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Effect of blunt nanocracks on the splitting transformation of grain boundary dislocation piled up at triple junctions

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ABSTRACT

Considering that grain boundary (GB) deformation is a structural element that hinders crack growth and promotes superplastic deformation in nanocrystalline materials (NCMs), a theoretical model is suggested to describe the effect of the blunt pre-nanocracks with surface stress on the splitting transformation of the first head grain boundary dislocation (GBD) within the pile-up at the triple junctions (TJs) of GBs in mechanically loaded NCMs. The analytic solution of the total energy change that characterizes this process of splitting transformation of GBD is derived quantitatively by the complex variable method, and then, the very beginning plastic deformation occurrence near the nanocrack tip is predicted. We theoretically evaluated the influence of the various parameters of blunt pre-nanocracks, such as nanocrack blunting and length, the characteristics of grain and GBs, such as grain size, the number of GBDs, and GB angles, and the surface stress at critical conditions for such a splitting transformation. Further analyses revealed that the positive (negative) surface stress significantly decreases (increases) the energy and obviously influences the critical conditions for splitting transformation. Our study identified the beneficial role of GB defect structure transformation, namely the splitting transformation, in enhancing the ductility and fracture toughness of NCMs. It also lays the foundation for investigating how the microstructures caused by GB deformation affect the novel mechanical properties of NCMs.

1. Introduction

Owing to the dramatically higher density of grain boundaries (GBs) and their triple junctions (TJs) that inherently accompany a reduction in grain size to the nanometer regime, the use of nanocrystalline materials (NCMs) has resulted in many improvements in vital technological and engineering properties such as susceptibility to corrosion (Telang et al., 2015), strengthening (Aifantis and Willis, 2005; Kedharnath et al., 2017), premelting (Lu et al., 2014), and creep damage (Barai and Weng, 2011; Mohamed, 2016; Roodposhti et al., 2016), which are closely related to the boundary structure. GBs and their TJs (including interphase boundaries between dissimilar phases) are known to occupy higher-energy regions as compared with atoms that occupy lattice sites within interior grains in NCMs and are preferential sites for metallurgical phenomena associated with fracture in polycrystalline materials (Zhang et al., 2017). Thus, different from that for conventional coarse-grained materials, GBs and TJs are crucial for the advanced performance of NCMs and must be comprehensively understood to design, model, and then predict the mechanical properties and novel physical deformation mechanisms of nanosized materials.

Extensive studies for decades have confirmed that when the average grain size reduces to the nanometer range, a crossover from intragranular dislocation-based plasticity (which is primary in coarse-grained materials) to GB-mediated plasticity occurs (Luo et al., al., 2009; Kahrobaiyan et al., 2014). The specific structural features of NCMs, such as nanoscopic size of grains, GBs and their TJs with their generic defects, such as grain boundary dislocations (GBDs) and disclinations, can effectively carry plastic flow, and stimulate, under special conditions, the generation and development of such deformation modes, including GB sliding, GB migration, Coble creep, TJ diffusional creep and rotational deformation (Tvergaard, 1985; Yamakov et al., 2002; Wei and Anand, 2004; Pan et al., 2007; Liu and Zhang, 2009; Liu and Ma, 2010; Wei and Kysar, 2011; Padmanabhan et al., 2014; Mompiou and Legros, 2015; Prokoshkina et al., 2017; Bobylev and Ovid'ko, 2017). Furthermore, GBs and their TJs instead become directly involved in the accommodation of strain and serve as active sources for dislocation emission (Shan et al., 2004; Monk et al., 2006; Bobylev et al., 2009; Ovid'ko and Skiba, 2012). Therefore, understanding and quantifying

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the relationship between these mechanisms and GB structure are critically important and a great step toward future GB engineering (Li and Chew, 2017).

In recent years, it has been clearly recognized that the features of GB deformations mentioned above are intensively related to TJs of GBs (Wu and He, 1998; Gutkin et al., 2005; Shi and Zikry, 2009; Zisman, 2017). TJs of GBs, where GB planes change their orientations, serve as obstacles for GBD motion and plastic flow occurring through GB deformation (Ovid'ko and Sheinerman, 2012). The transformation of GB structure into a neighboring energetically stable boundary must occur as GBDs are split from TJs. That is, in these circumstances, the splitting transformation of GB defects can occur at TJs and result in the formation of sessile, gliding or climbing GBDs, which can provide a further GB deformation, extremely affect the dominant deformation mechanism realized in mechanically loaded NCMs, and then play a constructive role in both the unique structure and properties of NCMs (Ovid'ko et al., 2000; Fedorov et al., 2003). From the viewpoint of thermodynamics, several works have suggested theoretical models to address the importance of motion and splitting transformation of GB defects at TJs to superplastic deformation of NCMs. For instance, Gutkin et al. (2003) and Gutkin and Ovid'ko (2003) considered a model of crossover from GB sliding to rotational deformation, which is realized by the very beginning transformation of a pile-up of gliding GBDs stopped by a TJ of GBs, into two walls of climbing GBDs (treated as the dipoles of partial wedge disclinations). The conditions necessary for such a transformation were then determined and discussed. Han et al. (2014) proposed a new composite model to describe the competition of deformation mechanism between stress-driven migration of GB and GB sliding, which is characterized by GBDs traversing through super TJs in mechanically loaded NCMs. Shimokawa et al. (2011) and Shimokawa and Tsuboi (2015) investigated the atomic-scale intergranular crack tip plasticity in tilt GBs, which act as an effective dislocation source. Ovid'ko and Sheinerman (2017) suggested a theoretical model to describe GB sliding and its accommodation through dislocation slip in ultrafine-grained and NC metals. The emission of lattice dislocations from TJs into interior grains characterizes the initial stage of dislocation slip accommodation.

