THE INFLUENCE OF DEFECTS ON INTERGRANULAR FRACTURE IN POLYCRYSTALLINE MATERIALS AT LOW TEMPERATURES

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The proportion of intergranular and cleavage fracture which occurs in high purity alpha-iron and ferritic steels which fail at temperatures below the ductile-brittle transition has been investigated using both theoretical models and high resolution fractography. Some intergranular fracture is necessary because cleavage cracks in adjacent grains do not meet in a line in their common grain boundary. Assuming that cleavage occurs on a single crystallographic plane in each grain, theoretical models predict that at least 30% of the fracture must occur on grain boundaries. Experimental work demonstrates that in practice the amount of intergranular fracture is much smaller than this. In this paper the ways in which microstructural features such as carbide precipitates and inclusions within grains or on grain boundaries could influence the predictions are explored. It is concluded that in practice cleavage must occur on more than one plane in many grains.

INTRODUCTION

At low temperatures single crystals fracture in a brittle manner by means of cleavage on well-defined crystallographic planes. In polycrystals, two brittle failure mechanisms are available, cleavage and intergranular fracture, and these might occur separately or in combination. Schematic representations of these four cases for two-dimensional specimens, regular hexagonal grains being used for the polycrystals, are shown in figure 1. Of particular interest is the case of 100% cleavage failure of polycrystals, illustrated in figure 1(c). In two-dimensions this is possible because a cleavage line in one grain meets a potential cleavage line in an adjacent grain at a point in their common grain boundary. In three-dimensions this is not generally possible, as illustrated schematically for a polycrystal consisting of two cubic grains in figure 2. Three possible cases are shown in which the two cleavage planes, shown lightly shaded, (a) meet at a grain edge, (b) intersect on the grain face and (c) do not meet. In each case an area of grain boundary, shown heavily shaded, must fail if the overall fracture surface is to become continuous.

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In recent papers (1,2) the present authors have investigated, using theoretical models, the proportion of grain boundary brittle fracture which on average, because of this effect, must accompany cleavage fracture of polycrystalline materials at low temperatures. In particular the case of alpha-iron and ferritic steels, in which cleavage occurs on one of the three variants of the {100} family of planes, has been considered in detail. The models consistently predict that about 30% of the fracture must be intergranular. In addition some grain boundaries may also fail completely, because for example they are particularly well-oriented relative to the stress axis, so that the overall proportion would then be even higher. However, interpretation of fractographs of materials which have failed at low temperatures has, in the past, suggested that in practice only a small amount of intergranular fracture occurs, typically a few percent.

One explanation for this discrepancy could be that the experimental work was carried out at relatively low magnifications at which the rather small but numerous partial grain boundary failures were not detected, particularly if they were approximately perpendicular to the overall specimen surface. Therefore new experimental measurements were made at high magnifications on alpha-iron specimens tested at temperatures below the ductile-brittle transition. These showed that the proportion of intergranular failure detected at high magnifications may approach 20%, but this included examples of complete grain boundary failure.(1) Also, corresponding observations on C-Mn steel specimens only gave proportions of up to about 6%. These results are for areas projected on to the image plane which could be misleading. Therefore additional experiments were carried out in which the steel specimens were tilted by up to 50° in two orthogonal directions. These revealed that the proportion of grain boundary failure could be as high as about 8% but in no way could it approach the theoretical value of 30% or more.(2)

It therefore appears that some of the basic assumptions made in the theoretical models are inappropriate, especially when applied to C-Mn steels, and need to be re-examined.. In particular it is the purpose of the present paper to explore whether the discrepancy can be explained by incorporating in the models cleavage crack initiation at microstructural features. In particular carbides and non-metallic inclusions have been identified as favoured initiation sites.(3) Examples of such sites on brittle fracture surfaces in alpha-iron and C-Mn steel are illustrated and the theory is developed to determine whether they can account for the discrepancy.

EXPERIMENTAL PROCEDURE AND RESULTS

Two ferritic materials were selected: (i) alpha-iron and (ii) C-Mn steel. The alpha-iron contained 230ppm oxygen and 260ppm nitrogen and this was heat treated at a temperature of 1243K for 900s and air cooled to produce a grain size of about 80μm (mean linear intercept). The C-Mn steel plate, composition 0.14C, 1.3Mn, 0.11Si, 0.029S and 0.012P (wt%), was cross-rolled and normalised at about 1213K, followed by heat treatment at 873K for $2.16\text{x}10^4$s, cooled at $0.003°s^{-1}$ to 523K and finally air cooled. This produced a grain size of about 50μm (mean linear intercept). The alpha-iron specimens were fractured at a temperature of about 100K and the C-Mn steel specimen was tested using a standard fracture toughness test procedure again at about

100K. The fracture surfaces were examined using a JEOL JSM80A scanning electron microscope operating in the secondary electron mode.

