BRITTLE FRACTURE OF POLYCRYSTALS: DEVELOPMENT OF A NEW THREE-DIMENSIONAL MODEL

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Abstract

A pseudo 3-d model of a polycrystal, based on a random array of columnar grains, has been developed further and applied to low temperature brittle fracture of ferritic steels. Cleavage fracture is allowed to propagate across the model but the results indicate that between 32% and about 60% of the overall fracture surface consists of accommodation, either brittle or ductile, at the grain boundaries. In addition, a genuine random 3-d model has been developed and is described. Further developments in the models and associated experimental work, which is currently being carried out, are discussed.

Introduction

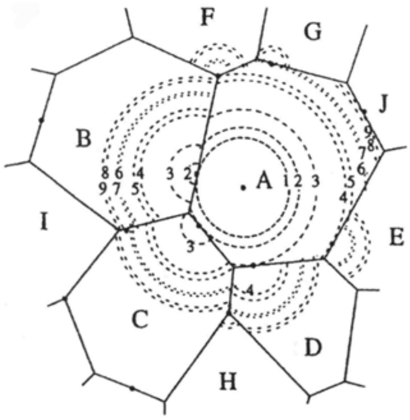
It has been reported previously that, in order to obtain a better understanding of the propagation of cleavage cracks across grain boundaries, a theoretical model of a polycrystal consisting of randomly-generated prismatic grains has been developed, Smith *et al*. [1]. In particular the case of ferritic steels, in which cleavage occurs on one of the three {100} planes, was considered. Using computer simulation a tensile stress was applied parallel to the prism axes and a brittle cleavage crack was allowed to nucleate and propagate across the model. As cleavage planes in adjacent grains do not in general meet in a line in their common grain boundary, propagation can only occur if some accommodating failure, brittle or ductile, takes place at this boundary. The results indicated that about 32% of the overall fracture surface consisted of this type of accommodation. This result was consistent with earlier predictions obtained using much simpler models, Crocker *et al*. [2], Smith *et al*. [3], Flewitt *et al*. [4], although it is much higher than that suggested by most experimental studies. However, fracture experiments carried out at a temperature of 77K on similarly loaded specimens containing columnar ferrite grains, which occur in the central regions of weld beads in C-Mn steels, do indicate that a substantial amount (between 10% and 20%) of grain boundary failure, in this case ductile, does occur [1].

The pseudo 3-d model has been developed in several ways and new predictions obtained. These provide valuable additional information on the fracture of columnar grain structures and also a useful insight into the accommodation of cleavage fracture at grain boundaries in other polycrystalline materials. Clearly however for many applications there would be great advantages in using a genuine 3-d model. The simplest example of this type of model is the body-centred cubic array of regular tetrakaidecahedra (14-hedra), each with six square and eight hexagonal faces, Crocker and Smith [5]. However, the regularity of this structure casts doubts on its value in modelling real polycrystalline materials. A method of generating models of polycrystalline materials consisting of irregular polyhedra has therefore been developed and is currently being used to investigate the propagation of cracks. The present paper describes these developments and discusses the results.

The Basic Pseudo Three-Dimensional Model

The original pseudo 3-d model [1] was generated by erecting polygonal columnar grains from the cells of a 2-d model created by constructing Wigner-Seitz cells around randomly located grain nuclei. The grain edges and grain faces were all parallel to the common axis of the columns, which were of infinite length. Each grain was given a random crystallographic orientation and a uniaxial stress was applied parallel to the prism axes. Fracture was initiated at a randomly selected point on the particular cleavage plane in the whole model which was closest to being perpendicular to the stress axis. As the cleavage crack spread outwards from this point it was assumed that its projection on the plane perpendicular to the stress axis was circular. When this crack met a grain face or a grain edge, it was further assumed that it immediately initiated a new crack which propagated into the next grain at the same speed as the original crack. However, once a grain had started to fail no further cracks were allowed to penetrate into it.

