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An energy analysis of the grain boundary behavior in cleavage cracking in Fe–3wt.%Si alloy

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Abstract

The resistance of high-angle grain boundaries to cleavage cracking in Fe–3wt.%Si bicrystals is discussed in context of linear elastic fracture mechanics based on an energy method. The grain boundary toughness is determined by the fracture work associated with the plastic shear along the grain boundary and the crack-trapping effect. The influence of the crystallographic misorientation and the size effect are analyzed. It is concluded that the toughening effect of the grain boundary is dominated by the tilt and twist angles and is more pronounced for shorter cracks. The numerical results fit with the experimental data quite well.

Keywords: Grain boundaries; Metals and alloys; Fracture toughness; Cleavage cracking

1. Introduction

The role of grain boundaries in cleavage cracking has been an active research area for decades. In engineering practice, the length of the strength-limiting microcracks in brittle materials was often assumed to be grain-sized, indicating that to propagate across a grain boundary, the microcrack must overcome significant resistance. The resistance offered by the grain boundaries is dominant in a variety of material failure phenomena, such as the catastrophic cleavage cracking across a field of grains [1–3], the brittle-to-ductile (BD) and ductile-to-brittle (DB) transitions [4,5], and so on.

In an early study on the microstructure dependence of the grain boundary toughness in hydrogen-charged Fe–3%Si alloy, Gell and Smith [6] concluded that among the twist, tilt, and rotation misorientations, the influence of the twist misorientation is most important and that of the rotation misorientation is negligible, which was attributed to the difficulty in the nucleation of the cleavage facets in adjacent grains. This result indicated that to take account for the effect of the crystallographic orientation on the toughening effect of the grain boundaries, the crack–boundary interaction must be considered. In a theoretical analysis of cleavage cracking after extended plastic deformation in polycrystals, McClintock [7] suggested that the overall fracture resistance is dominated by the work of separation of the grain boundaries.

In a recent grain boundary toughness measurement experiment, Qiao and Argon [8] observed the breakthrough process of cleavage cracks across the high-angle grain boundaries in a substantial set of Fe–3wt.%Si bicrystals. Fig. 1 is the SEM fractography showing the entry of a cleavage crack across a grain boundary along a series of twisted tiered cleavage strips. When the cleavage front encountered the grain boundary, it first penetrated through the grain boundary locally at a number of breakthrough points distributed along the front quasiperiodically. The distance between the breakthrough points was in the range of 1–50 μm and was quite independent of the crystallographic orientation. With increasing stress intensity at the crack tip, the penetration depth of the crack front across the grain boundary kept increasing, and when the peak resistance was reached, the grain boundary between the cleavage facets in the two grains was sheared apart and the crack "burst" into grain "B", as depicted in Fig. 2. During this process, both the separation of the grain boundary and the crack-trapping effect suppressed the crack advance, resulting in an about threefold rise of the fracture resistance over

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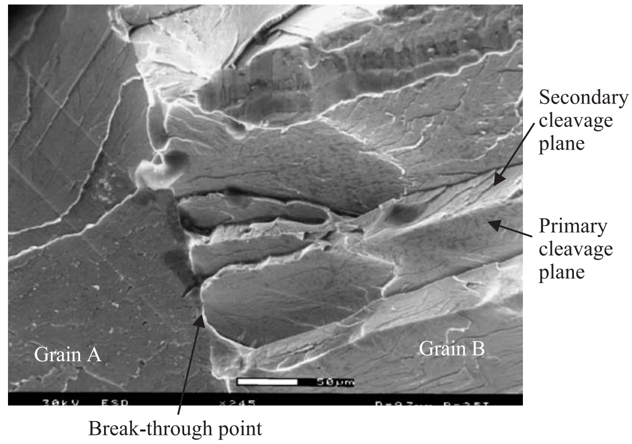

Fig. 1. SEM fractography of a high-angle grain boundary in a Fe−3%Si bicrystal.

the single crystal. While a number of numerical procedures (e.g., [9]) have been developed to simulate the evolution of the profile of the crack front across an array of regular-shaped obstacles, in the case of the grain boundary, the very high aspect ratio of the intersection area with the fracture plane makes the numerical calculation of the front behavior difficult.

