Brittle Fracture of Polycrystals: a New Pseudo Three-Dimensional Model

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ABSTRACT: *In order to investigate the propagation of cleavage cracks across grain boundaries, a theoretical model of a polycrystal, which consists of prismatic grains, has been developed. Using computer simulation a brittle cleavage crack is allowed to nucleate and propagate across the model. The results indicate that about 32% of the overall fracture surface consists of accommodation, either brittle or ductile, at the grain boundaries. This prediction has been examined by carrying out fracture experiments on specimens containing columnar ferrite grains formed within C-Mn steel weld metal. The results demonstrate that there is indeed a substantial amount of grain boundary failure, which in this case is ductile.*

INTRODUCTION

In single crystals of body-centred cubic materials, brittle fracture occurs by cleavage on well-defined crystallographic planes [1]. In polycrystals individual grains also fracture in this way [2] but an additional failure mechanism, particularly brittle or ductile grain boundary fracture is needed to link these cracks together. The proportions of cleavage and grain boundary failure which occur will depend on the number of cleavage planes available and the shapes of the grains so that different results will be expected in different cases. The present authors have developed a suite of theoretical models to investigate the ways in which fracture may occur in polycrystalline materials such as -iron and carried out specific experimental work to test the predictions [3-7].

Some of the theoretical work has been based on models consisting of body-centred cubic arrays of regular tetrakaidecahedra (14-hedra). This has indicated, simply from geometrical arguments, that about 30% of the overall fracture is on grain boundaries, much larger than anticipated [4, 5]. Some of the assumptions used in the modelling work must therefore be questioned and, indeed, the influence of the regularity of the model itself needs to be explored. Ideally this can be done using three-dimensional models with randomly generated grains and carrying out computer simulations describing the propagation of brittle cracks. These more realistic simulations are difficult to perform, visualise and interpret and it has been found that, in practice, to investigate many fracture phenomena in polycrystals two-dimensional models with irregular grains are adequate. For example, these models provide a valuable insight into the influence of grain boundary energy, grain elongation, preferred crystallographic orientation, precipitates, prior creep cavitation, boundary decoherence, and segregation of impurities to grain boundaries, on the propagation of brittle cracks [5-7]. However, being two-dimensional, the models are unable to help in obtaining a better understanding of the amount of grain boundary failure needed to accommodate the mis-match between cleavage cracks in neighbouring grains in three-dimensional materials.

It was therefore decided to make use of a pseudo three-dimensional model consisting of columnar grains. Previously a very simple model, consisting of a close-packed array of regular hexagonal prisms, was used and tended to confirm that about 30% of the failure is by grain boundary fracture [5]. However, these results are subject to the same or even greater concerns as those of the regular 14-hedra models and it was clear that computer simulations of more general models with irregular columnar grains were needed. This work is the subject of the first part of the present paper. The results again provide an insight into the fracture of genuinely three-dimensional polycrystals but are also directly relevant to the fracture of weld metal in weldments made in ferritic steels [5-6]. The individual weld beads have columnar grains and the remainder of this paper presents experimental results on new, specific, fracture tests carried out on specimens taken from such selected regions and compares the results with the predictions of the models.

MODELLING RESULTS

A cross-section of a few grains of the new model of a polycrystalline material which has been developed, is illustrated in figure 1. The polygonal cells have been generated randomly, prisms erected to generate the three-dimensional grains and a random orientation allocated to each. Therefore, lines in figure 1 represent vertical grain faces and three-fold nodes represent vertical grain edges. Three orthogonal cleavage planes were then allocated to each grain, corresponding to the {100} planes in ferrite. A uniaxial stress was applied parallel to the prism axes and fracture was initiated at a randomly selected point on the particular cleavage plane which is closest to being perpendicular to this stress axis. In figure 1 this is in grain A. As a cleavage crack spreads from this point it is assumed that its projection on the plane perpendicular to the stress axis is circular. When this crack meets the nearest grain face, at the dot on the face between grains A and B in figure 1, it is assumed that it propagates immediately into grain B at the same speed as the original crack.