An example of the use of this model is illustrated in Fig. 1. A cleavage crack is nucleated in grain A, spreads outwards as a projected circle and propagates across grain faces into grains B, C, D and E before meeting the vertical grain edge between grains A, B and F and propagating into F from this edge. It continues to propagate across a face into G, from edges into H and I and across a face into J. However, the arcs of circles shown in Fig. 1 are the projections of crack fronts on cleavage planes inclined differently in the different grains. Therefore, in order to link the separate cleavage cracks, some grain boundary failure must occur and Fig. 2 shows schematically four distinct mechanisms, I-IV, by means of which this may happen. When the crack propagates across a grain face, the grain boundary failure has the form of a double triangle, I, and when from a grain edge, a single triangle, II. When independent cracks meet a boundary from opposite sides two possibilities arise. They may cross, again giving a double triangle, III, or they may miss each other to give a quadrilateral,



IV. On average, IV has a greater area than II, which has a greater area than I and III so that the total area of grain boundary failure is governed by the proportions of these four mechanisms which arise in practice.

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 numbered sequentially 1 to 9.

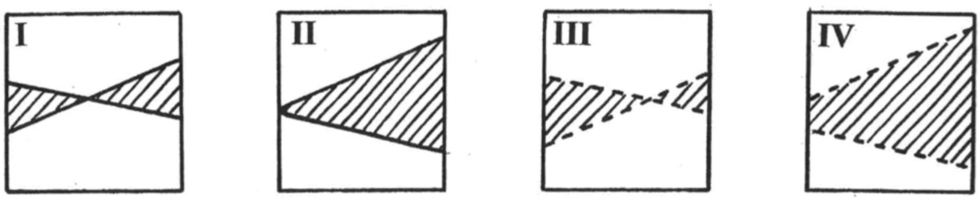


FIGURE 2. The four grain boundary failure mechanisms. The boundary is shown schematically as a square and the parts which must fail are indicated by shading, the straight edges of which are the traces of the two cleavage planes. In mechanisms I and II the crack crosses the boundary whereas in III and IV two cracks meet the boundary from opposite sides.

Developments of the Pseudo Three-Dimensional Model

Propagation from a single grain edge

The first development of the model was to assume that cracks could only propagate from grain edges. Physically, this means that the material has very strong grain boundaries but weak grain edges. To make comparisons easy, the same columnar polycrystal and crack nucleation site as that shown in Fig. 1 was used and the new sequence of events which arises is illustrated in Fig. 3(a). The crack first propagates simultaneously into B and C from the edge between A, B and C (ABC), it then propagates sequentially into D from ACD, E from ADE, F from ABF, H from CDH, G from AFG, I from BCI and J from AGJ. This is the same sequence as in Fig. 1, except that B and C are simultaneous and G and H are reversed. However, there is a significant difference in the proportions of mechanisms I to IV of Fig. 2 which occur. For a model in which a total of 31 grains have fractured by cleavage, when both grain boundary and grain edge propagation are allowed, it was shown previously that these proportions are 32%, 16%, 17% and 35% respectively [1]. These become 0%, 38%, 21% and 41% in the present case. Here the 0% for mechanism I arises because propagation across grain boundaries is not now permitted. This results in larger percentages for the other mechanisms, an increase in the proportion of grain boundary failure from 32% to 38% and an increase in the area of the fracture surface by 14%, with a corresponding increase in the overall fracture energy. If the model used was larger, the effect would have been greater as the proportion of mechanism IV, which involves on average the largest area of grain boundary failure, gradually increases as the fracture surface extends.

