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# Characteristic length scale in cleavage cracking across high-angle grain boundary

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**Abstract**

The factors that govern cleavage cracking across high-angle grain boundaries are investigated theoretically. According to previous experimental observations, a cleavage front overcomes the resistance of a high-angle grain boundary by first penetrating across it at a number of break-through points (BTP) and then separating apart persistent grain-boundary islands (PGBI). In the current study, this process is modeled as a competition between grain boundary shearing and crack front transmission. The numerical calculation shows that at a large grain boundary there exists an optimum BTP distance at which the grain boundary toughness is minimized, and when the BTP distance is relatively large its influence is secondary, fitting well with the experimental results.


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*Keywords:* Grain boundary; Cleavage; Fracture toughness; Break-through mode

## 1. Introduction

Fracture toughness of engineering materials is an important issue in design of structures that work under adverse conditions [1]. In the framework of the well established linear elastic fracture mechanics (LEFM), it is usually assumed that in a brittle material there are a large number of pre-existing microcracks. Under an external loading, propagation of one or a few of them would lead to catastrophic failure [2]. The microcracks may be induced by residual stresses or unexpected thermal or mechanical loadings during processing and manufacturing. In a polycrystalline material, they are often assumed grain-sized. That is, a microcrack can be initiated either inside a grain or at a grain boundary; and once it propagates and encounters the first grain boundary, its tip would be arrested since grain boundary usually offers a higher resistance than a single crystal. Under this condition, the fracture resistance of the material is actually determined by the grain boundary toughness.

In a recent experimental study, cleavage cracking processes across a number of high-angle grain boundaries in an iron–silicon alloy were examined in detail [3,4]. The difference between the grain boundary toughness and the toughness of a single crystal was attributed to the shift of fracture surface from the cleavage plane of one grain to that of the other, as well as the additional work required to separate grain boundary. It was observed that when the effective stress intensity at a crack tip was increased, the cleavage front would first penetrate across the boundary at a number of break-through points (BTP). The rest of the crack front in between the BTPs was left behind, arrested by persistent grain boundary islands (PGBI). The PGBI would be sheared apart once the penetration depth of the penetrating crack front reached a critical value. Since the cleavage planes in the two grains were of different orientations, the fracture surface across the grain boundary was sectioned, and further crack propagation would lead to formation of river markings.

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Clearly, the PGBI plays a critical role in the crack front transmission process [5–8]. Particularly, the crack trapping and bridging effects of PGBI are dominant, which is dependent on the PGBI width, or the distance between BTPs. One interesting phenomenon observed in fractography study was that along a large grain boundary the most probable distance between adjacent BTPs was 2–3 μm for all the samples (see Fig. 1a), somewhat independent of the crystallographic orientations [3]. However, occasionally the BTP distance can be much larger, as shown in Fig. 1b, while BTP distance larger than 100 μm have never been observed. When the BTP distance was large, it usually distributed quite uniformly in the range of 10–80 μm. That is, the BTP distance distribution curve consisted of a peak at 2–3 μm and a long, flat tail [3]. According to the river markings, in the large-BTP-distance area, the crack front penetrated all the BTPs nearly simultaneously, indicating that in this range the grain boundary resistance was insensitive to the BTP distance.

The lack of understanding of the factors governing BTP distance, $w$, has imposed considerable challenges to predicting grain boundary toughness. On the one hand, the most possible energetically favorable way for a crack to overcome PGBIs is to minimize $w$, i.e. the crack front should transmit from grain "1" into grain "2" simultaneously along the entire boundary, so that the area of grain boundary involved in this process is negligible. On the other hand, there is no characteristic length of grain boundary structure in the range of 2–50 μm [9]. In the past, in our discussions of grain boundary toughness, $w$ was taken as a material constant. In the current work, through a theoretical analysis, we show that the characteristics of BTP distance distribution can be explained by the competition between crack front penetration and PGBI shearing.