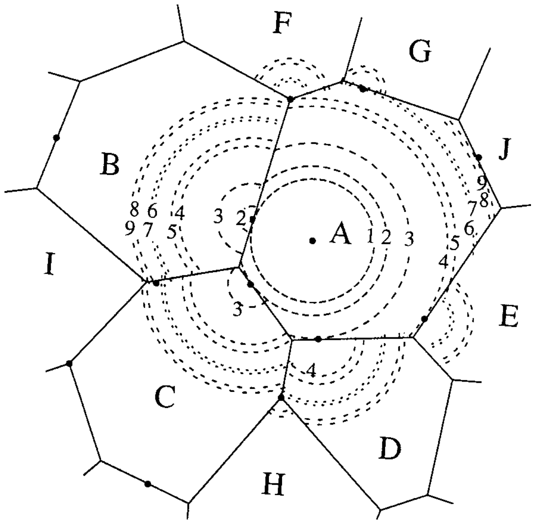


Figure 1: Cross-section of a few grains of a model polycrystal. A cleavage crack nucleates in grain A and propagates into neighbouring grains at the sites indicated by dots. The development of the crack is represented by the arcs of circles which are numbered sequentially 1 to 9.

Subsequent propagation events may occur at either grain faces or grain edges. Thus in figure 1, after meeting grain B, the expanding crack in A meets faces of C, D and E before meeting the edge between A, B and F and then the faces of G and J. However, before it propagates into J, the crack in D has met the edge between C, D and H and spread into H and similarly the crack in C has met the edge between B, C and I and spread into I. The positions of the projected crack-fronts at the times of these nine propagation events are indicated sequentially in figure 1 with the numbers 1 to 9.

By assuming that the propagation events occur immediately the crack meets any grain face or edge it is implied that all of these sites are equally favoured. Finally, it is assumed that fracture of a grain will propagate only from its first contact point with a crack. Thus when a crack meets a grain which has already started to fracture from another site, it is not allowed to propagate. For example, when the crack in B of figure 1 meets the edge between A, B and C, it will not nucleate a crack in C as this grain already contains a crack spreading from the face between A and C.

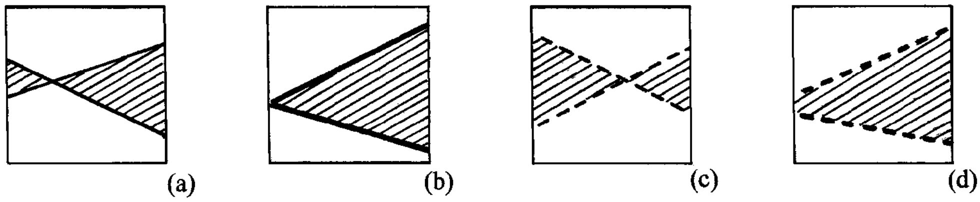


Figure 2: The four grain boundary failure mechanisms, arising from a cleavage crack propagating either (a) across the face of a grain or (b) from the edge of a grain or (c) meeting and (d) not meeting an approaching cleavage crack in a neighbouring grain.

As the polygons of figure 1 represent three-dimensional prismatic grains and as the cleavage planes in adjacent grains are not parallel, grain boundary brittle or ductile failure is needed to link the cleavage cracks together. In both cases four distinct possibilities arise and these are illustrated schematically in figure 2. When a crack propagates across a grain face, the grain boundary failure has the form of the double triangle shown in figure 2(a). The boundary between A and B is an example of this in figure 1. When a crack propagates from a grain edge the boundary failure has the form of a single triangle, as shown in figure 2(b). The boundary between A and F is an example. When independent cracks meet a boundary from opposite sides two possibilities arise. They may cross, again giving a double triangle as shown in figure 2(c), or they may miss each other to give a quadrilateral as shown in figure 2(d). The total area of grain boundary failure is then governed by the proportions of these four mechanisms which arise in practice and the average area involved in each case.

In order to reduce the amount of computation, it was decided to nucleate the first crack near the corner of the model rather than near its centre. A cross section of the actual model adopted is shown in figure 3(a). The bottom corner of this corresponds to the top right-hand corner of figure 1 but extra grains have been added. Also the grains to be considered have been labelled 0 to 18 which represents the sequence in which fracture occurred. These nineteen cells are those which lie wholly or partly within the area defined by the orthogonal axes which have been drawn through the nucleus of grain 0, corresponding to grain A in figure 1.

