# GRAIN BOUNDARY FRACTURE IN THE CLEAVAGE REGIME OF POLYCRYSTALLINE METALS

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In general, active cleavage planes in two adjacent grains of a polycrystal do not meet in a line in the common grain boundary. Therefore some grain boundary failure is necessary to link the two cracks. It is shown, using a three-dimensional model, that four different grain boundary failure mechanisms are possible. High resolution scanning electron microscopy of fracture surfaces in α-iron has confirmed that these mechanisms occur in practice. The model predicts that about 30% of the fracture will have occurred by grain boundary failure, whereas the experiments on α-iron give a value of about 20%. It is suggested that this discrepancy is because of the occurrence of cleavage steps and a proportion of ductile failure. These possibilities are being included in a computer based model currently being developed.

## INTRODUCTION

With decreasing temperature, the fracture mode of α-iron and ferritic steels changes from ductile to brittle, the latter occurring primarily by transgranular cleavage. However, brittle fracture may also occur by intergranular cracking and Abbott et al (1), using simple two-dimensional geometrical arguments, have shown that a small proportion of this mode of failure is also expected to occur. Moreover, intergranular fracture is promoted by the reduction of the fracture energy as a result of segregation of impurities to grain boundaries. The preferred cleavage planes are {100} and, in general, variants of these planes in adjacent grains will not meet in a line in their common grain boundary. Therefore, some localised grain boundary fracture will be necessary to link together cracks on these planes. Using three-dimensional theoretical models, it is shown that grain boundary failure may then occur by one of four distinct mechanisms, shown schematically and labelled I, II III and IV in Figure 1. Estimates are given of the proportions of these types which should arise and the extent of grain boundary failure which this implies. Results are

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then presented for observations on fracture surfaces of α-iron, which are relevant to ferritic steels, and these are compared with the predictions of the models.

## THREE-DIMENSIONAL GEOMETRICAL MODELS

To estimate the fraction of grain boundary failure acompanying cleavage, it is necessary to deduce first the average amount of failure associated with each of the four mechanisms shown in Figure 1. On average, the three potential cleavage planes (pcps) in the second grain will intersect the grain boundary at angles of 60° to each other. This means that, the angle between the trace of the cleavage crack in grain 1 and the trace of the nearest pcp in grain 2 will, on average, be 15°. However the nearest pcp may not be oriented favourably with respect to the stress axis so that it may be necessary for grain 2 to fail on the second nearest pcp, the corresponding angle being 45°. Assume that the occurrence of these two cases will be inversely proportional to the angles 15° and 45°, ie 3:1. The average angle between the traces of the two cracks will then be about 22½°. Thus, for mechanism I, on average, about 12½% of the boundary must fail. Mechanisms II and IV give, approximately, the same answer but mechanism III gives a value of about 37%.

Consider a crack nucleating within grain 1 and examine its propagation through the polycrystal. When it impinges upon grain 2 it may nucleate a second crack at its point of contact with boundary 1/2, Figure 2a. This would result in grain boundary failure mechanism I of Figure 1. Alternatively, it may spread further in grain 1 until it reaches the edge 1/2/3 between grains 1, 2 and 3. A cleavage crack in grain 2 may then nucleate at this point, Figure 2b. In this case grain boundary failure mechanism II will arise. The next stage of the process will involve the crack propagating into grain 3. This may occur either at face 1/3 or at edge 1/2/3, Figures 2c and 2d respectively. These cases will be labelled I/I and I/II respectively, indicating the types of failure arising at the two grain boundaries. If now the existing cleavage cracks in grains 2 and 3 extend they will meet boundary 2/3. Two possibilities arise as they may not intersect each other, giving the geometry of mechanism III, or intersect giving that of mechanism IV. The four distinct possibilities of Figures 2e-2h then arise and are defined by I/I/IV, I/I/III, I/II/III and I/II/IV. Finally if the mechanism II cracks of Figure 2b propagate into grain 3 from the edge 1/2/3, the arrangement II/II/II of Figure 2i is obtained. It can readily be shown that the same mechanisms arise if the initial crack nucleates at a grain face, a grain edge or a grain corner, rather than within a grain.

This model can now be used to estimate the proportions of mechanisms I, II III and IV which are likely to arise in an extended fracture surface. This involves a great deal of detailed analysis which will be presented elsewhere. The essential point is that, as fracture spreads, the crack front becomes straighter and therefore meets new grains at edges and not at faces. This implies that, overall, roughly half of grain boundary failure mechanisms are of type II. The other half are either of type III or of type IV. A rough calculation indicates that on average about two-thirds of these will be of type III and one-third of type IV. Therefore, over a general fracture surface, very few boundaries will fail by mechanism I, one-half by mechanism II and one-sixth by mechanism IV, in both of which approximately 12½% of the grain boundary area is fractured, and about one-third by mechanism III, in which approximately 37% of the area is fractured. On this basis, subject to the constraints and assumptions of this geometrical model, about 20% of the area of affected grain boundaries will fail.