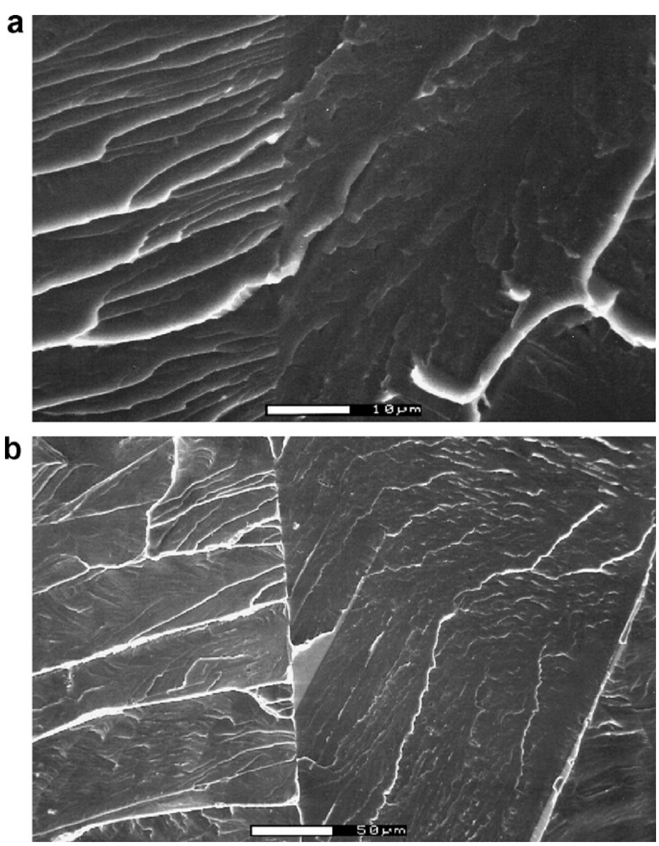


Fig. 1. SEM microscopy of cleavage cracking across a grain boundary in an iron–3 wt.% silicon alloy at different locations: (a) the distance between break-through points is smaller than a few microns; and (b) the distance between break-through points is 30–50 μm. The crack propagated from the right to the left.

## 2. Fracture resistance of persistent grain boundary islands

Fig. 2a depicts the cleavage cracking process across a high-angle grain boundary in a brittle material. The crack front first penetrates the boundary at the BTPs ("A" and "B"). As the penetration depth increases, the PGBI is sheared and thus the crack tip opens, as shown in Fig. 2b. The PGBI is left behind the verge of propagating, bridging across the fracture flanks, suppressing the crack advance through crack trapping effect. For the sake of simplicity, we analyze the crack trapping effect of a regular array of PGBI, where BTPs distribute along the grain boundary periodically. Without losing generality, assume that the crack is in a double-cantilever-beam (DCB) specimen. The height of the DCB arms, $h$, is much smaller than the initial crack length, $a_0$, so that the problem can be discussed in the framework of basic beam theory [10]. It will be shown shortly that the sample geometry has little influence on the calculation result of grain boundary fracture resistance.

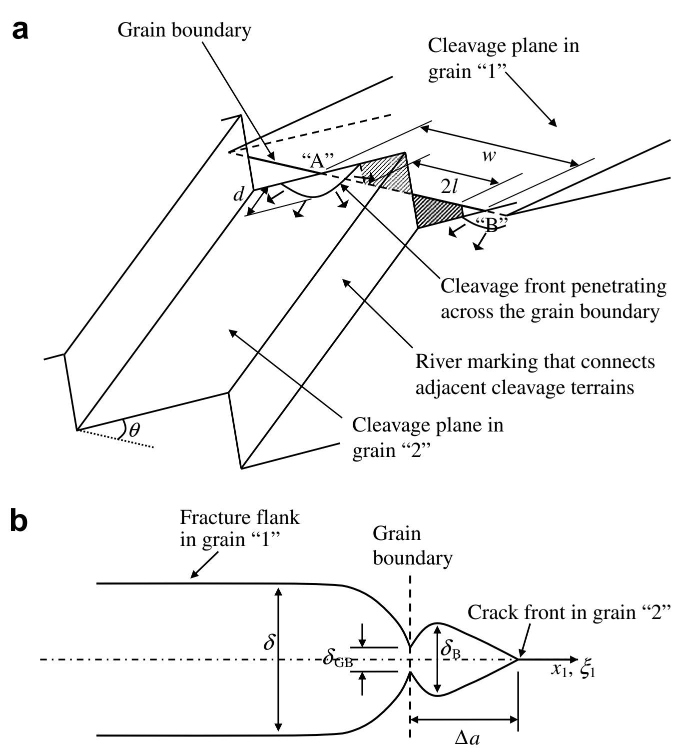


Fig. 2. Schematic diagrams of cleavage cracking across a high-angle grain boundary: (a) the three-dimensional view, where the crack propagates from the right to the left; (b) the side view, where the crack propagates from the left to the right.