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An atomistic insight into the fracture behavior of bicrystal aluminum containing twist grain boundaries

S. Chandra [a], N. Naveen Kumar [b], M.K. Samal [c,d,*], V.M. Chavan [a], S. Raghunathan [a]

[a] Refueling Technology Division, Bhabha Atomic Research Centre, Mumbai 400 085, India
[b] Materials Science Division, Bhabha Atomic Research Centre, Mumbai 400 085, India
[c] Reactor Safety Division, Bhabha Atomic Research Centre, Mumbai 400 085, India
[d] Division of Engineering Sciences, Homi Bhabha National Institute (HBNI), Mumbai 400 094, India

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ABSTRACT

Transgranular fracture in crystalline materials is strongly affected by the presence of twist misorientation of the grain boundaries and the plastic work ahead of the transgranular crack tip. Despite this, the underlying mechanisms associated with crack-twist grain boundary interactions during transgranular fracture remain rudimentary. In view of this, transgranular fracture behavior of precracked bicrystal Aluminum containing ⟨110⟩ twist grain boundaries is investigated using molecular dynamics simulations within the framework of embedded-atom method. The grain boundaries have been shown to act as both a cleavage as well as dislocation source. The first plastic evolution, if any, always occurs from the grain boundary region ahead of the penetrated crack tip, which is in contrast to the intergranular fracture behavior where dislocations are known to be emitted from both the crack tip as well as grain boundary region ahead of the crack tip. Further plasticity evolution in the neighboring grain that occurs after crack stagnation at the twist grain boundary deters further crack propagation. It is observed that the overall fracture resistance of bicrystal material is inversely related with the grain boundary energy. Consequently, the role of twist grain boundaries in affecting the fracture toughness of crystalline materials during transgranular fracture should not be ignored.

1. Introduction

The role of grain boundaries (GBs) as important microstructural features of polycrystalline materials has been well appreciated in a variety of contexts; one such example is the well known Hall-Petch relationship, where GBs themselves become important dislocation sources and sink [1,2]. This is attributed to the increase in GB volume fractions with decreasing grain size, that impede the free volume available for glide of dislocations. It has been suggested by Watanabe [3] that strong and ductile polycrystalline metals can be developed by suitable processing to produce specific frequency and configuration of GBs. Moreover, it has been well established that mechanical behavior of crystalline materials is also affected by the grain orientation and GB misorientation [4,5]. In general, the mechanical behavior of crystalline materials is strongly affected by the GB character. These effects are highly likely to be extended to the field of fracture mechanics also.

With respect to fracture, GBs can either serve as preferred paths for crack propagation (as in case of materials that fail by intergranular fracture), or may sometimes contribute to crack-growth resistance in transgranular fracture mode, where crack propagates on specific sets of crystal planes in individual grains. Studies on intergranular fracture (crack propagation along GBs), resulting from the nucleation and growth of wedge cracks and cavities, have shown that ductile or brittle response of GB to crack propagation depends upon the direction of crack advance [6–8]. Several experimental studies have also been conducted to determine the fracture toughness of individual GBs [9,10]. These experiments have shown that GBs are not weak per se, and thereby offer strong resistance to crack propagation. Complemented with a rich database of atomistic simulations of intergranular fracture [11–14], these studies have elucidated the importance of twist and tilt misorientations of GBs on fracture behavior of crystalline materials.

During transgranular fracture, from the perspective of misorientation, the phenomena of crack arrest at a GB stems from the fact that there is a misalignment between the preferential fracture planes in the two neighboring grains. When the crack arrives at the source of misalignment, it encounters a change in orientation

* Corresponding author at: Reactor Safety Division, Bhabha Atomic Research Centre, Mumbai 400 085, India.
E-mail addresses: mksamal@barc.gov.in, mksamal@yahoo.com (M.K. Samal).

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of the preferred plane in the adjacent grain. Subsequently, the crack growth is hindered and the material exhibits enhanced fracture resistance. The misalignment can be either (i) tilt, wherein the two adjacent grains are misoriented along an axis lying in both the GB plane and the fracture plane, or (ii) twist, where the rotation axis of misalignment lies in the fracture plane and perpendicular to the GB plane (Fig. 1). The effect of tilt misalignment between neighboring grains is well documented and understood: the crack forms a kink at the boundary to propagate along the weak fracture planes. In some cases, complete crack arrest may also occur at the boundary, following which the crack may re-nucleate in the neighboring grain with continuous application of load to form a bridging ligament. These effects have been successfully implemented in continuum solutions of crack growth in linear elastic solids [15–18]. All these calculations predict an increase in the transgranular fracture strength of the material due to tilt misorientation of the boundary.

In the case of twist misorientation, as is evident from the schematic shown in Fig. 1, the preferred crack planes intersect at a point (rather than at a line along the boundary for tilt misorientation which makes the fracture path continuous). Thus, in this case, the crack has to come to a complete halt at the boundary, and has to re-nucleate either at the boundary or in the neighboring grain along preferred fracture planes. These re-nucleated cracks would then need to link to cause complete rupture of the material. This phenomena has to be assisted by stress concentration, which requires additional energy to be expanded in plastic work. This signifies that twist misorientation of the boundary is likely to offer more crack growth resistance than tilt misorientation during transgranular fracture.