In order to estimate the proportion of grain boundary failure as opposed to cleavage failure, it is now necessary to deduce (a) the average area of the grain boundaries, (b) the average area of the cleavage planes and (c) the number of partially failed grain boundaries for each active cleavage plane. To obtain (a) assume that on average grains are regular tetrakaidecahedra of unit volume. These have six square faces and eight regular hexagonal faces, the average area being about 0.4. To obtain (b) it is convenient to replace the 14-hedron by a sphere of unit volume, which has an average cross-sectional area of about 0.8. The ratio of these areas is therefore about 1/2. To obtain (c), note that each cleavage plane will meet on average about six grain boundaries (Crocker and Smith (2)). However each of these is shared between two grains so that there are three partially failed grain boundaries for each cleavage plane. Hence the percentage of grain boundary failure is approximately 1/2 x 3 x 20% = 30%. This figure is surprisingly high and therefore the model and assumptions used need to be discussed thoroughly. However before doing this our experimental work will be presented.

## EXPERIMENTAL PROCEDURE AND RESULTS

The material selected was high purity $\alpha$-iron bar 3mm dia containing 230ppm oxygen and 260ppm nitrogen heat treated at 1243K for 900s and air cooled. This heat treatment produced a ~80μm (mean linear intercept) grain size. Each specimen was fractured at a low temperature (~100K) and the fracture surfaces were examined using a JEOL JSM 840A scanning electron microscope operating at an accelerating voltage of ~15KeV. The area fraction of intergranular failure was measured in the secondary electron imaging mode.

Observations of the fracture surfaces of the $\alpha$-iron specimens fractured at ~100K, which is below the ductile to brittle transition temperature, are summarised in Figure 3. The fracture mode is predominantly cleavage with a proportion of intergranular fracture. The area fraction of intergranular fracture was measured at low magnification x250 and this corresponded to ~15% of the fracture surface. At this low magnification only areas of significant intergranular fracture are measured and there is clearly evidence of small additional amounts of intergranular fracture associated with specific fractographic features of the cleavage crack when passing from one grain to the next. These were examined in detail at higher magnifications and at 1000x the total proportion measured approaches ~20%. Figures 4a-c are examples of the main interactions leading to the different types of grain boundary fracture geometries, Figure 1. In addition Figure 4d provides an example of a simple interaction where accommodation at the grain boundary is by multiple cleavage steps.

## DISCUSSION

The theoretical model of crack propagation in polycrystalline materials, which has been developed in this paper, is based on three-dimensional geometry and has shown that four different mechanisms of grain boundary failure may arise. The occurrence of these mechanisms has been confirmed in α-iron using high resolution scanning electron microscopy techniques. The model currently assumes that the misalignment between cleavage planes in adjacent grains is accommodated solely by intergranular cracking. This approach has yielded an estimate of about 30% for the proportion of grain boundary failure. Experimentally we have shown that this figure is about 20% for α-iron but it should be noted that in ferritic steels it can be as low as 2%. This difference may be accounted for by different methods of measurement. However it is probably more realistic to assume that it is because of the presence of cleavage steps and ductile fracture. Also, because the grains in polycrystals are multiply-connected, alternative routes for cracks are available so that grain boundaries which require large failure areas can be avoided. Clearly the magnitude of the grain boundary surface energy and the orientation of the applied stress are also important. These factors need to be taken into account more comprehensively in the model if a better correlation with experimental observations is to be obtained. However the present work does demonstrate that geometrical factors have a major influence on crack propagation in polycrystalline materials in the cleavage regime. More general computer based models of the phenomenon are currently being developed.

## ACKNOWLEDGEMENT

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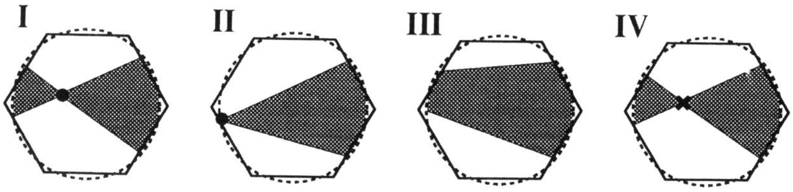


Figure 1 The four distinct mechanisms for grain boundary failure. The boundary is represented here by a regular hexagon but in practice the circle of equal area has been used. The part of the boundary which must fail is indicated by shading, the straight edges of which are the traces of the two cleavage planes. Crack nucleation and intersection points are shown by dots and crosses respectively.