2. Resistance of high-angle grain boundary to cleavage cracking

In order to calculate the grain boundary toughness, consider the bicrystal double-cantilever-beam (DCB) specimen depicted in Fig. 3. Initially, the crack tip is at point "1" at the grain boundary. The energy release rate rises with crack opening displacement. When the critical energy release rate G_{ICGB} is reached, the crack breaks through the grain boundary. Because, as will be shown shortly, the cracking resistance of the grain boundary is higher than that in grain "B", in a displacement-controlled test the crack

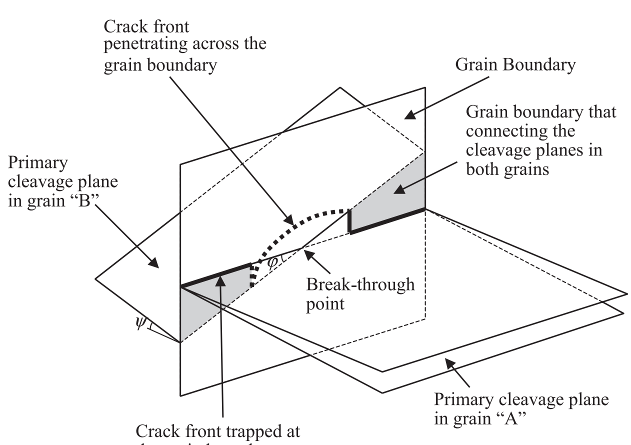

Fig. 2. A schematic diagram of the cleavage cracking across a high-angle grain boundary around a breakthrough point.

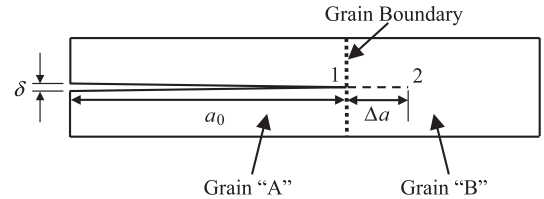

Fig. 3. The cleavage crack overcoming the resistance of the grain boundary in a bicrystal double-cantilever-beam specimen.

will propagate unstably by a distance Δa until it is stopped at point "2", where the energy release rate decreases to G_s, the critical value to arrest the propagating crack. According to dynamic fracture mechanics [10], if the crack jump length is small compared with the initial crack length, G_s is about the same as the fracture resistance of grain "B" to a stationary crack, G_{ICB}.

If the effects of the free edges and shear stresses are negligible, the critical energy release rate of the grain boundary can be obtained through the basic beam theory [11]:

$$G_{ICGB} = \frac{3}{16}\frac{Eh^2}{a_0^4}\delta^2 \tag{1}$$

where E is the Young's modulus, h is the height of the DCB arm, a_0 is the initial crack length, and δ is the critical crack opening displacement. During the dynamic crack jump, we assume that the crack opening displacement is constant. Thus,

$$G_{ICB} = G_s = \frac{3}{16}\frac{Eh^2}{a_1^4}\delta^2 \tag{2}$$

where $a_1 = a_0 + \Delta a$. Through Eqs. (1) and (2), we have

$$\tilde{G} = \frac{G_{ICGB}}{G_{ICB}} = \left(1 + \frac{\Delta a}{a_0}\right)^4 \tag{3}$$

The strain energy change associated with the crack jump is

$$\frac{\Delta U}{b} = \frac{Eh^3\delta^2}{16}\left(\frac{1}{a_0^3} - \frac{1}{a_1^3}\right) \tag{4}$$

where b is the specimen thickness. Substitution of Eqs. (1)–(3) into Eq. (4) gives

$$\frac{\Delta U}{b} = 3a_0 G_{ICB}(\tilde{G} - \tilde{G}^{1/4}) \tag{5}$$

The fracture work associated with the crack jump can be stated as

$$W = G_{ICB}\Delta a + \frac{1}{w}\chi S_{GB} \tag{6}$$

where χ and S_{GB} are the effective work of separation and the area of the grain boundary that must be sheared apart to connect the cleavage planes in grains “A” and “B”, respectively; and w is the average distance between the breakthrough points. The grain boundary area is

$$S_{GB} = \frac{w^2}{4}\sin\varphi\,\cos\varphi \tag{7}$$

with φ being the twist misorientaiton (see Fig. 2). Note that the strain energy change should be equal to the fracture work. Consequently, through Eqs. (3) and (5), (7), we have

$$\tilde{G} - 4\tilde{G}^{1/4} = S^* \tag{8}$$

where $S^*=3(Q-1)$, with $Q=\frac{\chi}{4G_{ICB}}\frac{w}{a_0}\sin\varphi\cos\varphi$. Fig. 4 shows the relationship between $\tilde{G}$ and Q. In the Fe–3%Si bicrystal experiments [8], if χ/G_{ICB} is taken as 1700, Eq. (8) fits with the experimental data quite well. Through Eqs. (3) and (8), it can be seen that in the range of Q under consideration, the crack jump length is indeed quite small compared with the initial crack length, indicating that the above analysis is self-compatible.

Because the fracture resistance of the single crystal Fe–3wt.%Si alloy is quite low when the process zone effect can be ignored, it is reasonable to take G_{ICB} as 10–20 J/m, which leads to an estimate of χ around 25 kJ/m. This relatively high work of separation of the grain boundary indicates that although the global fracture mode was cleavage, the local plastic shear deformation around the breakthrough points was significant, which is compatible with the experimental observation that the grain boundaries were separated mostly through plastic shear deformation ([12]; see Fig. 5).

