THE EFFECTS OF LATTICE ORIENTATION AND PROXIMITY TO A GRAIN BOUNDARY ON MICROSTRUCTURALLY SHORT CRACKS IN 316L STEEL

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ABSTRACT

The paper presents a finite element crystal plasticity model for microstructurally short cracks. The model is 2D plane strain and consists of 212 randomly shaped and sized grains with different crystallographic orientations. A stationary crack at an angle of 135° is then introduced to a surface grain and the model is monotonically loaded to a macroscopic equivalent strain of 1.45%. The crack tip opening (CTOD) and sliding (CTSD) displacements are then calculated for different crystal orientations in the crack-containing and surrounding grains. The results show that by rotating the crystallographic orientation of a crack-containing grain the CTOD value may vary by a factor of 1.73 and the CTSD by a factor of 1.26. A similar, albeit smaller, effect is observed when the crystallographic orientations of surrounding grains are rotated. Finally, the effect of the vicinity of the crack tip to the grain boundary is studied. No significant decrease in the CTOD/CTSD values is observed if the CTOD/CTSD values are calculated at a distance of 15% of the average grain size. As the distance is changed to 2.5% of the average grain size, the CTOD values decrease by 25%.

1 INTRODUCTION

The propagation of microscopically short cracks (i.e. cracks with length of up to a few grain sizes) is still not fully understood and measured crack propagation rates may vary significantly for nominally identical cracks [1]. Their behaviour strongly depends upon the surrounding microstructural features such as grain boundaries, crystal orientations, inclusions, voids, material phases etc. Grain boundaries tend to decrease the crack tip displacements as the crack tip approaches them [2]. The difficulty in propagating slip across an interface may gave rise to an incubation period, depending on the type of interface, e.g. high-angle grain boundary or interface with a second phase. Different crystallographic orientations of the grains may also increase, decrease or arrest the crack growth [4], [5]. A possible increase in closure stress as the crack tip crosses an interface can also influence the crack growth [5]. These factors may act independently or interactively, resulting in significant variability in crack growth rate.

In recent years several attempts were made to model the behaviour of short cracks using crystal plasticity material model[6], [7], [8]. However, to the best of our knowledge, with the exception of intergranular cracks in [9], no attempts have been made to combine modelling of short cracks with random grain geometry and the crystal plasticity. The present study explores this using the Voronoi tessellation technique for modelling grains. An angled short crack is then introduced in a surface grain and the model is subjected to a uniform monotonic tensile load. This paper presents and evaluates the results obtained.

2 MODEL LAYOUT

Microstructurally short cracks are analysed by calculating basic fracture mechanics parameters: crack tip opening (CTOD) and sliding (CTSD) displacements. K values are not used because the size plastic zone size is not small compared to the crack length. Due to the small size scale, crystal plasticity theory is used [10], [11] to describe the material's plastic behaviour. The material is assumed to deform plastically by simple shear on a specified set of slip planes. For the elastic deformation an anisotropic behaviour is used. In the example steel 316L, which has an f.c.c. crystal lattice and therefore 4 different slip planes and 3 different slip directions on each slip plane (thus creating 12 slip systems) is employed. The plastic deformation takes place along these slip directions. Deformation by diffusion, twinning and grain boundary sliding is not considered.

The global model is a simple rectangular block, which incorporates 212 randomly sized and shaped grains, see Figure 1. The generation of this grain structure is achieved through a process called Voronoi tessellation [12]. Each grain is assumed to behave as a continuum described by the anisotropic elasticity and crystal plasticity model [13]. The material orientations, which are defined by the crystallographic orientations of the lattices, are kept constant within a single grain but vary from grain to grain according to a uniform distribution with range 0 to 2π. The average grain size of 316L steel is between 50 μm and 80 μm [14]. In this study a value of 52.9 μm is used. The crystal plasticity model is implemented as a user subroutine into the finite element code ABAQUS [15]. Plain strain finite elements with a small strain formulation are used and the crystal orientation is such that plane deformation prevails. Crystal plasticity material properties are determined by a best fit between the numerical tensile test and the measured one.

