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Cleavage Resistance of Fine-Structured Materials

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Based on a previous bicrystal fracture experiment, the resistance offered by a narrow high-angle grain boundary to cleavage cracking is analyzed theoretically. It is predicted that, when the grain boundary width is smaller than the distance between break-through points, the grain boundary toughness will be highly dependent on the characteristic microstructure length. Analytical expressions are obtained for freestanding thin films and fine-grained materials.

Keywords: cleavage cracking, grain boundary, toughness

1. INTRODUCTION

The rapidly progressing processing techniques of fine-structured materials have received wide applications [1]. In general, decreases in grain sizes result in considerable increases in yield strengths [2]. However, this beneficial effect diminishes as the grain size becomes smaller than a few nanometers, probably due to the high defect density [3]. It is, therefore, important to understand the behaviors of materials with characteristic microstructure lengths at the sub-micrometer level. In this study, we analyze the cleavage cracking resistance.

In a previous bicrystal fracture experiment of a coarse-grained iron-silicon alloy [4], it was confirmed that, in a brittle polycrystalline material, the resistance to transgranular cleavage cracking is governed by the grain boundaries at the cleavage front, since the geometrically necessary crack front branching would lead to a 3-fold rise in fracture toughness over the single crystal. A grain boundary is overcome by the cleavage crack nearly simultaneously at a number of locations, namely, the break-through points [5,6], as shown in Fig. 1. Around each break-through point, the grain boundary yields as the crack front penetrates across it; farther away from the break-through points, the grain boundary is difficult to break apart and thus persistent grain boundary areas (PGBA), which will be separated later by shear fracture or ligament bending, are formed [7]. According to a statistical analysis, the distance between the break-through points, w, which is in the range of 0.1-10 μm, is somewhat independent of the crystallographic misorientations and therefore can be regarded as a material constant.

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If the grain boundary width is much larger than w, the grain-boundary fracture resistance, G_{GB}, is determined by the average effect of the break-through points; that is, the variation in w would not affect G_{GB}. In a thin film or a fine-grained material, on the other hand, the grain boundary width, d, is comparable with w, and the space is sufficient for only one break-through point along the boundary. Under this condition, as d varies, the area of PGBA changes accordingly, and consequently G_{GB} should be different. While the influence of microstructure length in plastic deformation has been studied extensively in the past several decades [8,9], the size effect in fracture, particularly cleavage fracture, has been rarely discussed. In this article, this phenomenon will be investigated through an energy balance analysis.

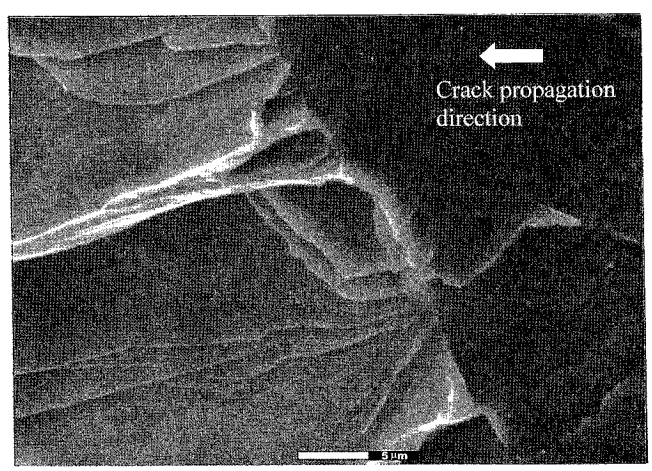

Fig. 1. A SEM image of the cleavage fracture across a large high-angle grain boundary in an iron-silicon alloy. The crack propagates from the right to the left.

2. ANALYSIS AND DISCUSSION

Consider the narrow bicrystal sample depicted in Fig. 2. Initially the tip of a cleavage crack of size a_0 is arrested at the grain boundary between grains "A" and "B". As the crack opening displacement, δ, increases, the crack growth driving force rises. When the energy release rate reaches the critical value of G_{GB}, the crack overcomes the grain boundary and "bursts" into grain "B". During this process, the fracture surface must transmit from the crystal plane of grain "A" to that of grain "B", which is misoriented by a twist angle, φ, and a tilt angle, θ. Due to the PGBA, the fracture resistance of the grain boundary is higher than that of grain "B", and thus with a constant δ the crack front would advance unstably by a distance of Δa, until the crack growth driving force is reduced to the critical value of crack arrest, G_B.

In a previous analysis [10], the condition of energy balance of the cleavage cracking across a large high-angle grain boundary was obtained as

$$\frac{1}{3}a_0 d G_B(\tilde{G}-\tilde{G}^{1/4}) = W \tag{1}$$

where $\tilde{G}=G_{GB}/G_B$, and W is the fracture work associated with the unstable crack advance [10,11]. The left hand side of Eq. 1 captures the variation in strain energy before and after the crack growth. Note that $G_B = G_0/(\cos\theta \cdot \cos\varphi)$, with G_0 being the effective surface free energy of the cleavage plane.

