Available online at www.sciencedirect.com

ScienceDirect

Acta Materialia 87 (2015) 233–247

Acta MATERIALIA

www.elsevier.com/locate/actamat

Atomic-scale intergranular crack-tip plasticity in tilt grain boundaries acting as an effective dislocation source

Tomotsugu Shimokawa[a,*] and Masaaki Tsuboi[b]

[a]*School of Mechanical Engineering, Kanazawa University, Ishikawa 920-1192, Japan*
[b]*Division of Mechanical Science and Engineering, Kanazawa University, Ishikawa 920-1192, Japan*

Received 3 October 2014; revised 25 December 2014; accepted 3 January 2015
Available online 28 January 2015

Abstract—The intergranular fracture toughness of plastic deformable crystalline materials is strongly controlled by the plastic work ahead of the intergranular crack tip. Therefore, in studies of intergranular fracture toughness, the grain boundaries (GBs) should be regarded as both a cleavage plane and dislocation source. Combining continuum analyses and atomic simulations, this study investigates the atomic-scale mechanism of intergranular crack tip plasticity in aluminum ⟨1 1 2⟩ tilt GBs as an effective dislocation source. To quantitatively predict the first plastic deformation near the intergranular crack tip, we first model the dislocation emission from the GBs ahead of the intergranular crack tip and analytically derive the critical stress intensity factor. If the predicted first plastic phenomenon is dislocation emission from the GBs, the resulting wedge disclination can shield the stress field near the crack. Dislocation emissions from the crack tip are accompanied by dislocation emissions from the GBs, despite the predicted difficulty of the latter. The lattice defect evolution nucleates a nanograin with a disclination at the triple-junction ahead of the crack tip, which can weaken the mechanical field near the crack tip. Consequently, when improving the intergranular fracture toughness of materials, the role of GBs as dislocation sources cannot be ignored.

Keywords: Grain boundary; Disclination; Dislocation; Interfacial fracture toughness; Molecular dynamics

1. Introduction

Owing to recent progress in manufacturing technology, nanostructured materials (NSMs) can now be manufactured in bulk [1]. NSMs include ultrafine-grained (UFG) materials [2], bimodal materials [3], and nanotwinned Cu [4]. To apply NSMs in high-strength, high-toughness structural components, we must understand their fracture phenomena [5–7]. Traditionally, fracture toughness is simply estimated from the relationship between the crack extension force and the resistance of the material [8]. In general, the former can be calculated within a continuum mechanics framework, whereas the latter is determined by physical properties such as the strength of interatomic bonding ahead of the crack tip. NSMs are characterized by a large volume fraction of grain boundary (GB) regions, the natural sites of cleavage fracture. Therefore, to understand the fracture toughness of NSMs in the above context, we must investigate the resistance of NSMs to both intragranular and intergranular cracking. Furthermore, since NSMs can plastically deform, we must consider the GB-related plastic phenomena ahead of intergranular crack tips.

First, we consider the transgranular fracture of plastic deformable materials in the absence of any GB effects. Based on the energy balance approach, crack propagation should satisfy the following condition [9–10]:

$$\mathcal{G}_c = \mathcal{G} > 2\gamma_s + \gamma_p. \tag{1}$$

Here $\mathcal{G}$ represents the strain energy release rate corresponding to the crack extension force and $2\gamma_s + \gamma_p$ represents the effective surface energy corresponding to the crack extension resistance. γ_s and γ_p represent the surface energy and the work done by plastic strain near the crack tip, respectively. A more specific description of plastic deformation that admits dislocations is provided by the stress intensity factor (SIF) approach. According to Griffith [11], ideal cleavage fracture requires that the local SIF k $(=K + K_D)$ be larger than the critical SIF K_G; that is,

$$K_c = K > K_G - K_D. \tag{2}$$

Here K and K_D are the SIFs caused by the applied stress and dislocations near the crack tip, respectively. K and $K_G - K_D$ can be regarded as the crack extension force and resistance, respectively. This concept is the well-known dislocation shielding theory [12]. Because the critical values of $\mathcal{G}_c$ and K_c correspond to the fracture toughness of deformable materials, materials with high fracture toughness exhibit large plastic strain with many shielding disloca-

* Corresponding author. Tel.: +81 76 234 4692; e-mail: simokawa@se.kanazawa-u.ac.jp

http://dx.doi.org/10.1016/j.actamat.2015.01.002
1359-6462/

tions near the crack tip. Moreover, the brittle–ductile transition behavior of materials can be determined by comparing the expansion rates of the crack expansion force and those of the plastic field.

Next, the influence of GBs on fracture toughness is incorporated by considering the intergranular fracture. In this case, a GB cleaves into two new surfaces, and the effective surface energy in Eq. (1) is modified to $(2\gamma_s - \gamma_{gb}) + \gamma_p$ [13], where γ_{gb} is the GB energy. Observed fracture toughness values indicate that although the first term depends on the GB structure [14], it is generally dominated by the second term ($(2\gamma_s - \gamma_{gb}) \ll \gamma_p$) [15]; therefore, fracture toughness appears to be relatively unaltered by the GB structure if γ_p is a constant parameter of the material. However, fracture toughness strongly depends on GB segregation that changes the first term [16], and GB strength is strongly correlated with GB energy [17], indicating that GB structure influences the fracture toughness in practice. These results clearly show the discrepancy between the estimated and observed influence of GB structure on intergranular fracture toughness. To resolve this discrepancy, Jokl et al. expressed γ_p as a function of $(2\gamma_s - \gamma_{gb})$ [18]; specifically, they proposed that the plastic work γ_p caused by dislocations emitted from the crack tip increases with the ideal cleavage fracture resistance $(2\gamma_s - \gamma_{gb})$. Yamaguchi and Kameda have explained the strong dependence of the fracture toughness on the type and coverage of segregated solute observed by the experiments with a thermodynamic approach aided by first-principles calculations [19].