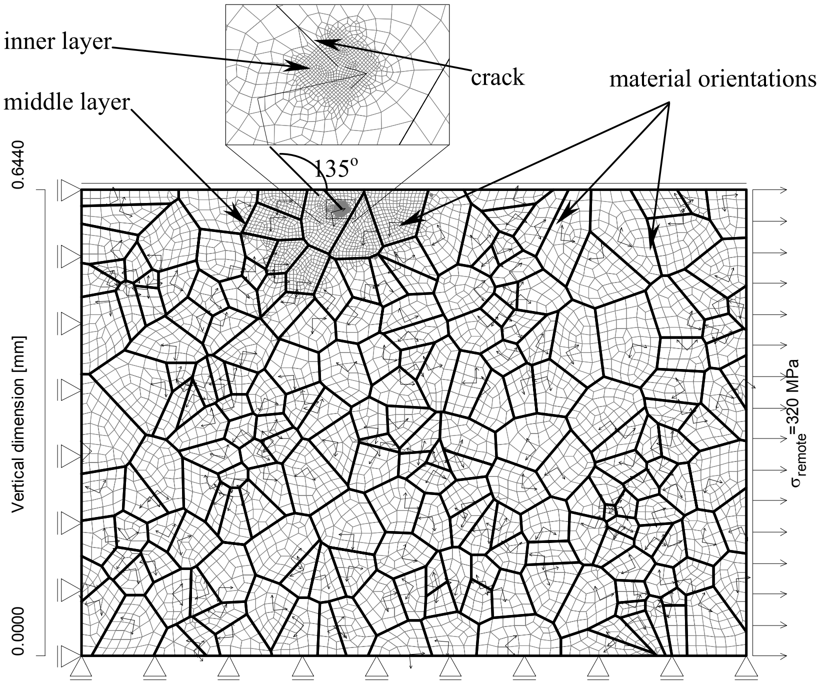


Figure 1: The finite element model, indicating the displacement boundary conditions and remote applied load; details of the crack are shown in the insert.

A maximum tensile remote load of 320 MPa with zero shear tractions is applied on the right edge of the model, which corresponds to a macroscopic equivalent strain of 1.45%. The right edge is only allowed to move parallel to the left edge. Similarly, the top edge is only allowed to move parallel to the bottom edge. Figure 1 shows the model used in this study. A stationary crack at an angle of 135° to the surface can be seen within one grain at the top of the model. This particular crack angle is considered typical for Stage 1 fatigue crack growth because it has the same direction as the maximal shear stresses.

Unless stated otherwise, the CTOD and CTSD are calculated at a distance of 15% of the average grain size behind the actual crack tip (i.e. 7.9 μm). A number of meshes with different refinement levels were generated to ensure that the mesh refinement does not significantly affect the results. The final mesh uses three levels of mesh refinements to achieve desired accuracy and minimize the total number of elements, cf. Figure 1 and Figure 2.

3 RESULTS

Figure 2 a) shows crack tip displacements as a function of the material orientations of the cracked grain at the maximum load. Crack length equal to half the cracked grain size is used. Material orientations of the cracked grain were steadily increased by 2° increments from 0° to 360°. Due to periodicity only results up to 180° are presented. Material angles are defined from the X-axis with anti clock-wise positive direction. For all neighbouring grains a value of 269.4° was used. This value was obtained by averaging the original material orientations of these grains that were generated by a random process. Other grains are oriented arbitrary. One can observe that the CTOD values differ by a factor of 1.73 and the CTSD values by a factor of 1.26 as the angle varies, pointing to a significant effect of the material lattice orientation. The periodicity of the response at 180° intervals is attributed to the symmetries in the crystal lattice. At a period of 90° the response is almost identical-the small differences are the result of slightly anisotropic elastic material properties. For isotropic elastic material properties the period would be 90°.

In Figure 2 b) material orientation of the cracked grain was set to 170° (at this angle maximum CTOD value was obtained), while the material lattice orientation of the surrounding grains were simultaneously increased by 2° increments. This rotation of material properties also has a significant effect on the calculated CTOD and CTSD values (differences of factor 1.4 and 1.53). From these results we conclude that the material orientation of the cracked grain as well as the surrounding grains have a significant influence on the crack tip opening and sliding displacements.

The second phase of the study considered the variation in the CTOD and STSD as the crack tip approaches the first grain boundary. For this purpose several models with different crack lengths were generated. The material orientation of the cracked grain was set to 170° (for this value maximum CTOD were obtained, see Figure 2 a)). The material orientations of all the surrounding grains were equal and set to 46° (minimum CTOD, see Figure 2 b)). This combination of material lattice angles was expected to give the strongest grain boundary effect. As the crack tip approached the grain boundary no significant reduction in the CTOD and CTSD values were observed. Given the large influence of the material orientation of the cracked and surrounding grains depicted in Figure 2, a much more pronounced grain boundary effect was expected [2]. Similar results have, however, also been reported by Potirniche et al. [6]. They also used a 2D model in combination with the crystal plasticity but they did not consider the random grain geometry. In their case the CTOD values are calculated at a distance of 2.5% of the average grain size.