In a freestanding thin film with a through-thickness grain structure, the lateral facets shown in Fig. 2 are free surfaces. Thus, the fracture work, W, consists of contributions of the cleavage plane in grain "B" and the separation of PGBA, i.e.,

$$W = G_B \cdot d \cdot \Delta a + \chi \cdot d^2 \cdot \tan\varphi/4 \tag{2}$$

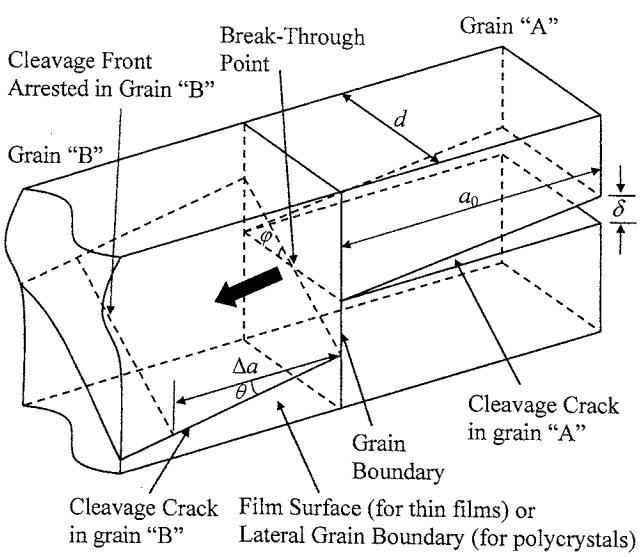

Fig. 2. A schematic diagram of the cleavage fracture across a narrow grain boundary.

where χ is the specific work of separation of the grain boundary. The grain boundary width equals the film thickness.

In the context of linear elastic fracture mechanics, the crack jump length, Δa, can be related to the initial and final energy release rates, G_{GB} and G_B, through [10],

$$\tilde{G}^{1/4} = 1 + \Delta a/a_0 \tag{3}$$

Substitution of Eqs. 2 and 3 into 1 leads to

$$\tilde{G} - 4\tilde{G}^{1/4} = \alpha \tag{4}$$

where $\alpha = 3\chi d/4G_B a_0 \tan\varphi - 3$. Note that $\tilde{G}$ is a function of a single parameter, α. It is remarkable that α is dependent on the film thickness, d, and the initial crack length, a_0, which in turn affects $\tilde{G}$, as shown in Fig. 3, where w is set to 1 μm. The factor of a_0 comes in because the model is scalable; that is, for a longer crack, the film looks "thinner", and vice versa. However, the calculation results indicated that, when $a_0 > 10d$, the crack length effect was only secondary compared with other parameters. In Fig. 3, the value of a_0 was somewhat arbitrarily set to 1 mm, which, when changed by a factor of 100, caused a variation of less than 5 % in $\tilde{G}$. On the other hand, as d is increased from about 0.2 μm to more than 1 μm, G_{GB} can be significantly increased by around 80 %. This change can be attributed to the fact that, the thicker the film, the more PGBA would be involved in the crack front transmission. Once d exceeds 2-3 μm, the cleavage front would break through the grain boundary at multiple break-through points. The process is reduced to a coarse-grained case, and the grain boundary toughness becomes size insensitive. The grain boundary fracture resistance is also related to the crystallographic misorientations, as it should be. The value of G_{GB} increases with both the twist

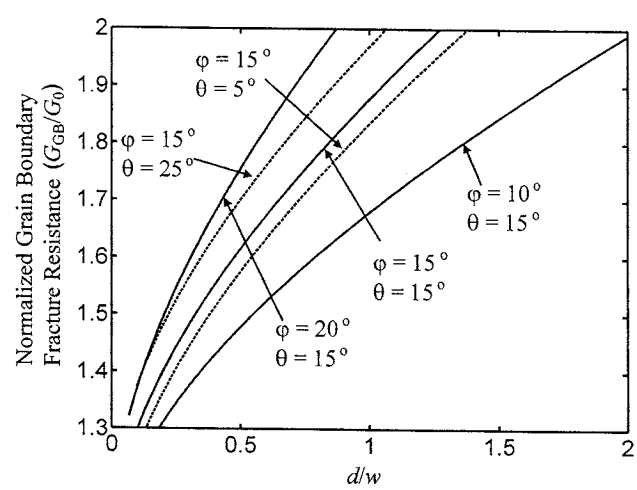

Fig. 3. The grain boundary fracture resistance as a function of the film thickness in a free-standing thin film. The values of χ/G_0 and a_0 are taken as 0.8 and 1 mm, respectively.

and tilt angles; however, as shown in Fig. 3, the influence of the former is more pronounced, which suggests that the PGBA plays a critical role.

