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Recresistance of high-toughness grains to cleavage cracking in a polycrystalline, brittle material †

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Abstract

As a cleavage crack propagates through a field of randomly oriented grains, due to the variation in local fracture resistance, the crack front advance is nonuniform. The crack would first penetrate into the low-toughness grains, leaving the high-toughness ones behind its front. In this article, the barrier effect of the high-toughness grains is investigated in considerable detail through a computational analysis. The dominant factors are the grain size and the effective content of high-toughness grains.

Keywords: Fracture toughness; Grain boundary; Cleavage; Crack trapping effect

1. Introduction

In a few experimental studies [1-3], transgranular cleavage cracking in polycrystalline materials was analyzed in detail. Iron-silicon alloys were employed as the model materials. Around room temperature, the dislocation mobility in an iron-silicon alloy is quite low and, therefore, the material is brittle and cleavage cracking is the dominant failure mode [4, 5]. When the crack front encountered an array of grain boundaries, grain boundaries of relatively low fracture resistances that are exposed to the cleavage front sections of relatively high local stress intensity would be first broken through, and the high-toughness grain boundaries would be left behind, bridging the crack flanks together, which, with the increasing of the external loading, would eventually fail through plastic shearing or secondary cracking, as shown in Fig. 1.

One interesting phenomenon observed in the experiment was the large difference between the fracture resistances of single crystals and polycrystalline materials. For instance, as will be discussed shortly, the low-temperature cleavage resistance of a brittle iron-silicon alloy was measured to be 9.6 kJ/m^2, much higher than the critical energy release rate of its single-crystal counterpart. In previous analyses [6, 7], this effect was attributed to the accumulation of fracture resistance offered by all the grains encountered by the crack front. When a cleavage front penetrates across a grain boundary, very often

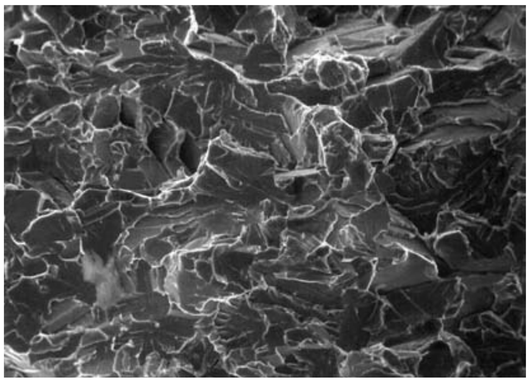

Fig. 1. SEM fractography: The crack propagates from the left to the right.

it would first enter into the grain ahead of the boundary at a number of break-through points (BTPs). The BTPs distribute quasi-periodically along the boundary [6]. The persistent grain boundary areas (PGBA) in between the BTPs offer additional fracture resistance, and would be separated apart either through plastic shearing or mode-II fracture [8]. Such type of crack front behavior will be referred to as the "regular" mode in the following discussion. For the regular mode, the concept of linear elastic fracture mechanics (LEFM), such as the critical energy release rate, G_{cr}, works well (e.g. Ref [8]). If the formation of break-through points is difficult, e.g. when the increase rate of local stress intensity is too high or the grain boundary is only partly exposed to the cleavage front, "irregular" break-through modes would be observed [9, 10], in which the crack front first enters the second grain in the central sec-

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tion of the boundary, and then overcomes the rest of boundary via inverse cracking or shearing/bending. Another possible cleavage fracture mechanism is the "self-similar" mode [11], which might be regarded as the combination of the "regular" and the "irregular" modes.

In a quasi-static cracking process, the steady-state of crack-boundary interaction can be reached and the "regular" mode should be dominant, which will be the focus of the current study. Under this condition, the effective grain boundary fracture resistance, i.e. the critical energy release rate for a cleavage front to bypass a grain boundary, can be calculated by a simple energy analysis [6]:

$$\frac{G_{\mathrm{GB}}}{G_{\mathrm{A}}}=\frac{\sin\theta+\cos\theta}{\cos^2\psi}+C\frac{\sin\theta\cdot\cos\theta}{\cos\psi} \tag{1}$$

where G_{A} is the effective surface free energy of cleavage plane; θ and ψ are the twist and tilt misorientation angles across the boundary, respectively; and C is a material parameter collectively capturing the influences of grain boundary separation and crack front profile. For the iron-silicon alloy under investigation, $C = 0.25$ [1].