To assess whether the results were affected by where the CTOD was calculated, the distance from the crack tip to the point where we calculate the CTOD/CTSD was decreased from 15% of the average grain size to 2.5% of the average grain size (i.e. from 7.9 μm to 1.3 μm). A reduction of 25% was then obtained in CTOD values as the crack approached the grain boundary. Because the crystal lattice (direction of 46°) in the second grain is almost aligned with the crack, the CTSD values actually increase, see Figure 3.

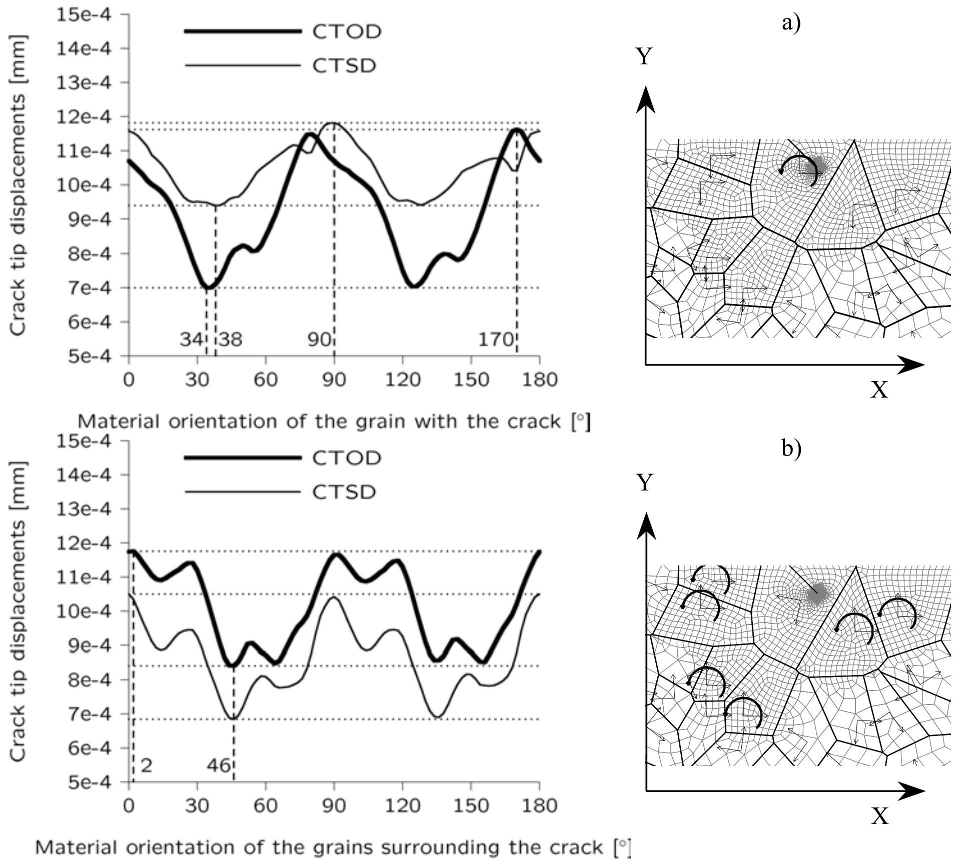


Figure 2: Crack tip displacements as a function of the material lattice orientations of a) the cracked and b) surrounding grains.

