

Acknowledgements

This research is supported by the Swedish Research Council (VR).

References

[1] S. Pearson: Engng Fracture Mech. Vol. 7 (1975), p. 235

[2] E.R. de los Rios, Z. Tang and K.J. Miller: Fatigue Engng Mater. Struct. Vol. 7 (1984), p. 97.

[3] P.C. Paris, M.P. Gomez and W.E. Anderson: The trend in Engineering Vol. 13 (1957), p. 361.

[4] D.S. Dugdale: J. Mech. Phys. Solids Vol. 8 (1960), p. 100.

[5] A. Navarro and E.R. de los Rios: Fatigue Fract. Engng Mater. Struct. Vol. 11 (1988), p. 383.

[6] J.R. Rice and R. Thomson : Phil. Mag. Vol. 29 (1974), p. 73.

[7] I.-H. Lin and R. Thomson: Acta Metall. Vol. 34 (1986), p.187.

[8] R. Pippan: Acta Metall. Mater. Vol. 39 (1991), p. 255.

[9] F.O. Riemelmoser, R. Pippan and O. Koeldnik : Comp. Mech. Vol. 20 (1997), p. 139.

[10] V.S. Deshpande, A. Needleman and E. van der Giessen : Scripta Mater. Vol. 45 (2001), p. 1047.

[11] Y.W. Zhang and T.C. Wang: Modelling Simul. Mater. Sci. Engng Vol. 4 (1996), p.231.

[12] P. Hora, V. Pelikán, A. Machová, A. Spielmannová, J. Prahl, M. Landa and O. Červená: Engng Fracture Mech. Vol. 75 (2008), p. 3612.

[13] D. Hull and D.J. Bacon: *Introduction to dislocations*, 4th edition. (Butterworth-Heinemann, Oxford, UK, 2001.)

[14] P. Hansson and S. Melin: Crack growth rates for short fatigue cracks simulated using a discrete dislocation technique: submitted for publication (2008).

[15] C. Bjerkén: Int. J. Fatigue Vol. 27 (2005), p. 21.

[16] C. Bjerkén and S. Melin: Engng Fracture Mech. Vol. 71 (2004), p. 2215.

[17] C. Bjerkén and S. Melin, in: *Proc. 15th European Conf. Fracture (ECF15)*, Stockholm, Aug (2004)

[18] C. Bjerkén and S. Melin: Int. J. Fatigue Vol. 25 (2003), p. 559.

[19] D.A. Hills, P.A. Kelly, D.N. Dai and A.M. Korunsky: *Solution of Crack Problems: The distributed dislocation theory.* (Kluwer Academic Publisher, 1996)

[20] S. Suresh: *Fatigue of materials*. (Cambridge University Press, Cambridge, UK, 1991).