A perspective view of the fracture surface which developed across the twelve complete prismatic grains in this model is shown in figure 3(b). The grains are labelled 0 to 11 and, as in figure 3(a), grain 0 is in the foreground. Also, the angle of tilt of each cleavage plane is given, ranging from 8° in grain 0 to 46° in grain 8 with an average of about 30°. This immediately demonstrates the danger of assuming that fracture surfaces are relatively flat.

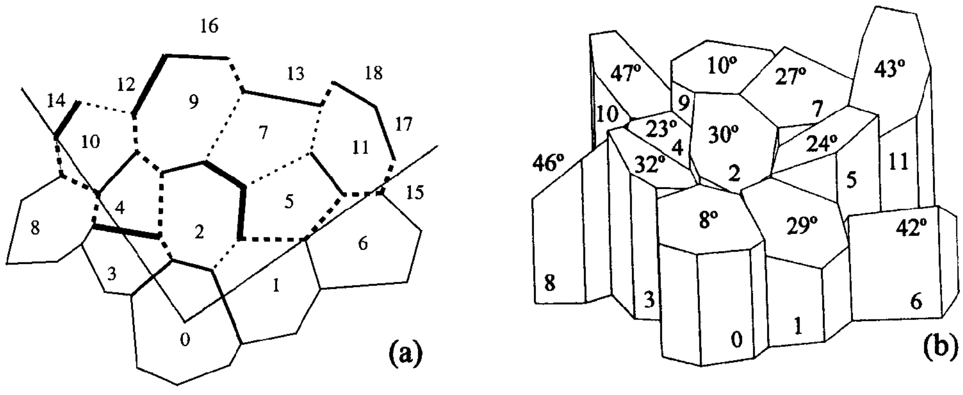


Figure 3: (a) Cross-section of the model. The crack propagates sequentially from grain 0 into grains 1 to 18. The grain boundary failure mechanisms are shown using the notation introduced in figure 2. (b) Perspective view of the fracture surface across the twelve complete prismatic grains of the model.

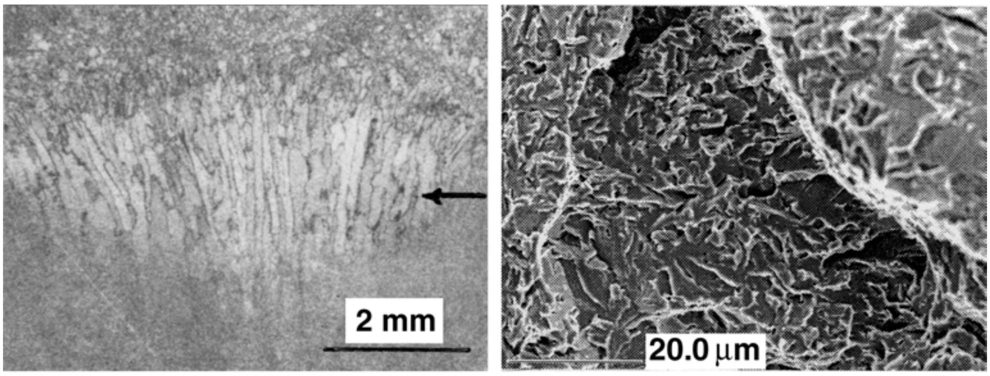
Examples of all four different mechanisms of grain boundary failure are present and are indicated on figure 3(a) for each grain face which lies wholly or partly within the designated area. Of the 32 relevant boundaries, 25 lie wholly and seven partially within the quadrant of interest. Dividing these between the mechanisms, there are 8, 4, 5 and 8 complete and 2, 1, 0 and 4 partial examples of (a), (b), (c) and (d) respectively. This means that, if the first crack had nucleated at the centre of a model rather than near a corner, 36, 18, 20 and 40 examples of complete boundaries would be expected, giving 32%, 16%, 17% and 35% respectively. Similar figures are obtained when the projected lengths of the boundaries which fail by means of the different mechanisms are measured. Also, if the proportions are determined sequentially as the fracture surface expands it appears that the figures have, at least approximately, reached a steady state. Thus, about one-third of the boundaries fail by each of mechanisms (a) and (d) and about one-sixth by each of mechanisms (b) and (c).