Apart from forming a cleavage plane, do GBs play other important roles in the transgranular fracture of NSMs? Recently, a dislocation source role has been identified for GBs, providing clues into the unique mechanical properties of NSMs [20–23]. For example, the fracture toughness of UFG metals is improved at low temperatures [24,25]. This phenomenon may be explained by dislocation emission from GBs near the transgranular crack tip [26]. Furthermore, atomic simulation studies have elucidated the mechanism of dislocation emission from GBs and its dependence on GB structure [27–29]. These studies have sparked an interest in GBs as a dislocation source and their effect on intergranular fracture toughness. Because dislocations emitted from GBs contribute to the plastic work γ_p and their characteristics greatly affect the K_D, the relationship between the intergranular fracture toughness and GB structures must be reconsidered from the perspective of GBs as a dislocation source. Such a reinterpretation is essential for the material design of NSMs based on GB engineering [30].

In this study, we investigate the atomic-scale intergranular crack tip plasticity in tilt GBs acting as an effective dislocation source. Our investigation combines continuum analyses and atomic simulations. In Section 2, after briefly introducing the GB properties used in the atomic simulations, we model the dislocation emission from GBs ahead of the intergranular crack tip and analytically derive the critical SIF. From the critical SIF, we quantitatively predict the first plastic deformation phenomenon near the intergranular crack tip. Section 3 examines the intergranular crack tip plasticity in atomic simulations and investigates how the microstructures caused by dislocation emission from GBs affect the fracture toughness. The investigated microstructures are a wedge disclination [31] at the GB and a nanograin with a disclination at the triple junction near the crack tip. Discussions and conclusions are presented in Sections 4 and 5, respectively.

2. Theories and computational methods

In this study, we use the theory of isotropic linear elasticity to derive the critical SIF to dislocation emission from GBs, and predict the first plastic deformation near the intergranular crack tip in atomic models. Therefore, the analyzed material is aluminum (Al), which can be considered as an isotropic elastic body. In the atomic simulations, we adopt the embedded atom method (EAM) proposed by Mishin et al. [32]. The anisotropic factor of the atomic potential, calculated as $c_{44}/(c_{11} - c_{12})$, is 1.25.

2.1. Grain boundary structure

The intergranular crack tip plasticity is investigated in four Al symmetrical $\langle 1\,1\,2\rangle$ tilt GBs: Σ175, Σ73, Σ77, and Σ15. These GBs exist close to the stable Σ11 GB and easily emit dislocations under tensile loading applied perpendicular to their planes [29]. The structural and physical properties of the GBs are summarized in Table 1. The detailed atomic structures and the dislocation emission mechanism are briefly described below.

Among the GBs close to the analyzed GBs, the most stable is Σ11 GB that misorientation angle $\theta_{GB} = 62.96°$. The structure of Σ11 GB can be represented by structural units (SUs; yellow symbols in Fig. 1(a)). This SU is called a *B*-SU [29]. The colors in Fig. 1 denote the stacked atomic layers at different depths along the $\langle 1\,1\,2\rangle$ direction. Note that the GB has a six-layer periodicity. In terms of the depth of atoms constituting the *B*-SU, the periodic structure of Σ11 GB is $|B^1B^2B^3B^4B^5B^6|$. However, because the results of this study were independent of atomic depth, the depth information was ignored when determining the GB structure with SUs. To represent the GB structures of Σ175, Σ73, Σ77, and Σ15, we regularly introduce SUs into Σ11 GB, as shown in Fig. 1(b–d). This SU is called *C*-SU. The density of *C*-SU and the GB energy increase with increasing deviation of the misorientation angle $\Delta\theta$ from Σ11 GB, as shown in Fig. 1 and Table 1. Setting Σ11 GB as a reference structure, we can consider *C*-SU to be a GB dislocation that forms the deviation from Σ11 GB [29].

When these GBs are deformed under tensile loading applied perpendicular to their planes, the GB dislocation (κ) in *C*-SU decomposes into a lattice edge dislocation (ζ) emitted into a grain and glissile GB dislocation (ζ″) with a Burgers vector parallel to the GB plane: $\boldsymbol{b}^{\kappa} = \boldsymbol{b}^{\zeta} + \boldsymbol{b}^{\zeta''}$ (see Fig. 3(b)), e.g., $\boldsymbol{b}^{\kappa} = \frac{2}{11}[\bar{3}\,1\,\bar{1}]$, $\boldsymbol{b}^{\zeta} = \frac{1}{2}[\bar{1}\,1\,0]$, and $\boldsymbol{b}^{\zeta''} = \frac{1}{22}[\bar{1}\,\bar{7}\,\bar{4}]$ in this study. Since this type of decomposition rarely occurs under compressive loading, dislocation generation by GBs is asymmetric. This asymmetry arises from the relationship between the Burgers vector components of the lattice dislocation ζ and the GB dislocation κ. Because dislocation emission transforms *C*-SU to *B*-SU, it structurally transforms the original GB into Σ11 GB. The tensile stress required for GB dislocation emission decreases with increasing spacing *h* of the *C*-SUs [29]; hence, dislocations are most easily emitted from Σ175 GB in this study.

2.2. Atomic simulation setups

Fig. 2(a) is a schematic of the analysis model used in the atomic simulations. In all models, initial L_y and L_z are set