Based on Eq. (1), when the grain orientation is random, a closed-form expression can be obtained to assess the fracture resistance of a polycrystalline material, G_{PC0} [2]:

$$\frac{G_{\mathrm{PC0}}}{G_{\mathrm{A}}}=1.45+3.03\frac{\Delta x_{\mathrm{c}}}{D_0}+B \tag{2}$$

where Δx_{c} is the critical penetration depth of crack front across a high angle grain boundary (typically one to a few μm) [6]; D_0 is the grain size and $B = k^*\delta_c\xi/G_{IC}$ is a material constant, with k^* being the "cleavage-like" shear fracture resistance of the boundary, δ_c the critical "preparatory" opening displacement of cleavage planes, and $\xi = \Delta h/D_0$ is the ratio of the average crack tip opening distance, Δh, to the grain size. If the grain size is much larger than Δx_{c}, the second term at the right-hand side becomes negligible and Eq. (2) is reduced to

$$G_{\mathrm{PC0}}=\alpha\cdot G_{\mathrm{A}} \tag{3}$$

where $\alpha \approx 3.2$ is a material constant.

While Eq. (3) predicts that the fracture resistance of a polycrystalline material would be higher than that of a single crystal by the factor of α, it still does not fully capture the broad gap between them. Note that Eq. (3) reflects the line average of fracture resistances of all the grains exposed to the crack front. That is, it is implicitly assumed that the front overcame all the grain boundaries simultaneously, which is contradictory to the experimental observation. If the non-uniform nature of crack front advance is taken into consideration, since the local fracture toughness at the protruding crack front segments would be lower than elsewhere [12], to keep the front propagating, the applied stress intensity must be much higher.

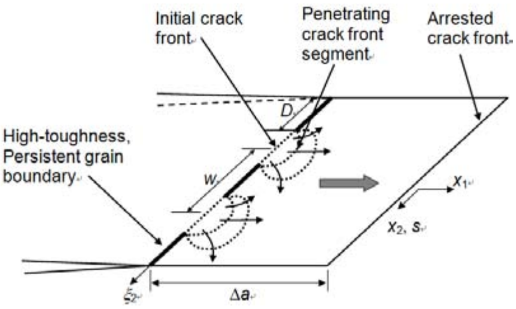

Fig. 2. Schematic of the cleavage cracking process in a field of randomly oriented grains. The crack propagates from the left to the right.

2. Crack tapping effect of high-toughness grains

Fig. 2 depicts the process that a crack bypasses a row of grain boundaries. The cleavage front first stably penetrates between the persistent grain boundaries, similar to the regular case discussed by Gao and Rice [13]. The boundaries of relatively low toughness, shown as the dashed lines, are broken through first. The high-toughness boundaries are persistent to the cracking process, shown as the solid lines. The initially straight crack front must be curved in the penetration segments when it advances locally in between the persistent grain boundaries. As the persistent grain boundaries are left behind the verge of propagating front, the required local crack growth driven force increases, leading to an increased overall fracture toughness. This toughening effect caused by the heterogeneous components is similar with the crack trapping effect commonly observed in composite materials of strongly bonded reinforcements [14].

The local cracking resistance offered by the low-toughness boundaries in between the persistent boundaries can be estimated as G_{PC0}. When the critical penetration depth is reached, the crack trapping effect is overcome and the crack would propagates unstably by a distance Δa until the stress intensity at the crack tip decreases to a critical value, G_{a}, so that the advancing crack is arrested again. For a long crack, since Δa is much smaller than the initial crack length (a_0), G_{a} is about the same as G_{PC0} [15].

The change of the strain energy associated with the unstable crack advance is

$$U_1-U_0=G_{\mathrm{PC0}}\cdot\Delta a\cdot b \tag{4}$$

where U_0 and U_1 are the values of strain energy before and after the crack jump, respectively, and b is the sample thickness. The value of U_0 can be calculated through

$$U_0=Ebh^3\delta^2/16a_0^3=a_0bG_{\mathrm{PC0}}/3 \tag{5}$$

where E is the Young's modulus of the material, h is the height of the double cantilever beam (DCB) arm, and δ is the critical crack opening displacement to overcome the crack trapping effect. The value of U_1 can be estimated as