In a polycrystalline material, the grain boundary width is equal to the grain size. In addition to the two terms at the right hand side of Eq. 2, the work of separation of lateral grain boundaries must be taken into consideration. If the grain orientation is random, the tilt angles of the grains adjacent to "B" are distributed uniformly in the range of $-\pi/4$ to $\pi/4$, and the average fracture work can be stated as

$$W = G_B \cdot d \cdot \Delta a + \chi \cdot d^2 \cdot \tan\varphi/4 + \chi \cdot \Delta a^2 \cdot f(\theta)/2 \qquad (5)$$

where

$$f(\theta) = \frac{2}{\pi}\int_{-\pi/4}^{\pi/4} |\tan\hat{\theta} - \tan\theta| d\hat{\theta} = \frac{2}{\pi}\left[2\theta \cdot \tan\theta + \ln\cos_2\theta - \ln\frac{1}{2}\right].$$

Note that, for the sake of simplicity, the dimension of grain "B" along the crack growth direction is assumed to be larger than Δa. The post-critical crack advance process has little influence on the calculation result of G_{GB}.

Combination of Eqs. 1, 3, and 5 gives

$$\tilde{G} + (2\beta - 4)\tilde{G}^{1/4} - \beta \cdot \tilde{G}^{1/2} = \beta + \frac{9}{8}\left(\frac{\chi}{G_B}\right)^2 \frac{\tan\varphi}{\beta} f(\theta) - 3 \qquad (6)$$

with $\beta = \frac{3}{2}\frac{\chi}{G_B}\frac{a_0}{d} f(\theta)$. The relationship between the grain size, d, and the grain boundary fracture resistance, G_{GB}, is shown in Fig. 4, where the parameter values are the same as those of Fig. 3. Due to the additional resistance caused by the lateral boundaries, the G_{GB} of the polycrystalline material is higher than that of a film of the same grain boundary width. The difference between them is of the order of 10-30 %. The grain boundary toughness increases with d, since the area of PGBA is higher in a larger grain. This size effect is stronger if d is smaller than about 0.2 μm; in the higher d range, the size sensitivity of G_{GB} is reduced by a factor of about 2-3. Increasing φ or θ is of a beneficial effect to the fracture toughness, though the effect of φ is more important, which is in agreement with the fact that the contribution of the lateral boundaries is less significant than that of the boundary directly penetrated through by the cleavage front.

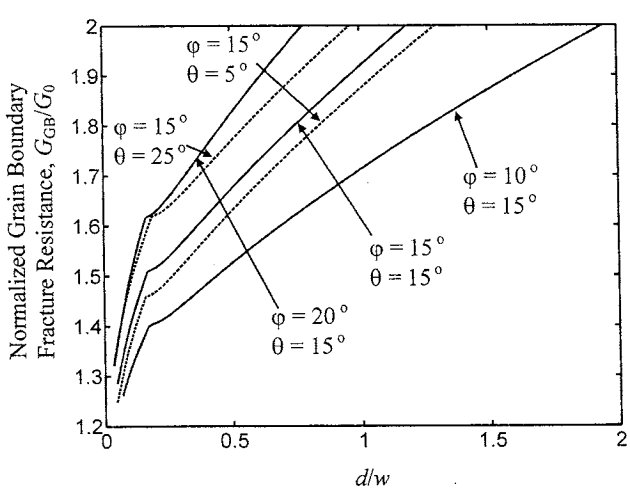

Fig. 4. The grain boundary fracture resistance as a function of the grain size in a fine-grained material. The values of χ/G_0 and a_0 are taken as 0.8 and 1 mm, respectively.

Currently, the experimental data of the film thickness or grain size dependence of fracture toughness at the length scale discussed above are scarce. Therefore, this analysis is merely a theoretical prediction that needs to be verified. Nevertheless, it provides a basis for the fracture testing of fine-structured materials, and it indicates a potential risk of low toughness as the characteristic microstructure length is decreased. Note that in Eq. 1 the effects of recalcitrant grain boundaries [12] and irregular fracture mode [13] are ignored.

3. CONCLUDING REMARKS

In summary, according to an energy analysis, as film thickness or grain size becomes smaller than 1-2 μm, such that along a grain boundary there is only one break-through point, the fracture toughness of a brittle polycrystalline material will decrease if the grain boundary width is reduced. Analytical expressions of the relationship between G_{GB} and d were obtained. Other factors that influence the fracture toughness include the crystallographic misorientations, the effective surface free energy of a grain boundary, as well as the initial crack length. In a polycrystalline material, the work of separation of lateral boundaries is about 10-30 % of the total fracture resistance.

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