Observations of the fracture surfaces of these two materials have been described elsewhere.(4) However with respect to cleavage crack initiation figure 3 shows a cleavage fracture facet immediately adjacent to the fatigue pre-crack introduced prior to fracture toughness testing of a C-Mn steel specimen. The initiation occurs at a small carbide precipitate of 0.5mμ diameter positioned within the ferrite grain. The pattern of the "river lines" emanating from the carbide precipitate is consistent with initiation and the location with respect to the pre-crack confirms it to be a primary initiation site. The second example, figure 4, shows initiation from a grain boundary feature, in this case a non-metallic inclusion, which is marked with an arrow. Here the inclusion is certainly responsible for the initiation of the cleavage facet in the alpha-iron since the pattern of "river-lines" again emanates from this feature. However since the inclusion is located at a grain boundary site it may also have initiated the associated intergranular fracture.

THEORETICAL MODELS AND RESULTS

The aim of the models is to deduce the proportion of partial grain boundary failure which must occur to link cleavage cracks in adjacent grains. The first step in the theory is to calculate the average proportion of the grain boundary area which will fail in each of the three schematic mechanisms shown in figure 2. This clearly depends upon the average angle between the traces of the cleavage planes in the boundary. Assuming that cleavage occurs on one of the three variants of {100}, it can be shown that the smallest available angle will on average be 15°. However, the corresponding cleavage planes may not be favourably oriented relative to the stress axis so that in practice the second or third smallest angle may be selected. Computer simulations have been used to deduce the overall average angle and this is about 30°. The other variable is the point of intersection of the two traces and the results of simulations are that for mechanisms (a), (b) and (c) respectively, on average, about 17%, 17% and 45% of the area of grain boundaries must fracture.

The next step is to deduce what proportions of mechanisms (a), (b) and (c) actually occur in practice as brittle fracture spreads across a polycrystalline material. To do this it is necessary to use a more realistic model of a grain than that shown in figure 2 and the one adopted is the regular polyhedron with six square and eight hexagonal faces. As shown in figure 5 such tetrakaidecahedra (14-hedra) stack together in a body centred cubic array to fill all space. Depending on its orientation and position, a cleavage crack crossing one of these grains has any number of edges from three to ten and computer simulations have shown that the average is six.(2) Thus the propagation of fracture through a polycrystal may be represented topologically using a diagram consisting of a regular array of hexagonal prisms, or even more conveniently by a regular array of hexagons.

Several different developments are now possible depending on the sites where cleavage cracks are assumed to nucleate. We shall here concentrate on cracks being nucleated at precipitate particles and consider in detail the case where these particles are within grains, corresponding to figure 3. A possible sequence of events is then shown schematically in figure 6, which is a cross section of a model consisting of hexagonal prisms. The initiation point of the first cleavage crack is unimportant, so assume that it occurs at a particle at the centre of grain 1. As this crack spreads, new cracks will be nucleated at particles in the surrounding grains which experience high stress concentrations. These are likely to be near the boundaries with grain 1 and the resulting cracks will tend to meet the original crack by means of mechanism (a) of figure 2. These are indicated by fine lines in figure 6. However, the particles in grains 2 and 3 are remote from the boundary between them so that either mechanism (a) or (c) will operate, as indicated by a bold line. The crack in grain 4 will be initiated by stress concentrations arising either from grain 2 or grain 3 and the latter has been selected. Hence boundary 3/4 exhibits mechanism (a) and boundaries 4/5 and 4/6 mechanism (a) or (c). As the fracture surface develops, the proportions of the two types of boundary is found to be one-third mechanism (a) and two-thirds of either (a) or (c). This simple relationship is to be expected as there is one initiation site for each cell and, as faces are shared between adjacent cells, there are three edges per cell. Also a simulation has shown that in the "either (a) or (c)" boundaries about one-third will be (a) and two-thirds (c). Therefore the overall result is 56% of (a) and 44% of (c). Alternatively the particles which initiate cleavage cracks may lie on grain faces, as in figure 4, on grain edges or at grain corners. However models similar to that given above for the grain interior case give at least approximately the same result.

The models therefore indicate that, overall, approximately 17% of the area of 56% of the grain boundaries and 45% of 44% of the grain boundaries must fracture to link cleavage cracks together. On average this give a result of 29%.. To estimate the proportion of intergranular failure as opposed to cleavage failure it is now necessary to deduce the average area of a grain boundary and of a cleavage plane. If it is assumed that the volume of the 14-hedral grains is unity it can easily be shown that the average area of the square and hexagonal faces is about 0.4. Also approximating the 14-hedron by a sphere the average area of a cleavage plane is found to be about 0.8. The ratio is therefore about one-half. Also each cleavage plane intersects on average 6 grain boundaries, each of which is shared between two grains. Thus there are three times as many partially failed grain boundaries as cleavage planes. Hence the proportion of grain boundary failure is about $(3 \times 0.5 \times 0.29)/(1+ 3 \times 0.5 \times 0.29)$ or 30%.

