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The role of grain boundary structure and crystal orientation on crack growth asymmetry in aluminum

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ABSTRACT

Atomistic simulations have shown that the grain boundary (GB) structure affects a number of physical, mechanical, thermal, and chemical properties, which can have a profound effect on macroscopic properties of polycrystalline materials. The research objective herein is to use atomistic simulations to explore the role that GB structure and the adjacent crystallographic orientations have on the directional asymmetry of an intergranular crack (i.e. cleavage behavior is favored along one direction, while ductile behavior along the other direction of the interface) for aluminum grain boundaries. Simulation results from seven ⟨110⟩ symmetric tilt grain boundaries (STGBs) show that the GB structure and the associated free volume directly influence the stress–strain response, crack growth rate, and crack tip plasticity mechanisms for middle-tension (M(T)) crack propagation specimens. In particular, the structural units present within the GB promote whether a dislocation or twinning-based mechanism operates at the crack tip during intergranular fracture along certain GBs (e.g., the 'E' structural unit promotes twinning at the crack tip in Al). Furthermore, the crystallography of the adjacent grains, and therefore the available slip planes, can significantly affect the crack growth rates in both directions of the crack – this creates a strong directional asymmetry in the crack growth rate in the Σ11 (113) and the Σ27 (552) STGBs. Upon comparing these results with the theoretical Rice criterion, it was found that certain GBs in this study (Σ9 (221), Σ11 (332) and Σ33 (441)) show an absence of directional asymmetry in the observed crack growth behavior, in conflict with the Rice criterion. The significance of the present research is that it provides a physical basis for the role of GB character and crystallographic orientation on intergranular crack tip deformation behavior.

1. Introduction

Atomistic modeling and simulation methods have dedicated considerable effort towards understanding the brittle versus ductile behavior of materials, including the dynamic instabilities that occur during fracture [1–11]. To understand this behavior, a number of studies have focused the deformation process that occurs at the crack tip, i.e., brittle (cleavage) versus ductile (nucleation of partial and full dislocations, and deformation twinning) behavior and dislocation burst in single crystal and bicrystal metals, in particular [6]. These simulations have clarified the effects of applied load orientation and slip planes on dislocation nucleation or twinning at/ahead of the crack tip, both in the single crystal and at the grain boundaries (GBs).

In general, atomistic simulations have helped in understanding that crack tip propagation is primarily governed by the dislocation process (emission versus cleavage) and in some metals, such as aluminum and copper, deformation may be accommodated through deformation twinning [12,13,10,14]. Deformation twinning, especially in aluminum, has been a subject of debate due to discrepancies in experimental and atomistic modeling results, regardless of the time and length scale issues [2,3,10,13]. For example, Tadmor and Hai [15] used a quasi-continuum method to suggest that deformation twins form ahead of the crack tip in single crystal aluminum when $T = \lambda_{crit}\sqrt{\gamma_{us}/\gamma_{ut}} > 1$, where λ_{crit} is the normalized critical load for the nucleation of a trailing partial dislocation, γ_{us} is the energy associated with unstable stacking fault energy, and γ_{ut} is the unstable twinning partial nucleation energy. Farkas et al. [2] and others [6,16,17] have used atomistic simulations to observe similar twinning behavior in Al. However, it has been well-established experimentally that Al does not twin except under certain loading conditions and at relative small time scales, primarily due to the high stacking fault energy of the material [13,17,18]. On the other hand, this discrepancy between simulations and experiments regarding deformation twinning does not occur in nanocrystalline (NC) metals (grain

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size $< \sim 100$ nm), as observed by Zhu et al. [12,19] and others [16,17,20–22], where deformation twinning is indeed one of the experimentally-observed deformation mechanisms, along with the GB rotation/sliding and dislocation glide [12,17,21]. This behavior may be partially attributed to GB interfaces and networks that contribute significantly to the properties of metals. Furthermore, onset of plastic deformation is complicated due to the dissociated and faceted structure present in GB interfaces [23,24]. Hence, the local structure and character of the GB was important for understanding interfacial crack mechanics.

Research has shown that GB properties are affected by both the macroscopic degrees of freedom and the microscopic local structure [25–30]. The term GB character is often used to refer to the macroscopic GB degrees of freedom. The GB character refers to the five degrees of freedom associated with the misorientation between the crystallographic orientations of the two adjoining grains. Hence, GB character encompasses not only the misorientation angle, but also the GB plane as well as information pertaining to GB type (e.g., low angle versus high angle, Σ value, etc.). In terms of microscopic local structure, the translations between adjoining grains are important, as is the localized dislocation structure of the boundary. Historically, many efforts have focused on developing a method to characterize GBs [31–36] and their influence on the physical properties of polycrystalline material (e.g. [37–39]). These models utilized dislocation arrays, disclinations, and coincident site lattice (CSL) to describe microscopic and macroscopic degrees of freedom of GBs. Based on identifying the favored GB for the corresponding GB systems, these methodologies [25,28,40–46] described the structural elements comprising symmetric tilt, asymmetric tilt, twist, and twin GBs. They determined that the favored GBs are entirely composed of unique structural units (SUs) that cannot be decomposed into other GB structures.