3. Discussion

In Eq. (8), the toughening effect of the grain boundary consisting of the crack-trapping effect and the fracture

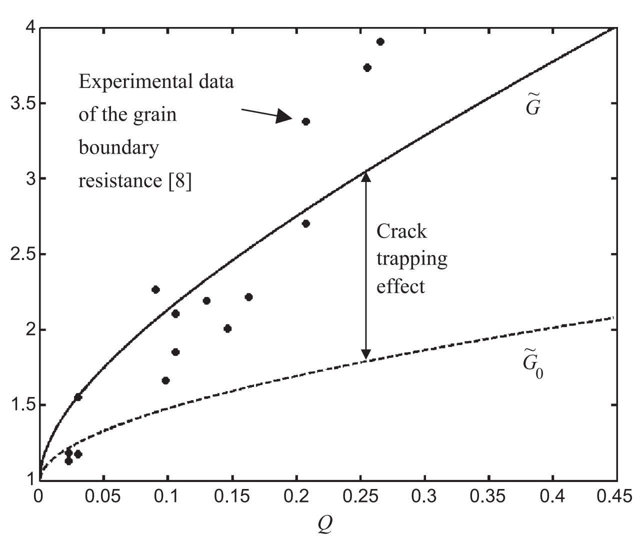

Fig. 4. The relationship between the grain boundary toughness and the parameter Q.

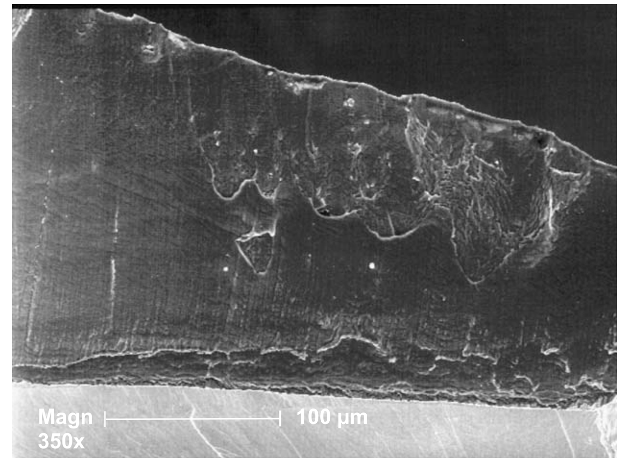

Fig. 5. SEM fractography of the separation of a grain boundary. Most of the surface shows signs of plastic shearing [12].

work associated with the grain boundary separation is considered as a whole. If we only consider the influence of the grain boundary separation, the grain boundary resistance can be estimated through the area–average method [13]

$$G_{ICGB0} = (\chi S_{GB}/w + G_{ICB}\Delta a)/\Delta a \tag{9}$$

Based on Eq. (3), Eq. (9) can be rewritten as

$$\tilde{G}_0 = Q/(\tilde{G}^{1/4}-1)+1 \tag{10}$$

where $\tilde{G}_0=G_{ICGB0}/G_{ICB}$. The comparison of $\tilde{G}$ and $\tilde{G}_0$ is also shown in Fig. 4. The difference between them should be attributed to the crack-trapping effect, which in Fe–3%Si alloy was about 60% of the overall grain boundary resistance.

By considering both the primary and the secondary cleavage planes in grain “B”, G_{ICB} can be stated as

$$G_{ICB} = G_0(\sin\varphi+\cos\varphi)/\cos^2\psi \tag{11}$$

where ψ is the tilt misorientation (see Fig. 2) and G_0 is the critical energy release rate of the single crystal. Thus, the grain boundary toughness is

$$\hat{K} = \sqrt{\tilde{G}\cos^2\psi/(\sin\varphi+\cos\varphi)} \tag{12}$$

where $\hat{K}=K_{ICGB}/K_0$ and $K_0=\sqrt{EG_0^2/(1-\nu^2)}$ is the critical stress intensity factor of the single crystal. The influence of the crystal misorientation on $\hat{K}$ is shown in Fig. 6. It can be seen that the larger the extent of the crystal misorientation, the higher the grain boundary toughness, and the influence of the twist misorientation is more important.