CONCLUSIONS

The theoretical model now incorporates crack nucleation at precipitate particles but this does not influence predictions of the earlier work. Therefore other explanations must be sought for the major discrepancy between the predictions and experimental results. One possibility is that cleavage is effectively occurring on planes other than {100}. For example, if it occurred on {110} six crystallographically distinct variants rather than three would be available. This would reduce the predictions to about 15%. Also if both {100} and {110} were available, giving a total of nine variants, the predictions would be further reduced to about 10%. However, much of the observed intergranular failure appears to involve the fracture of complete boundaries, which is not included in the predictions, so that there is still a large difference between theory and experiment. A plausible explanation is that, in at least some grains, cleavage occurs on a combination of two or more planes. Experiments are currently being carried out to test this proposal.

ACKNOWLEDGEMENT

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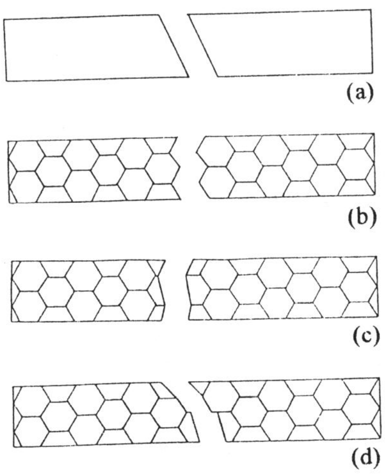

Figure 1. Schematic representations of cleavage and intergranular fracture in: (a) a single crystal, (b-d) polycrystals.

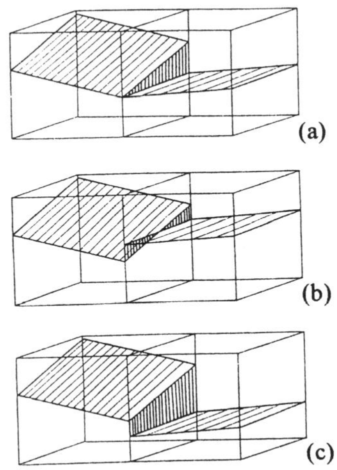

Figure 2. Schematic representations of intergranular fracture linking cleavage cracks in two adjacent cubic grains.

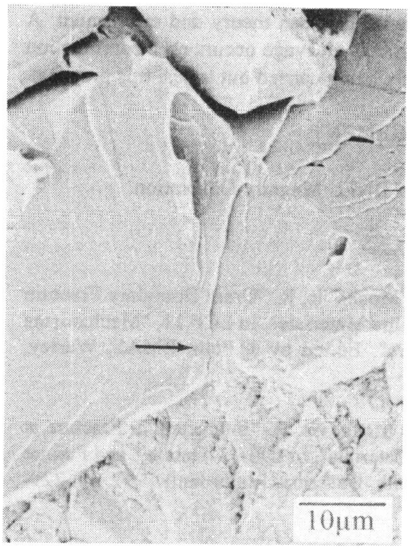

Figure 3. Fracture surface in C-Mn steel. Cleavage crack initiation from a carbide precipitate within a grain.

Figure 4. Fracture surface in alpha-iron. Cleavage crack initiation from a grain boundary non-metallic inclusion.

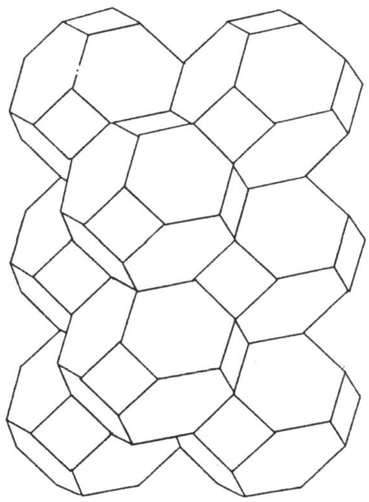

Figure 5. Eight space-filling regular 14-faced polyhedra stacked to form a body centred cubic array.

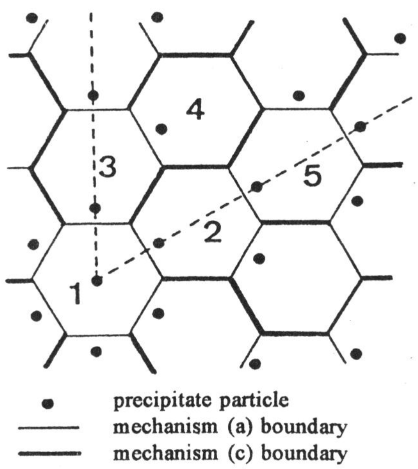

Figure 6. Schematic illustration of the propagation of a brittle crack across an hexagonal-prism model polycrystal.