$U_1 = \hat{U}_1 + U_b$, where

$$\hat{U}_1 = a_1 b G_{trap}/3 \tag{6}$$

is the strain energy if the persistent grain boundaries did not exist and U_b is the strain energy caused by the bridging effect, with $a_1 = a_0 + \Delta a$ and G_{trap} being the critical energy release rate to overcome the crack trapping effect. For a long crack, Δa is much smaller than a_0, and Eqs. (4)-(6) can be reduced to

$$G_{trap}/G_{PC0} + 3U_b/(a_0 G_{PC0} b) = 1 + 3\cdot\Delta a/a_0 b\,. \tag{7}$$

Based on the weight function method, the wedging stress, $\tilde{P}(\xi)$, at the persistent grain boundary that locally pin together the fracture flanks can be calculated through

$$0 = \tilde{U}(\bar{x}') + \int_\Gamma \hat{U}(x', \xi)\tilde{P}(\xi)\mathrm{d}\xi \tag{8}$$

where $\tilde{U}(\bar{x}')$ and $\hat{U}(\bar{x}', \bar{\xi})$ are weight functions of crack opening displacement, Γ is the domain of the persistent grain boundaries in the crack plane, and x' and ξ are points in Γ. With the wedging stress, the stress intensity along the arrested crack front is

$$K(s) = K^\infty + \int_\Gamma H(s, \xi)\tilde{P}(\xi)\mathrm{d}\xi \tag{9}$$

where $H(s, \xi)$ is the stress intensity at s due to a pair of unit wedging force at ξ, and K^∞ is the stress intensity factor at the arrested crack front if there were no persistent grain boundaries, which can be calculated through, $K^\infty = \sqrt{E a_0^4 G_{trap}/[(1-\nu^2)a_1^4]}$ with ν being the Poisson's ratio. The forms of $\tilde{U}(\bar{x}')$, $\hat{U}(\bar{x}', \bar{\xi})$, and $H(s, \xi)$ were given by Ulfyand as [16]:

$$\tilde{U}(\bar{x}') = 2\tilde{K}\frac{1-\nu}{\mu}\sqrt{\frac{\Delta a}{2\pi}}$$

$$\hat{U}(\bar{x}', \bar{\xi}) = \frac{1-\nu}{\mu\rho\pi^2}\arctan\left(\frac{2\sqrt{x_1\xi_1}}{\rho}\right)$$

$$H(s, \xi) = -\sqrt{\frac{2}{\pi^5}\frac{\sqrt{\Delta a}}{s^2 + \Delta a^2}}$$

where μ is the shear modulus, and ρ is the distance between $\bar{x}$ and $\bar{\xi}$. Note that the average of $K(s)$ along the arrested crack front should be equal to $\sqrt{EG_{PC0}/(1-\nu^2)}$.

Substituting Eqs. (8) and (9) into (7) gives G_{trap}. In the current study, the equation set was solved numerically by using the Ritz method, where the integration equations were enforced at the 3rd points in Γ. Further increasing the resolution would result in converged results. The wedging stress parameter was assumed constant along Γ and periodic boundary condition was employed. By considering the critical bridging strength [17], the numerical results can be regressed as

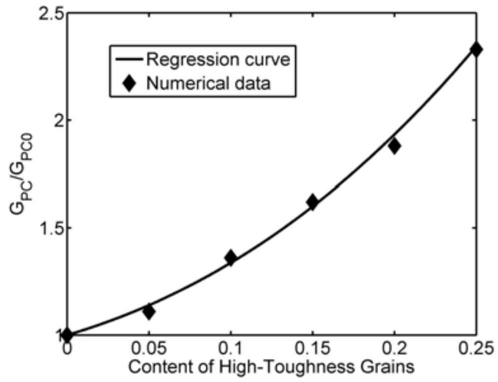

Fig. 3. The fracture resistance as a function of the content of high-toughness grains.

