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MINIMUM SURFACE FORMATION ENERGY FOR THREE-DIMENSIONAL INTERGRANULAR FRACTURE

E. A. HOLM, G. N. McGOVNEY
Sandia National Laboratories, Albuquerque, NM 87185-1411

ABSTRACT

The minimum expended energy for fracture is the free energy required to form two new surfaces. For intergranular fracture, the minimum surface formation energy is complicated by the rough fracture surface, with area greater than the specimen cross-section. We utilize network optimization algorithms (max-flow/min-cut) to determine the minimum surface formation energies and surfaces for intergranular fracture in 3D polycrystals. For equiaxed grains and uniform boundary strength, the minimum energy fracture area is independent of grain size and is 45% larger than the specimen cross-section, and intergranular fracture will occur when surface energy is less than 1.6 times the grain boundary energy. The 3D fracture area is larger than projected from 2D systems. In systems with microcracked boundaries, the fracture surface deviates to preferentially include microcracked boundaries, creating interlocking grain configurations. Two-dimensional percolation of microcracks occurs at about 80% microcracked boundaries.

INTRODUCTION

In brittle materials, the energy for fracture includes a variety of thermodynamic and kinetic contributions. The minimum energy E_f which must be expended to fracture a specimen is the free energy required to form two new surfaces

$$E_f = \Delta E A \tag{1}$$

where ΔE is the surface formation energy per unit area and A is the surface area of the fracture.

For a material which fractures by cleavage (transgranular fracture), ΔE is the energy of forming two new surfaces from the bulk, 2σ, where σ is the surface free energy per unit area. For materials which fracture along grain boundaries (intergranular fracture), ΔE is the energy for forming two new surfaces minus the free energy per unit area of the original grain boundary γ, so

$$\Delta E = 2\sigma - \gamma \tag{2}$$

In transgranular fracture, the surface formation energy is computed assuming the crack is planar; thus, A is the cross-sectional area of the specimen. For intergranular fracture, the surface formation energy is complicated by the rough fracture surface, with area greater than the specimen cross-section.

Dynamic processes such as plasticity, crack branching, crack bridging and healing all add to the fracture energy. However, the surface formation energy E_f provides a minimum expended energy below which fracture cannot occur. Therefore, it is useful to characterize E_f for systems and fracture processes of interest. In this paper, we determine and analyze E_f for intergranular fracture in three-dimensional (3D) equiaxed polycrystals with and without microcracks.

FRACTURE MODEL

To find the minimum surface formation energy for intergranular fracture, we must identify a surface which divides a polycrystal into two parts while conforming to the grain boundaries and minimizing surface formation energy. Such surfaces may be found by various

network algorithms. A two-dimensional (2D) approach, which uses Djikstra's algorithm on the graph of grain vertices and edges, is described in [1]. That scheme cannot be used on 3D grain structures, however.

To solve the 3D problem, we use a graph which is the dual of the grain boundary structure. The grain centroids are the nodes of the graph. Centroids of neighboring grains are connected by edges of the graph, so that each edge represents the boundary between two grains. Each edge is given a capacity that corresponds to the surface formation energy for fracturing that boundary. This scheme is shown in Figure 1.

This graph is a capacitated network, defined as a graph consisting of nodes, edges which connect nodes, and capacities associated with each edge. The top and bottom surfaces of the sample are defined as source and sink nodes. The maximum flow (max-flow) a network can sustain is the largest numerical flow which can move from the source to the sink, node to node via the connecting edges, with no edge carrying more flow than its capacity. The minimum cut (min-cut) is the separation of the network into two networks, with the source in one new network and the sink in the other, such that the sum of the capacities of the broken edges is minimal. Ford and Fulkerson [2] proved that the max-flow in a network occurs across the min-cut and developed a polynomial-time algorithm to determine the max-flow. Edmonds and Karp [3] modified the algorithm to guarantee convergence in the case of non-integer capacities.

The max-flow/min-cut algorithm proceeds by associating a flow value with each edge in the network, initially set to zero. An attempt is made to push an infinite amount of flow out of the source, limited by the flow available in the edges leaving the node. This process is repeated for each node reached by the new flow until some incremental flow reaches the sink. When this happens the flow values of all edges in the path that this new flow took are updated to reflect the increase. This procedure is repeated, each time augmenting the flow from the source to the sink, until a path to push even the smallest flow increase to the sink cannot be found. The resulting flow reaching the sink is the max-flow, and also the value of the min-cut.