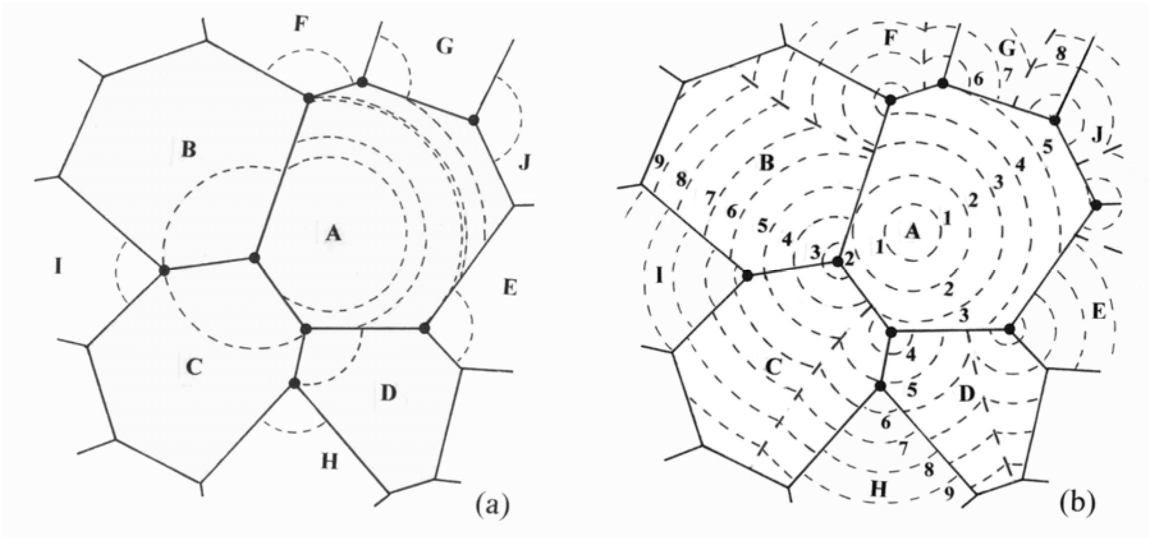


FIGURE 3. Cross-sections of a few grains of a model pseudo 3-d polycrystal. A cleavage crack nucleates in grain A and propagates into neighbouring grains at the sites on grain edges indicated by dots. In (a) only one crack is allowed in each grain but in (b) two parallel cracks from two different edges may nucleate and give rise to stepped cleavage planes, time increments being indicated by numbered broken circles and possible steps by bold slightly curved broken lines.

Propagation from two or more grain edges

In previous simulations, once a crack has propagated into a grain no other cracks have been allowed to penetrate it [6]. In practice however this may occur and therefore the above model has been extended to examine what ensues. It was again assumed that cracks would only propagate from grain edges and the same model was used. Fig. 3(b) shows the resulting propagation sequence. The crack nucleates in grain A and after 2.5 increments of time reaches edge ABC and immediately propagates into B and C. However, at time 3.3 the crack in A reaches ACD and propagates into C and D. There are then two cracks on parallel cleavage planes in C and at 4.3 the fronts of these lie vertically above one another in grain boundary AC, as shown in Fig. 3(b). As time progresses this superposition extends in a curved line across C until it meets its outer boundary. Meanwhile the crack in A reaches, in turn, edges ADE (at 4.5), ABF (4.6), AFG (5.0), AGJ (6.0) and AEJ (6.2) and parallel pairs of cleavage cracks are generated in D, B, F, G, E and J respectively. However before the last two events, at 5.2, the cracks propagating in C and D from ACD meet CDH and one or both of them propagates into H. Similarly at 5.6 the cracks in B and C propagating from ABC reach BCI and again one or both propagates into I. As the fracture surface continues to grow, three or more parallel cracks may occur in some grains. For example the cracks propagating in C and D from ACD reach two edges of H before the crack already propagating in H from CDH. Both therefore propagate into G, resulting in three cracks on parallel planes in this grain.

If a grain does have two or more parallel cleavage cracks, in order to complete the fracture process it is necessary to link them together. This generates steps on the fracture surface which may, for example, arise from failure on different variants of the cleavage plane. However, the simplest situation to consider is when vertical cracks, parallel to the prism axes, form along the slightly curved superposition lines marked in Fig. 3(b). In a particular grain the cleavage crack then has a single large vertical step. When this stepped crack meets a grain boundary it propagates from the two bounding grain edges so that the next grain also has a pair of parallel cleavage cracks. These will again be linked by a vertical step but in general this will not meet the first step. The area of the necessary grain boundary failure, and hence the energy, is substantially less than if there was only one unstepped cleavage plane in each grain. However, the total energy may be increased because of the areas of the steps on the cleavage planes within the grains. Stepped cleavage planes of the type discussed here have been observed in ferritic materials but their propagation into adjacent grains needs to be examined experimentally for the present geometry.

Bypassing an unfavourably oriented grain

The computer simulation procedures used above assume that, when a cleavage crack reaches a grain boundary or grain face, it immediately propagates into the next grain, regardless of the orientations of the possible cleavage planes in that grain. Clearly however, the grain is sometimes very badly oriented for cleavage. Also, neighbouring grains may have preferred cleavage planes inclined steeply in opposite directions resulting in large areas of grain boundary failure and leading to further large areas at later stages of the fracture process. In such cases the fracture surface may propagate entirely around a grain before it eventually fails. This failure may then be nucleated at any point around the surface of the grain and not be restricted to the place where the propagating crack first meets it. In this way the amount of grain boundary failure may be reduced substantially.