The above line of reasoning has sparked an interest in GBs as toughening mechanisms in transgranular fracture studies. For instance, Argon and Qiao [19] conducted experiments on Fe-3 wt % Si alloys and reported a profound increase in cleavage cracking resistance across a GB due to twist misorientation. Both the authors later confirmed that this increase in cracking resistance was more profound for twist than for tilt misalignment at the GB [20]. Wang et al. [21] investigated the crack growth behavior of lamellar Ti-46Al alloy, and found that twist misorientation across colony boundaries offers higher resistance than the tilt misorientation. This phenomena has also been extended to the area of fatigue as well, and has been documented in the works of Zhai et al. [22] on Al-Li alloys and Schaef et al. [23] on CMSX-4 alloy. Specifically, these authors have argued that the area between the traces of crack plane and GB plane has to be fractured for complete failure, which manifests itself in the form of increased fracture resistance of the material. Single crystals and bicrystals of NiAl alloys have also been used to understand crack interaction with GBs by performing *in situ* deformation in a scanning force microscope (SFM) [24].

Although the above review is not intended to be comprehensive in itself, the consensus is that a significant amount of experimental work has been dedicated to investigate intergranular [9,10] and transgranular [19–24] fracture in metallic specimens. In addition, it has been unraveled that twist misorientation across a boundary is more effective than tilt misorientation in toughening the material to transgranular fracture. Often however, precise recognition of sequence of deformation and cracking events in such experimental studies is a challenging enterprise. Although *in situ* observations of crack growth in a scanning electron microscope (SEM) have already proven their utility in this regard, such observations are made on the specimen surface and assumptions are usually made regarding the crack path and subsurface microstructure [25]. Precise introduction of a crack along a particular GB and then studying its pre/post interaction behavior with the boundary poses another challenge. A detailed real-time monitoring of the deformation and fracture processes remains mostly unresolved.

Molecular dynamics (MD) simulations, in this respect, allow the investigation of deformation processes at the atomic scales of inception. These methods allow to focus on the evolution and interaction of plasticity and damage mechanisms at a high resolution, and have, therefore, been exploited to study crack-GB interactions as well. MD studies on intergranular fracture have shown that the crack will propagate along the boundary in either ductile or brittle manner, depending upon the direction of crack advance [6–8,11–14,26–29]. In contrast, the underlying mechanisms of crack propagation across GBs in transgranular fracture mode are not well understood. Terentyev and Gao [30] investigated the interaction of a brittle crack with low and high angle GBs in BCC Fe. They found that the GB resistance to crack propagation is controlled by the ability of the boundary to slide and emit dislocations. Gao et al. [31] reported that twist angle of a GB has a particular effect on crack growth dynamics in nanocrystalline Al. Very recently, Fang et al. [32] showed that crack propagation and growth behavior are more sensitive to twist than to tilt misorientation of GBs in bicrystal Al. Thus, the studies describing the fracture properties of crystalline materials in the presence of twist GBs are, indeed, rare.

The existing literature also indicates that significant efforts have been devoted to the field of grain boundary engineering to ameliorate GB corrosion resistance and boundary embrittlement [3,33]. We believe that an in-depth understanding of the underlying crack-GB physics of transgranular fracture can pave the way to improve the fracture resistance of materials through grain boundary engineering.

We, therefore, have attempted to develop a nanoscale understanding of the transgranular fracture behavior of metallic bicrystals containing twist GBs within the framework of atomistic simulations employing embedded-atom method (EAM). Face centered cubic (FCC) structure is selected as the suitable candidate

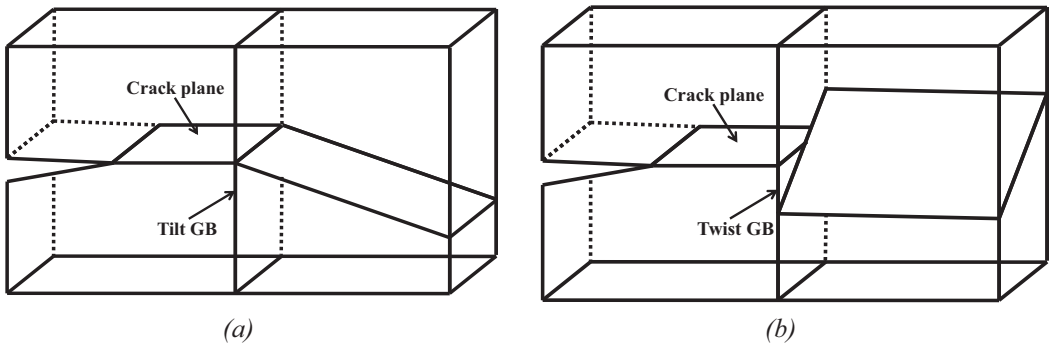

Fig. 1. Schematic representation of misorientation at a (a) tilt and (b) twist boundary.