For a grain structure graph, the minimum surface formation energy fracture is the surface which divides the graph into two pieces while cutting edges with the minimum total edge capacity, i.e. the min-cut. Therefore, the max-flow/min-cut algorithm can provide both the position and surface formation energy for the minimum energy fracture.

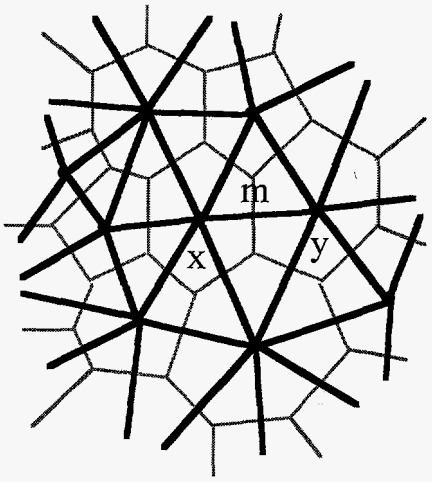

Figure 1. A grain structure (gray lines) represented by the graph of its dual. Nodes of the graph (dots) are the grain centroids; edges (black lines) connect centroids of neighboring grains. The capacity of an edge is its surface formation energy. Here, the boundary between grains x and y has surface formation energy of m units.

DISCLAIMER

All grain structures in this study were equiaxed, single phase polycrystalline microstructures produced using a 3D Monte Carlo Potts Model grain growth simulation [4-6]. Although the fracture model can operate on digitized experimental microstructures, simulated microstructures were used to allow a consistent 3D representation and to ensure equivalence between specimens in all but the desired varying characteristics.

Because we are interested only in surface formation energy, we ignore mechanical processes in crack propagation, including plasticity, crack branching, crack bridging and healing.

RESULTS AND DISCUSSION

Equiaxed Polycrystals

Figure 2 shows a typical intergranular fracture surface which globally minimizes surface formation energy in an equiaxed microstructure with uniform boundary strength. The crack forms a relatively smooth surface, and interlocking grain configurations which could cause crack bridging are absent.

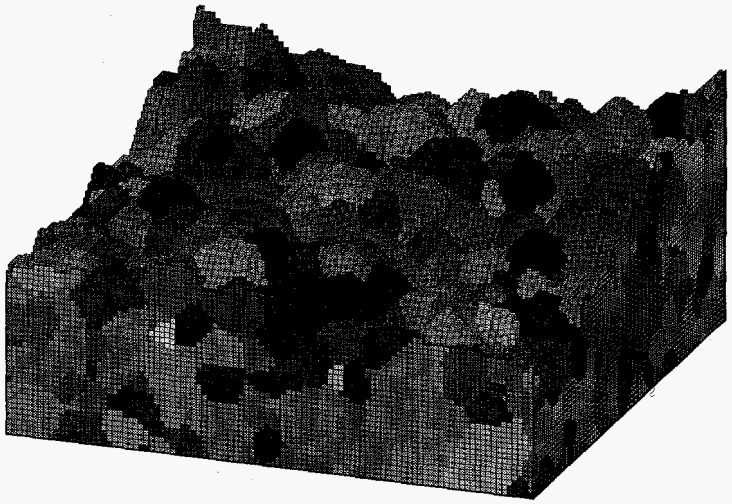

Figure 2. Intergranular fracture surface of minimum surface formation energy for an equiaxed 3D polycrystal with uniform boundary strength. Sample size is 200x100x100 sites, and the average grain radius is 6.6 sites.

The minimum energy fracture area is about 1.45 times the cross-sectional area and does not vary with grain size, as shown in Figure 3. Therefore, in equiaxed structures, the minimum energy intergranular crack surface is about 45% larger than a cleavage fracture.

Also plotted in Figure 3 is the minimum surface formation energy crack length for 2D grain structures. In two dimensions, the minimum energy fracture is about 1.1 times the sample width (very close to the length expected for a perfect hexagonal array of grains) and does not vary with grain size [1]. A 2D path 1.1 times as long as its end-to-end width extrapolates to a 3D surface of area 1.2 times the cross-sectional area. Actual 3D fracture surfaces are of considerably larger area. This indicates that 2D and 3D fracture surfaces are fundamentally different. This is not surprising considering the difference in boundary topology in two and three dimensions. In particular, the requirements of connectivity prevent each slice of the 3D surface from being a minimum length 2D path. Since the 3D minimum energy fracture is not a composite of 2D minimum fractures, its area is necessarily larger than that extrapolated from the 2D results.