There have been several studies that examine the role of GB structural units on GB plasticity and deformation mechanisms. For instance, Sansoz and Molinari [47] used quasi-continuum simulations on Al and Cu bicrystals to show that deformation sliding was accommodated through atomic rearrangement of 'E' SUs in the GB structure for the ⟨110⟩ symmetric tilt grain boundary (STGB) system. Additionally, Spearot et al. [23,48] have used molecular dynamics (MD) simulations at 10 K and 300 K to examine how GB structural units impacted the process of dislocation nucleation. However, the role of GB character on plastic events such as dislocation emission, twin formation, and atomic displacements at the interface with a preexisting crack has received less attention, especially in Al with varying types of GB SUs. In fact, in Cu and Fe bicrystals, it has been shown experimentally that there exists a strong directional dependence on the fracture behavior along the interface [49–54]. Moreover, the crack growth asymmetry is governed by the relative angle of the slip plane to the crack plane (θ) and the angle between normal to the crack tip *and* slip direction (ϕ) [55], as depicted in Fig. 1a. The critical energy release rate (G) required for a dislocation emission can be expressed as follows:

$$G_{disl} = 8\left(\frac{1+(1-\vartheta)\tan^2\phi}{(1+\cos\theta)\sin^2\theta}\right)\gamma_{us} \tag{1}$$

where γ_{us} is the unstable stacking fault energy for the slip plane and is ϑ the Poisson's ratio. Furthermore, the Rice–Thompson criterion for dislocation nucleation versus cleavage failure (i.e., $G_{cleav}=2\gamma_s$) is given by

$$\frac{\gamma_s}{\gamma_{us}} > 4\left(\frac{1+(1-\vartheta)\tan^2\phi}{(1+\cos\theta)\sin^2\theta}\right) \tag{2}$$

where γ_s is the surface energy required to create a free surface along the GB interface. Wang et al. [49,51] used the Rice–Thompson condition to examine experimentally-observed directional crack growth behavior in Fe–Si and Cu bicrystalline interfaces and found that the large variation in crack growth behavior was attributed to the relative orientation of slip system ahead of crack tips. Furthermore, the larger crack growth along certain directions was observed when the ratio of γ_s/γ_{us} was the lowest. For example, using the Rice criterion, Wang et al. [49,51] calculated the G_{disl} for a dislocation nucleation from the Σ9 (221) GB in Cu and G_{disl} was $\sim$5.5 J/m^2 and $\sim$2.4 J/m^2 along the $-X$ and $+X$ directions, respectively. On the other hand, the critical energy for the cleavage (G_{clea}) in the Σ9 (221) GB interfaces was $\sim$2.5 J/m^2. These predictions for the Σ9 (221) GB suggest that the fracture behavior changes from a ductile to brittle or vice versa, when the crack propagation direction along the interface changes, which was further corroborated with experimental findings. However, a complete understanding of the fundamental mechanisms associated with asymmetric deformation are inaccessible with experimental techniques, especially the atomic deformation ahead of the advancing crack, the role of GB character, and the resulting directional intergranular fracture. Thus, this presents significant challenges to developing unique state variables (e.g., free volume, GB energy and SU present along the grain boundary etc.) capable of being hierarchically transferred to higher-order models for predictive modeling.

Therefore, the objective of the present research is to understand the relationship between the local atomic structure and the crack mechanics at the GB interface. In this work, the directional anisotropy of an intergranular crack was studied for ⟨110⟩ STGBs in Al to clarify the role of interface character on dislocation emission, formation of twins, and/or atomic displacement. The GB structural description corresponding to the minimum energy was characterized using the structural unit model (SUM) [25,42,56–58], and the initial free volume of each interface was calculated using a previously-described method [59]. The Rice criterion predictions for the directional behavior of incipient plastic event ahead of a crack tip in these GBs were compared against the observed crack tip event. A middle tension – M(T) – specimen was modeled using molecular dynamics with a constant tensile strain rate applied normal to the GB plane at 300 K. The tensile stress–strain response of these M(T) GB specimens were analyzed to correlate the mechanical response to the GB structure. Subsequently, the crack tip plasticity and the directional crack tip response of these GB interfaces were examined. The incipient crack tip event observed deviates from the Rice criterion predictions in certain interfaces (e.g., Σ9 (221), Σ11 (332), and Σ33 (441) GBs). Furthermore, the crack growth during the fracture process was calculated and a noticeable variation in crack growth was observed for the $+X$ direction and $-X$ direction (from the center of the specimen).

This paper is organized as follows. Section 2 briefly summarizes the simulation approach utilized herein. The results and discussion are presented in Section 3, including the atomic structure of GBs at 0 K, the stress–strain responses of the interfaces, the crack growth along both $+X$ and $-X$ directions of each interface, and the atomic deformation for GB interfaces displaying interesting crack growth features. The simulation results reveal several interesting observations: (1) there was a strong asymmetry in crack growth due to the difference in crystallographic orientation of the {111} slip planes on adjacent grains and the crack growth directions, (2) in some cases, the GB volume ahead of the crack tip underwent significant structural rearrangement, which subsequently influenced the crack propagation mechanism, (3) in most GBs, crack propagation was caused by alternating mechanisms of dislocation emission, followed by propagation of dislocation (blunting) and cleavage/crack advance, (4) the crack growth rates along the GB interface were strongly influenced by the initial free volume at the interface, i.e., faster crack growth was observed along interfaces with higher initial free volume, (5) the 'E' SU GBs show a distinct deformation