The areas of grain boundary brittle fracture which have occurred within the 32 complete and partial boundaries which lie within the model have also been determined. The proportions corresponding to mechanisms (a), (b), (c) and (d) are 10%, 4%, 10% and 76% respectively and are thus dominated by mechanism (d). This was not unexpected and was in any case suggested by figure 3(b). It arises in part because the prismatic grains are of unlimited height. The proportions of cleavage and grain boundary failure which have occurred can now be determined. For cleavage the true areas rather than the projected areas, which overall are 14% lower, have been used. Also, for grain boundary failure only one-half of the contributions from the ten outer boundaries have been included, as these are shared with grains outside the model. The result is that 32% of the failure has occurred on grain boundaries. This is remarkably close to the result of about 30% estimated from earlier models.

EXPERIMENTAL RESULTS

The predictions of the model have been examined with respect to the columnar grains formed within a C-Mn ferritic steel weldment. A multipass manual metal arc weldment was made between C-Mn steel plates with a single V butt preparation using C-Mn steel weld metal. The nominal composition of the weld metal is (wt%) 0.035C, 0.70Mn, 0.13Si, 0.01S, 0.03Ni and 0.03Cr. The individual weld beads are typically 10mm across and contain a central region of "as cast" columnar grains of typically 5mm cross section, figure 4(a). Generally the crystal growth in the weld bead tends to be along the steepest temperature gradients in the weldment. In practice the growth is also along a preferred crystallographic direction which for ferrite is 100 .[8] However, the complex heat flow path means that there is an overall preferred direction of growth and there is also a measure of misorientation between grains. Moreover, in addition to the grain-refined regions generated by the deposition of successive beads, there will be heat treatment of the "as cast" columnar material. Hence the columnar grains were ferrite with many inter- and intra-granular carbide precipitates. Specimens 5 mm x 5 mm x 50 mm long were extracted with columnar grains parallel to the long axis. Notches 1.5 mm deep and 1mm wide were cut across the centre of one face of the specimens and therefore across some columnar grains. The specimens were fractured in 3-point bend loading at 77K and examined using an Hitachi S-2300 scanning electron microscope operating at 15keV in the scanning electron imaging mode.

The SEM results revealed, as shown in figure 4(b), that the failure mechanism in each grain was quasi-cleavage, there being multiple initiation of cleavage cracks at many carbide precipitates. However the fracture surface in each grain was approximately planar. At the boundaries between the columnar grains, the mismatch of the meeting quasi-cleavage fracture surfaces was accommodated by ductile grain boundary fracture, see figure 4(b). In many cases there was a considerable height difference between the quasi-cleavage facets such that when tilted the region of ductile grain boundary fracture could be up to twice the grain cross section, 50μm, of the columnar grains. It was not possible to make quantitative measurements on the areas of these ductile failures, but the general impression obtained was that the proportion of grain boundary fracture can be, on average, between 10 to 20% of the total fracture area.



(a) (b)

Figure 4: (a) Optical micrograph showing the columnar grains in a weld bead; the arrow indicates the fracture path. (b) Scanning electron fractograph of the corresponding fracture surface.

CONCLUSIONS

Simulations of brittle fracture of polycrystalline materials have been carried out using a pseudo three-dimensional model consisting of columnar grains. Cleavage cracks in adjacent grains are assumed to be linked by brittle or ductile grain boundary fracture. Four different mechanisms of boundary failure are possible and all four have occurred in the simulations. The models predict that about 32% of the overall failure is on the grain boundaries. Fracture tests using three-point bending at 77K have been carried out on specimens containing columnar grains formed within a C-Mn ferritic steel weldment. Scanning electron microscopy revealed that the failure mechanism in each grain was quasi-cleavage, there being multiple initiation of cleavage cracks at carbide precipitates. The mis-match of the meeting quasi-cleavage fracture surfaces was accommodated by ductile grain boundary fracture. The proportion of grain boundary failure is considered to be between 10% to 20% of the total fracture area. Because the axes of the columnar grains probably have a preferred 100 orientation this result is not inconsistent with that obtained from the theoretical model.

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