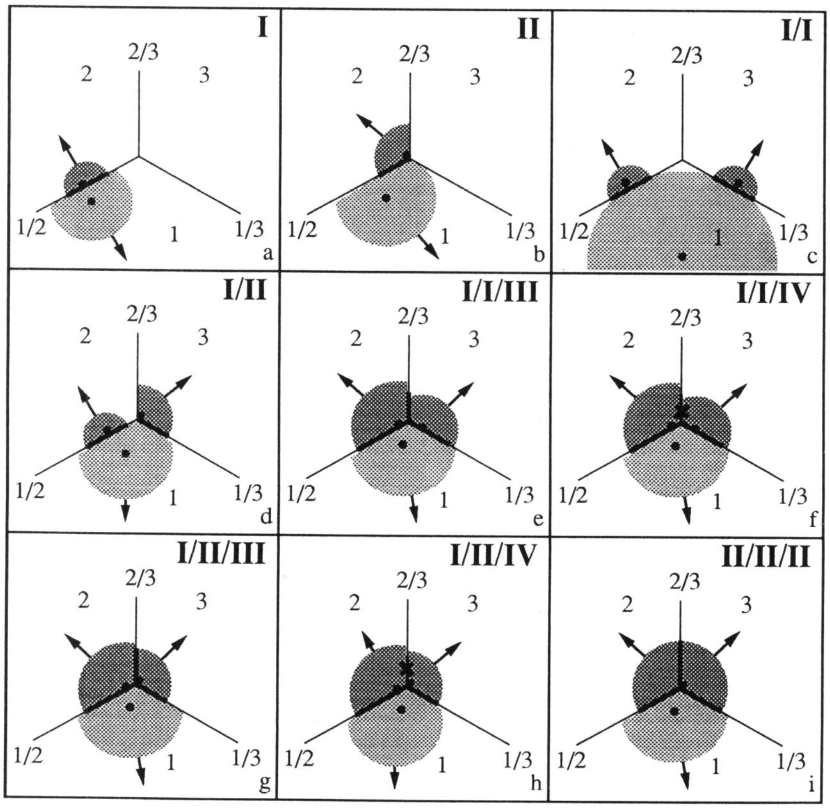


Figure 2 Schematic mechanisms for the propagation of a cleavage crack (shaded) from grain 1 into grains 2 and 3. Grain boundary failure is indicated by bold lines. Mechanisms I, II, III and IV and the dots and crosses are defined in Figure 1.

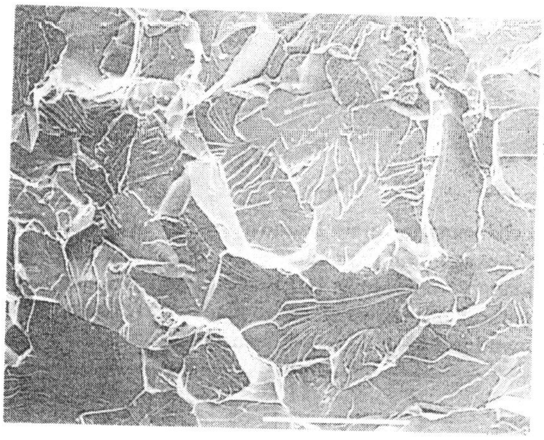

Figure 3 Secondary electron image of an $\alpha$-iron fracture surface showing, predominantly cleavage fracture. The marker equals 100μm.

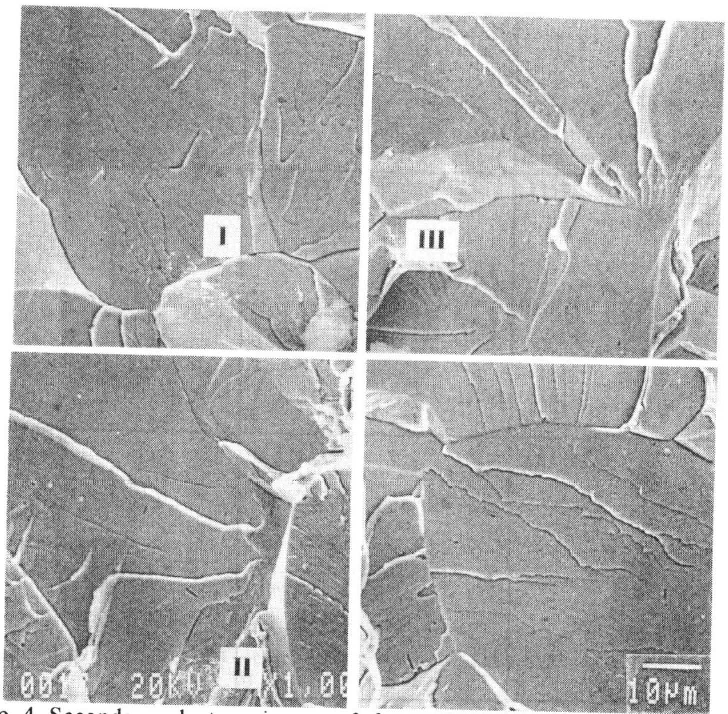


Figure 4 Secondary electron image of fracture surface showing intergranular cracking by means of mechanisms I, II and III (see Figure 1) and also cleavage step accommodation across boundaries.