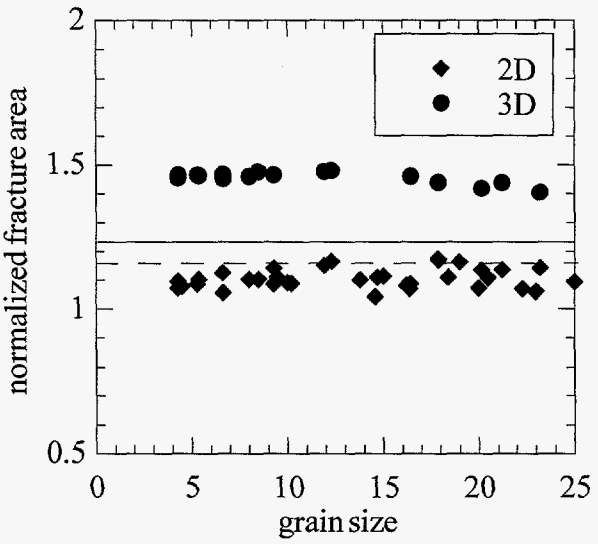

Figure 3. Minimum surface formation energy intergranular fracture surface size as a function of equiaxed grain size in 2D (diamonds) and 3D (circles). Fracture size is shown normalized by the sample width (2D) or cross-sectional area (3D). Fracture size does not change with grain size. In 2D, fracture length is approximately the same as for a perfect hexagonal grain array (dotted line). In 3D, fracture area is much larger than extrapolated from the 2D result (solid line).

The observation that the minimum energy intergranular fracture is 1.45 times larger than a transgranular cleavage plane allows us to calculate an energetic criterion for intergranular fracture in 3D. Intergranular fracture is preferred when the intergranular fracture energy E_i is less than the transgranular cleavage energy E_t. From equations (1) and (2), this occurs when

$$(2\sigma - \gamma)A < 2\sigma A_0 \qquad (3)$$

where A is the intergranular fracture area and A_0 is the cross-sectional area of the specimen. If $A = 1.45A_0$, intergranular fracture is energetically preferred when

$$\sigma < 1.6\,\gamma \qquad (4)$$

When surfaces are energetically inexpensive, the crack will follow a more tortuous path to eliminate grain boundary. In typical pure metals, $\sigma \sim 3\gamma$ [7]; therefore, we do not expect intergranular fracture in equiaxed microstructures. This is consistent with experimental observations. However, if the grain boundary energy is increased or the surface energy is decreased (i.e. by contamination of grain boundaries), intergranular fracture can and does occur.

Microcracked Polycrystals

Anisotropic effects such as thermal expansion anisotropy or preferential solute segregation can cause grain boundaries to have non-uniform properties. In particular, the surface formation energy of boundaries may vary across a polycrystal, with some boundaries having a very low surface formation energy. As surface formation energy decreases, boundaries become similar to microcracks and can dramatically affect intergranular fracture.

We consider a system in which special boundaries have a surface formation energy ΔE_s which is much lower than the surface formation energy for normal boundaries ΔE_n; here $\Delta E_s = 0.01\Delta E_n$. We assign a fraction f of the boundaries in the system at random to be special

boundaries, and the average surface formation energy in the system is $<\Delta E> = f\Delta E_s + (1 - f)\Delta E_n$.