Although the above discussion is based on the analysis of the DCB specimen, the result is independent of the speci-

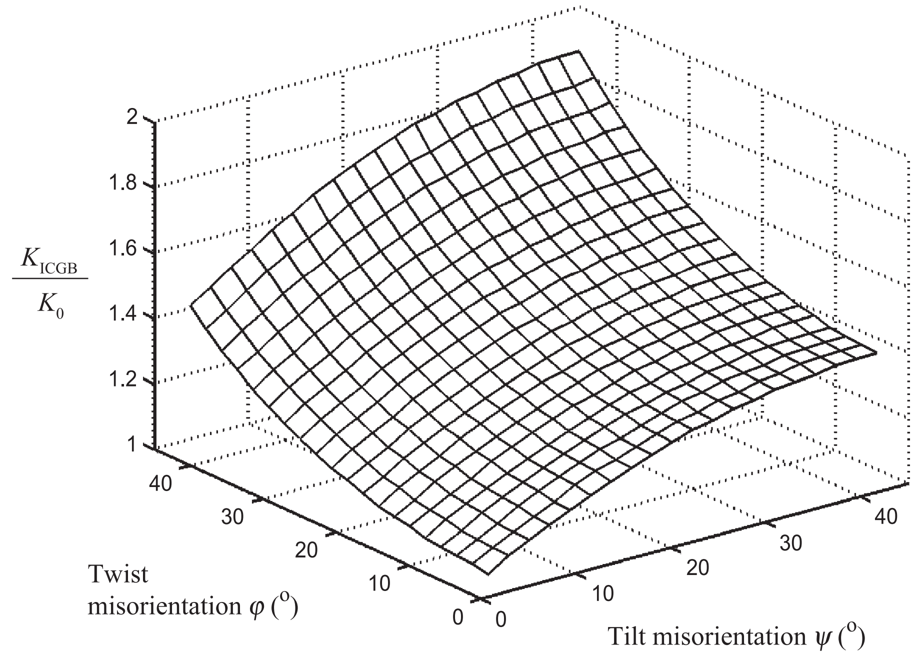

Fig. 6. The relationship between the grain boundary toughness and the crystal misorientation.

men geometry, because all the specimen parameters, E, h, and b, vanish in Eq. (8). However, according to Eq. (8), $\tilde{G}$ is crack length-dependent. This size effect is more pronounced for shorter cracks, as shown in Fig. 7. When the crack length is below $100w$, $\tilde{G}$ decreases with increasing crack length; if the crack length is larger than $1000w$,

$$G_{ICGB} \approx G_{ICB} \tag{13}$$

that is, the toughening effect of the grain boundary and the crack length effect become negligible. This phenomenon is quite similar to the result of the well-known R-curve analysis, where the second derivative of the strain energy is essential to the onset of the unstable crack advance. In the case of the grain boundary, because the fracture resistance of

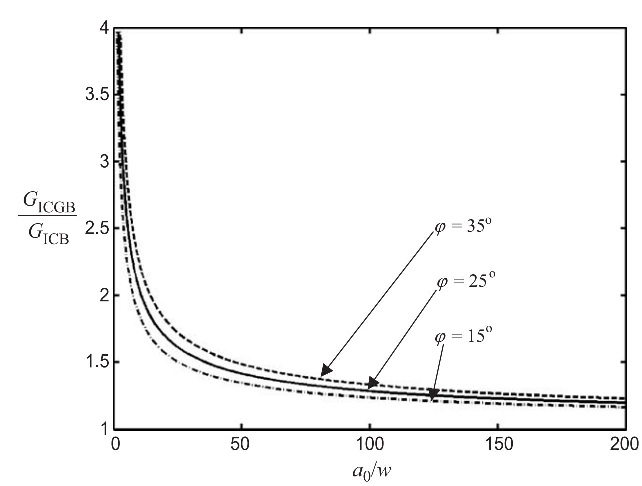

Fig. 7. The crack length dependence of G_{ICGB}.

the single crystal does not change, the effect of the crack length should be attributed to the fact that the crack is not scalable if the crack length varies while the crack front behavior remains the same. It can be seen that if w changed with a_0 such that the a_0/w ratio kept constant, $\hat{K}$ is independent of a_0.

4. Conclusions

To summarize, in this study, the influence of the crystal misorientation on the grain boundary toughness is quantified. The plastic shear deformation along the grain boundary is important even when the temperature is well below the ductile-to-brittle transition temperature. The following conclusions are drawn:

(1) The grain boundary toughness is dominated by a single parameter Q collecting together factors including the crystal misorientation, the work of separation of the grain boundary, and the breakthrough mode of the cleavage front.
(2) About 60% of the grain boundary resistance is due to the crack-trapping effect, and about 40% is caused by the work of separation of the grain boundary areas connecting the cleavage planes in the adjacent grains.
(3) The toughening effect of the grain boundary is pronounced only for short cracks. For cracks longer than $1000w$, which is about 10 mm for the Fe−3%Si alloy, the grain boundary toughness tends to be given by G_{ICB}. For cracks shorter than $100w$, the grain boundary toughness decreases as the crack length increases.

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