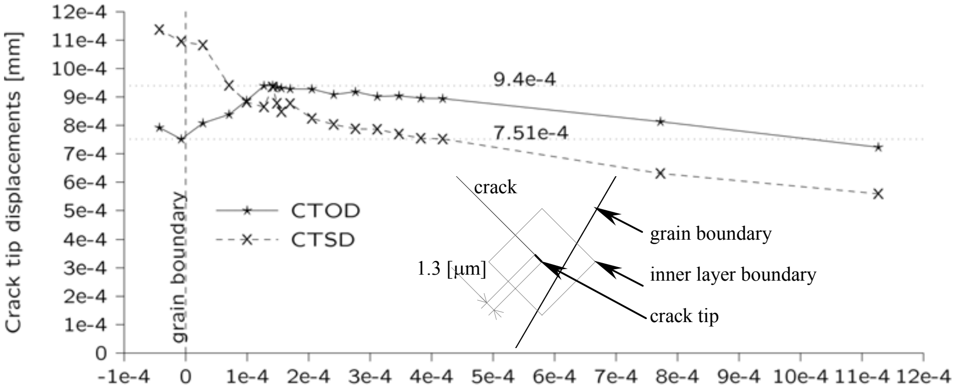
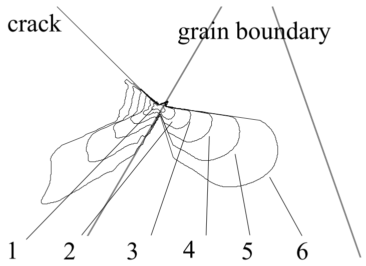


Figure 3: The influence of proximity to the grain boundary on the crack tip displacements.



Case	Macr. eq. strain [%]	Macr. eq. stress [MPa]
1	0.0223	45.01
2	0.0334	67.52
3	0.0446	90.03
4	0.0558	112.55
5	0.0670	135.06
6	0.0782	157.59

Figure 4: The size of the plastic zone. Isocontours at $\sigma_{r0.2}$=250 MPa.

The effect of the grain boundary on the growth of the plastic zone was also studied. Figure 4 shows plastic zones for different loads and for a crack length of 51.38 μm (distance to the grain boundary 1.08 μm). The initial development of the plastic zone in the direction of the crack (length direction) is not blocked by the grain boundary. The grain boundary, however, blocks the plastic zone growth along the grain boundary, i.e. perpendicular to the crack direction. External load has to be sufficiently high for the plastic zone in the direction of grain boundary to extend across it.

4 DISCUSSION

Since the present model is limited to 2D plane strain, the orientations of the grains are only rotated around the Z-axis (out of plane axis). This effectively limits the slip angle (minimal angle between the slip planes and the X-axis) to $35.26^o \leq \phi \leq 54.73^o$. The maximum difference in the slip angle between the cracked and the surrounding grains is therefore only 19.47^o. This could be one of the reasons why a higher decrease in the CTOD values was not observed as the crack approached the grain boundary. Several studies indicate that this affect could be larger, see [2], [3] and [4]. To allow for full 3D rotation of the material properties a 3D model is currently under development, in which the grains are extruded to produce a thin slice of material. With full 3D rotation of the material coordinates a system can be generated where there is the highest possible difference in the slip angles between the cracked and surrounding grains. A further proposed development is the extension of the crystal plasticity material model to account for certain aspects of material cyclic behaviour. At a first stage elastic unloading is implemented whereas in later stages also more complex effects such as Bauschinger effect, cyclic hardening and softening will be considered.

5 CONCLUSION

A method for modelling short cracks within randomly sized and shaped grain structures is presented. Since the behaviour of short cracks strongly depends upon the surrounding microstructural features it is important to be able to model them. In this paper the influence of the crystal orientations and the proximity of the grain to the crack tip displacements has been studied. Crystallographic orientations of the cracked and surrounding grains have a significant influence on the crack tip opening and sliding displacements. Rotating the crystallographic orientation of a cracked grain changes the CTOD values by a factor of 1.73 and CTSD values by a factor of 1.26. Similar, albeit smaller, impact is observed when rotating the crystallographic orientations of surrounding grains. Such differences could partly explain the apparent variations in crack propagation rate for microstructurally short cracks.

The effect of the vicinity of the crack tip to the grain boundary has been studied. If the CTOD/CTSD values are calculated at a distance of 15% of the average grain size from the crack tip, no significant decrease in the CTOD/CTSD values is observed. As the distance is changed to

2.5% of the average grain size, the CTOD values decrease by 25%. A larger effect of the grain boundary is expected for a model with larger difference in slip angles. To be able to increase the slip angles a 3D model that supports full 3D rotation of material properties has to be built.

Finally, the effect of a grain boundary on the crack tip plastic zone has been examined. Plastic zone growth in the crack direction does not appear to be significantly affected. However, the grain boundary is shown to block the plastic zone growth along the grain boundary, i.e. perpendicular to the crack direction. External load has to be sufficiently high for the plastic zone in the direction of grain boundary to extend across the boundary.

6 REFERENCES

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