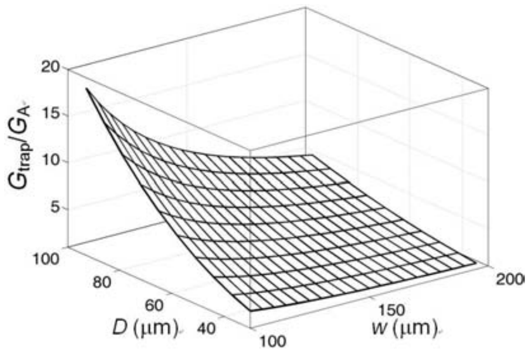

Fig. 4. The effective fracture resistance as a function of the grain size (D) and the average spacing between high-toughness grains (w).

$$\frac{G_{PC}}{G_{PC0}} = \left(1 - \frac{D}{w}\right) + \left(1.8 + 2.9\frac{D}{w}\right)^2 \cdot \frac{D}{w} \tag{10}$$

where w is the center-to-center distance of the adjacent persistent grain boundaries. Figs. 3 and 4 show the influences of D and w on G_{trap}. Note that in Eq. (10), D denotes the effective grain size exposed to the cleavage front. Because the crack front may not move across the main circle or every grain in its path, in average $D = D_0/\sqrt{3}$ [18].

3. Results and discussion

Experimental observation (e.g. Fig. 1) indicates that the content of high-toughness grain boundaries in the array of boundaries encountered by a cleavage front is usually in the range of 0.05 to 0.25 [19]. Its governing factors are still under investigation. It is likely that D/w is associated with the loading mode. Under a mode I or mode II loading, the twist misorientation across grain boundary determines the boundary toughness, and, therefore, the ones of the largest θ are effectively much tougher, becoming persistent boundaries. Under a mode III loading, the crack propagation is more related to the in-plane stresses and the crystallographic misorientation angles may be less important; that is, the distribution of local fracture resistance along the boundary array tends to be more uniform, so that D/w is relatively small. Other vital factors may include the crack propagation rate, texture and grain shape, etc.

If the D/w value is 0.1, i.e. if 10% of the grain boundaries are persistent and left behind the crack front, from Fig. 3 it can be seen that, compared with G_{PC0}, the overall fracture toughness increases by nearly 50%, due to their trapping effect. Even if the content of persistent grain boundaries is at its lower limit, 0.05, the increase in G_{trap} is still quite significant, around 20% of G_{PC0}. As D/w rises, G_{trap} rises rapidly. When the content of high-toughness grain boundaries is 0.25, in the upper range of experimental observation, the overall fracture resistance, G_{trap}, is nearly 3 times higher than G_{PC0}, the resistance offered by a material where $D/w = 0$. Eq. (3) indicates that even when there were no persistent boundaries, a polycrystalline material is of a critical energy release rate about 3.2 times more than its crystallographic cleavage plane. Therefore, as the effects of crack trapping of the high-toughness grain boundaries are taken into consideration, the overall fracture resistance is an order of magnitude higher than that of single crystals, closer to the fracture toughness of grain boundary arrays discussed by McClintock [8].

When the effects of the effective grain size and the distance between adjacent high-toughness grain boundaries are analyzed separately, from Fig. 4 it can be seen that, with a constant value of w, the influence of D is more pronounced, especially when w is relatively small. Under this condition, increasing the grain size may cause a beneficial effect on the overall fracture toughness, as the width of the persistent grain boundary island along the crack front becomes larger, while G_{PC0} is no longer sensitive to D. It has been shown in a previous analysis [6] that as long as the grain size is sufficiently large so that multiple break-through points can be activated simultaneously, the grain boundary toughness is governed by the average contribution from all the break-through points and is quite independent of D. At the higher end of the range of w that we investigate, when D increases from about 40 μm to about 80 μm, the overall fracture resistance increases by nearly 5 times. As the grain size is larger, this effect is promoted. Note that the grain size should not exceed the range allowed by the content of high-toughness boundaries; otherwise the weight function method may break down. If the grain size is constant, the increase in w would result in a reduced overall fracture resistance, as it should. This effect is less evident when the grain size is relatively small, collectively described by Eq. (10).

4. Conclusion

To summarize, according to a numerical analysis on the fracture resistance of a row of grain boundaries of various local boundary toughnesses, the persistent grain boundaries that cannot be directly broken through by the crack front offer an important crack trapping effect, which can partly explain the large difference between the measured high toughness of polycrystalline materials and the prediction of surface free energy of crystallographic cleavage planes. A vital factor is the content of high-toughness grain boundaries. With a constant distance between the high-toughness grain boundaries, increasing grain size is of a beneficial effect to the overall fracture resistance. With a constant grain size, as the content of high-toughness boundaries decreases, the material becomes less tough.

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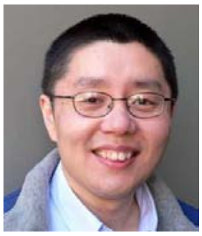

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