Grain I in the model shown in Fig. 1 has been used as an example of this situation. In the basic model a cleavage crack entered this grain from edge BCI. In the new model all five of its neighbouring grains were allowed to fail by cleavage propagation, either from grain faces or from grain edges. Then grain I was cleaved independently on the most favourably oriented cleavage plane at the height in the model which minimised the total grain boundary area that needed to fail in its five vertical grain faces. This reduced the area by 24% and hence the proportion of grain boundary failure to about 26%.

Stress axis not parallel to prism axis

In all previous applications of the pseudo 3-d model the stress axis has been assumed to be parallel to the common axis of the columnar grains. This restriction has now been removed in order to enable the results to be compared with related experimental observations. The same model as that illustrated in Fig. 1 was adopted and stress axes at approximately 45^{o}, 60^{o} and 80^{o} to the prism axes investigated. It is again assumed that in each grain the fracture front is circular when viewed in the plane perpendicular to the stress axis but these circles will, of course, now project as ellipses in the plane perpendicular to the prism axis. The results are very scattered as they depend critically on the orientation of the stress axis relative to the active cleavage planes as well as to the prism axis. However in all cases a substantially higher proportion of grain boundary failure is found, increasing on average from 32% for 0º tilt, to 48% for 45º, 63% for 60º and 59% for 80º. Again in a few cases grain I was treated as a rogue grain and this reduced the proportion of grain boundary failure by a few percent. In all of these cases, but especially for 80^{o} tilt, the total area of the fracture surface increases substantially and the fracture facets are elongated.

The Basic Three-Dimensional Model

The model of a 3-d polycrystalline material which has been used previously is the body centred cubic array of identical tetrakaidecahedra (14-hedra), with six square and eight regular hexagonal faces. A single 14-hedral grain is shown in Fig. 4(a). It has 36 edges and 24 vertices, satisfying the well-known Euler formula V - E + F = 2, where V, E and F are the numbers of vertices, edges and faces respectively. On average the faces have 5.14 vertices. This model describes a structure in equilibrium if all the square faces have the same energy Es, all the hexagonal faces have the same energy Eh, and Es/Eh = 1.1548. The case of Es/Eh = 1 can be simulated by allowing the hexagonal faces of the 14-hedra to become curved and other modifications have been considered.[5,7]

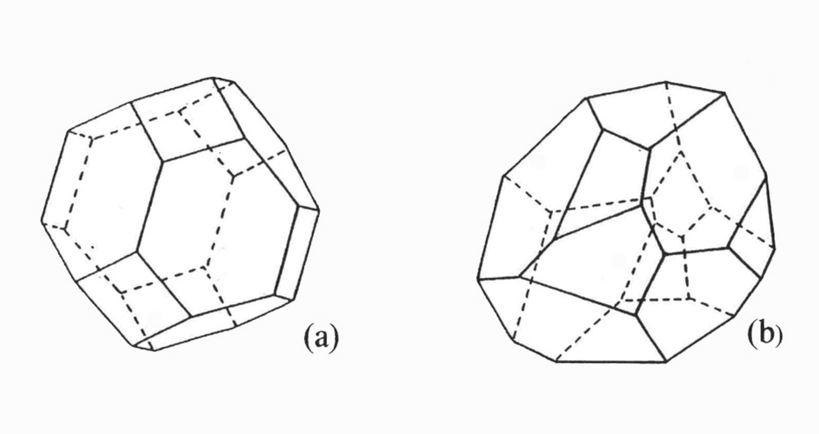


FIGURE 4. Individual grains of model 3-d polycrystals: (a) the regular 14-hedron, (b) a randomly generated polyhedron with 16 faces. The bold lines represent faces on the front of the model and the broken fine lines those on the back.