In general, GBs are recognized as one of the major barriers to crack growth in most engineering materials, and grain refinement increases the fracture toughness of materials (Xiao and Chen, 2001b; Pook, 2007; Legros et al., 2008; Zhou et al., 2008; Jin et al., 2015; Fang et al., 2016; Vetterick et al., 2018). Thus, the role of GBs and their TJs as dislocation sources must be known to elucidate the fracture phenomenon in fine-grained materials (Shimokawaa and Tsuboi, 2015). Bobylev et al. (2010) theoretically described two scenarios for the evolution of GBDs at a TJ near a microcrack tip in creep, similar to that in tests specified by constant and comparatively low applied stresses in a NCM. In the first case, such dislocations are immobile, and their stress fields compensate, in part, for local stresses near the microcrack tip. In the second case, GBDs at the TJ climb along adjacent GBs and promote microcrack blunting. Both these cases suppress microcrack growth and enhance ductility and toughness of NCMs. Kim et al. (2013) performed in situ tensile experiments to investigate the interaction of an advancing crack with GBs in thin copper foils. They found that certain GBs are effective in arresting the crack growth, and the stress field of the arrested crack then activates multiple deformation modes in the grain ahead of the crack tip. Hosseinian et al. (2018) performed in situ TEM experiments to investigate the combined effects of thickness (30 vs. 100 nm) and average grain size (40 vs. 70 nm for the thicker films) on the crack propagation mechanisms in ultrathin NC gold microbeams. They found that for the thinner specimens, secondary nanocracks are generated (as a result of GB sliding) ahead of the main crack and coalesce together. Instead, secondary nanocracks do not form ahead of the main crack for the thicker specimens; the main crack extends as a result of sustained GB sliding at the crack tip.

From the above data, it can be well established that GBs could interact with cracks during the process of fracture in polycrystalline materials and NCMs. GBDs piled up at TJs can shield the stress field near the crack tip. Consequently, a mechanical response of the splitting transformations of GBD is different from that without cracks. However, the aforementioned theoretical models of splitting transformations of GBDs piled up at TJs operate without pre-existent cracks. Furthermore, GB defect structure transformation, namely the splitting transformation, can shield the stress intensity factor near the nanocrack tip. This implies that when dislocation emission from the crack tip stops because of the presence of neighboring GBs, the dislocation reactions at TJs can additionally reduce the stress intensity factor, thereby hindering crack growth. Therefore, hereinafter, the main aim of this work is to theoretically describe in detail the splitting transformation of GBDs piled up at TJs of GBs near a pre-existent or growing blunt nanocrack with surface stress in plastically deformed and mechanically loaded NCMs, with focus on one of the transformations of GBD, which serves as an elementary act of the very beginning of the GB deformation, and is relatively most energetically favorable (Fedorov et al., 2003). In the framework of the model, stress concentration near nanocrack initiates the splitting transformation of GBD. The total energy change is analytically derived, and the critical conditions for splitting transformation are quantitatively predicted in plastically deformed NCMs. Special attention is paid to quantify the effect of blunt pre-nanocracks, the characteristics of grain and GB, and the surface stress on the presented type of splitting transformation of GBD piled up at TJ. The results provide a greater depth of understanding the GB-crack-dislocation interaction, which is essential for investigating how the microstructures formed because of the splitting transformation of GBDs affect the crack propagation behavior and the fracture toughness and then for designing better GB engineered materials.

2. Model

The geometric features of a blunt nanocrack and GBD pile-up at TJ A are critical to understand the splitting transformation of GBD piled up at TJ in plastically deformed NC solids. In this section, a deformed elastically isotropic NC specimen with shear modulus μ and Poisson ratio υ is considered under the action of remote tensile loading σ_0 applied perpendicular to the nanocrack growth direction. This specimen consists of nanoscale grains divided by GBs and contains a pre-existent mode I blunt nanocrack, schematically shown in Fig. 1. Here, we assume that the nanocrack has already been blunted because of previous consecutive processes of dislocation emission and nanocrack advance (Ovid'ko and Sheinerman, 2010). Thus, for more reasonable and realistic description of crack stability and growth, an elliptically pre-cracked two-dimensional grain structure of a typical fragment of the solid is schematically shown in Fig. 1a. In doing so, we model the blunt nanocrack as an elongated ellipse, which is oriented along x and y axis of the Cartesian coordinate system (xOy) with the origin at the ellipse center (Fig. 1a). The curvature radius $\rho(=q^2/p)$ characterizes the "bluntness" of the nanocrack tip, and at the nanocrack tip, the radius is much smaller than the crack half-lengths p and q. To read and analyze easily, using the relationship $z=z_1+p-\rho/2$, the stress field in the Cartesian coordinate system (xOy) can be transited to the coordinate system ($x_1O_1y_1$), whose origin is of $\rho/2$ away from the tip of the elliptically blunt nanocrack. The elliptical representation will lead to a quantitative estimate of nanocrack blunting effect.