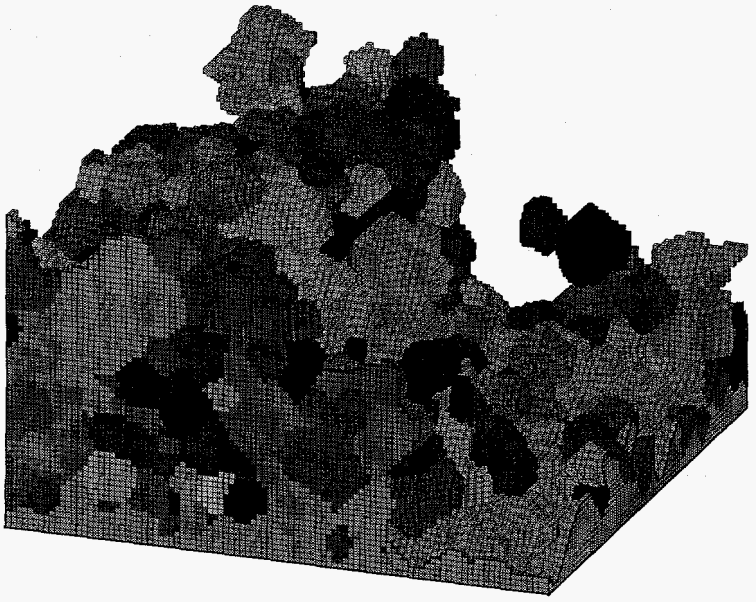

Figure 4. Intergranular fracture surface of minimum surface formation energy for an equiaxed 3D polycrystal with $f = 0.8$ very low surface formation energy boundaries (microcracks). Sample size is 200x100x100 sites, and the average grain radius is 6.6 sites. Note the convoluted fracture surface which includes geometrically interlocking grains.

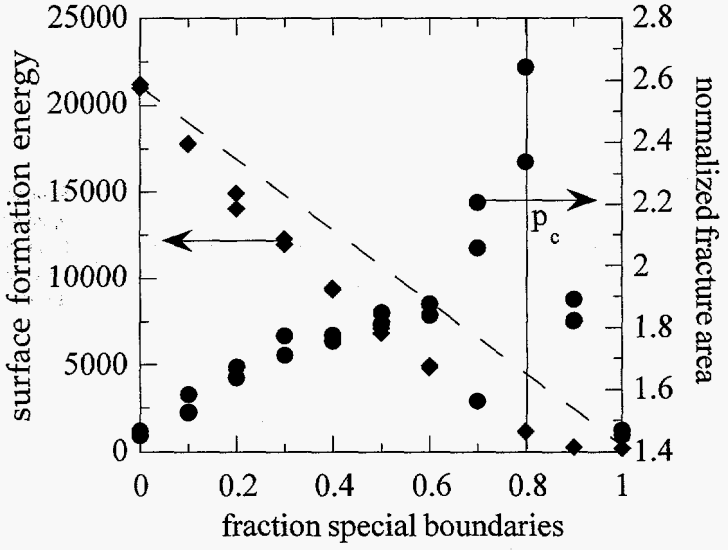

Figure 5. Intergranular fracture surface area (circles) and surface formation energy (diamonds) as a function of fraction microcracked boundaries. Fracture area is shown normalized by the cross-sectional area. The maximum surface area fracture occurs at the 2D percolation threshold for microcracks, p_c. Surface formation energy is lower than predicted from the average surface formation energy per unit area in the system (dashed line), indicating that low surface formation energy boundaries are preferentially included in the fracture surface.

Because the special boundaries have significantly lower surface formation energy per unit area, the fracture surface may deviate in order to include them, as shown in Figure 4. These

deviations may lead to geometrically interlocking grains (i.e. crack bridging). The minimum energy fracture area is significantly higher than the uniform boundary case for all mixtures of special and normal boundaries, with a peak near $f = 0.8$, as shown in Figure 5. In addition the surface formation energy for fracture is smaller than predicted from the average surface formation energy in the system, indicating that fracture surfaces preferentially choose the low surface formation energy special boundaries. There is no effect of grain size on these results.

The percolation threshold, where a connected surface of special boundaries spans the system, occurs when $f \sim 0.8$. At this point, the minimum energy fracture surface has the largest area and the highest roughness. Note that typical percolation problems entail the formation of a one-dimensional path across a specimen. Fracture percolation, however, is the formation of a continuous 2D surface. Such percolation problems are computationally challenging; in fact, the max-flow/min-cut algorithm used here is an efficient way to find such percolation thresholds.

CONCLUSIONS

Max-flow/min-cut network optimization algorithms allow efficient determination of the minimum surface formation energies and surfaces for intergranular fracture in 3D polycrystals. For equiaxed grains and uniform boundary strength, the minimum energy fracture area is independent of grain size and is 45% larger than the specimen cross-section. For such systems, intergranular fracture will occur when surface energy is less than 1.6 times the grain boundary energy. The 3D fracture area is larger than projected from 2D systems, indicating that the propagation of linear and planar cracks is fundamentally different. In systems with microcracked boundaries, the fracture surface deviates to preferentially include microcracked boundaries, allowing interlocking grain configurations. Two-dimensional percolation of microcracks occurs at about 80% microcracked boundaries.

ACKNOWLEGEMENTS

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