When this model is used to simulate low-temperature fracture propagation in ferritic materials, a crystallographic orientation is allocated randomly to each grain. Fracture on one of the three {100} cleavage planes is then allowed to occur and it has been shown that cracks in adjacent grains meet their common grain boundary in traces which, on average, are at an angle of about 22.5^{o} to each other. These cracks meet in one of the four configurations shown in Fig. 2 and it has been deduced that in order to link the cracks together, overall, about 20% of the area of the affected boundaries needs to fail. Also, the average area of a cleavage crack is about twice as large as that of a grain boundary and there are, overall, three times as many partially failed grain boundaries as cleavage cracks. It is then concluded that the percentage of intergranular failure is 0.5 x 3 x 20%, i.e. 30%. A slightly different procedure gives 35%.[3]

Developments of the Three-Dimensional Model

Clearly any predictions concerning fracture or any other phenomenon in real polycrystalline materials, which are based on a 3-d model consisting of a regular array of 14-hedra, are open to question. A much more general model in which the grains are represented by irregular polyhedra is therefore now being developed. This model is based on a random distribution of grain nuclei around which Wigner-Seitz cells are drawn to define the grain faces, edges and vertices. Unfortunately, it is not easy to portray the resulting structure graphically and therefore, in the example given in Fig. 4(b) only one complete grain is shown. This particular grain has 16 faces, four with 4 edges, four with 5 and eight with 6, giving an average of 5.25. In all there are 42 grain edges and 28 vertices, again satisfying the Euler formula.

Returning to the whole model, which may contain a large number of grains, a scale is chosen which defines the average grain size. A distribution of crystallographic orientations, random or otherwise, is then allocated to the grains. Next, an appropriate family of potential cleavage planes and a cleavage fracture energy are selected. A distribution of fracture energies is then allocated to the grain boundaries and a stress axis is specified. The grain with the most favourably oriented cleavage plane is selected for failure and a crack is nucleated at a random point on this plane. This is allowed to spread until it reaches the surrounding grain boundaries, which will number between 3 and 10 or more, and the corresponding grain edges. Criteria are then used to decide if and how the crack will propagate across or around the surrounding grains. For example, cracks may cross grain boundaries or continue from grain edges, as in the cases considered for pseudo 3-d models discussed above. Alternatively, cracks may follow grain boundaries or new cracks may be nucleated ahead of the crack tips within neighbouring grains. These criteria are based on appropriate energies for the different defects.

As discussed above, cleavage cracks in adjacent grains will not meet in a line in their common boundary and therefore partial grain boundary failure by one of the mechanisms illustrated schematically in Fig. 2 will have to occur. The model enables the extent of this to be determined and therefore the proportion of cleavage to grain boundary failure established. The simulation is repeated many times and average values obtained. As yet only preliminary results using this generalised 3-d model have been obtained and it is not appropriate to report them in detail here. However they do tend to support the general conclusions of earlier 2-d and pseudo 3-d simulations.[1-6]

Discussion

This paper has examined several ways in which computer simulation studies of fracture in polycrystalline materials based on geometrical considerations have been and are being extended. Other modifications have also been made or are being considered. These include restricting the height of the prisms and delaying the propagation of cleavage cracks across grain boundaries and edges in the pseudo 3-d models and introducing substructure into the grains of the 3-d models. In addition the effect of grain size on fracture, particularly at the nano-scale, is being investigated. Again, much of the research has concentrated on brittle fracture but recently the ductile-to-brittle transition region in ferritic steels has been investigated.[8] However all of these simulations depend on the availability of detailed and reliable experimental observations to use as input data.

There are two areas, in particular, that would validate and challenge the predictions of these 3-d geometrical models. To date, the model for fracture in columnar grains has been compared with the technologically important low temperature brittle crack propagation in a bead of C-Mn steel weld metal [1]. However the comparison has been restricted to fracture when the stress is applied parallel to the direction of the columns. These experiments revealed that at a temperature of 77K the propagation of cleavage cracks from grain to grain was accommodated by ductile fracture at the near vertical grain boundaries. There is a need to examine the effect of varying the direction of the applied stress from this orientation through to being normal to the columns on the overall fracture path. This may lead to a change from the ductile accommodation fracture to brittle intergranular fracture as the shear stress across the grain boundaries reduces. In the second area considerations have been associated with bcc polycrystalline ferritic materials where there are three variants of the {100} cleavage planes in each grain. It would be instructive to examine both columnar and equiaxed polycrystalline hcp metals such as zinc or zirconium where there is a restriction of cleavage to the basal plane. This would test rigorously aspects of the role of grain orientation described above. Close collaboration between those carrying out experimental work on fracture and those using models to simulate the propagation of cracks is essential if a better understanding of the underlying processes is to be developed.

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