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Nanoscale rotational deformation effect on dislocation emission from an elliptically blunted crack tip in nanocrystalline materials

H. Feng [a], Q.H. Fang [a,*], Y.W. Liu [a], C.P. Chen [b]

[a] State Key Laboratory of Advanced Design and Manufacturing for Vehicle Body, Hunan University, Changsha 410082, China
[b] College of Civil Engineering and Architecture, Xiamen University of Technology, Xiamen 361024, China

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ABSTRACT

A grain size-dependent model is theoretically established to describe the effect of a special physical micromechanism of plastic flow on the dislocation emission from an elliptical blunt crack tip in nanocrystalline solids. The micromechanism represents the fast nanoscale rotational deformation (NRD) occurring through collective events of ideal nanoscale shear near crack tips, which as a stress source is approximately equivalent to a quadrupole of wedge disclinations. By the complex variable method, the grain size-dependent criterion for the dislocation emission from an elliptical blunt crack tip is derived. The influence of the grain size and the features of NRD on the critical stress intensity factors for dislocation emission is evaluated. The results indicate that NRD releases the high stresses near the crack tip region and thereby enhances the critical stress intensity factor for dislocation emission. The NRD has great influence on the most probable angle for dislocation emission. The critical stress intensity factor will increase with the increment of the grain size, which means the emission of the dislocation becomes more difficult for larger grain size due to the effect of NRD.

1. Introduction

In recent decades, crack growth and fracture processes in nanocrystalline (NC) and ultrafine-grained materials showing superior strength, hardness and good wear resistance have attracted tremendous attention motivated by both fundamental interest to specific deformation mechanisms operating in these solids and their technological applications (Aifantis and Dempsey, 2005; Dao et al., 2007; Kumar et al., 2003; Meirom et al., 2012; Ovid'ko and Sheinerman, 2010, 2007; Yang and Yang, 2008; Zhou and Wu, 2006; Zhou et al., 2008a,b, 2007, 2006). The specific properties of the ultrafine-grained and NC solids are controlled by their specific structural features, such as nanoscopic sizes of grains and large amounts of grain boundaries (GBs), because these features cause operation of specific structural deformation and fracture mechanism. For instance, due to large amounts of GBs, alternative deformation modes such as intergrain sliding, GB migration, triple junction diffusional creep, Coble creep, rotational deformation and nanoscale twin deformation effectively operate in NC solids (Bobylev et al., 2011; Gutkin and Ovid'ko, 2005; Juan et al., 2012; Morozov et al., 2010; Ovid'ko and Sheinerman, 2012, 2011, 2010). These mechanisms of plastic deformation can not only cause relaxation of high-concentrated stresses, thereby hampering the nucleation of nanoscale cracks, but also slow down or arrest the growth of the formed cracks. It has been proposed that these deformation modes can play an important role in the toughening of NC materials. This is in agreement with computer simulations and experimental data showing the enhancement of fracture toughness of several materials compared to those of their microcrystalline counterparts (Kuntz et al., 2004; Meirom et al., 2012; Zhao et al., 2004).

Of particular interest is the experimentally documented phenomenon of the nanoscale rotational deformation (NRD) – a plastic deformation accompanied by crystal lattice rotations, which operates in NC solids characterized by superior strength (Cheng et al., 2010, 2013; Cui et al., 2009; Ke et al., 1995; Liu et al., 2011; Shan et al., 2008). For instance, Ke et al. (1995) *in situ* observed grain rotations (crystal lattice rotation within grains) of up to 15° ahead of growing crack tips in nanocrystalline Au films under tensile deformation. With a thin film tensile technique, Liu et al. (2011) reported on *in situ* observation of grain rotations near crack tips in a nanocrystalline, textured, columnar-structured Au film during its plastic deformation. In parallel with crystal lattice rotations in nanograins, the associated formation of perfect lattice dislocations (carrying an extra tilt misorientation) at GBs near a crack tip was observed. These experimental data provided convincing evidence that NRD effectively operates in highly stressed regions near crack tips in NC materials with finest grains. Recently, a theoretical model (Fang et al., 2012; Feng et al., 2013b; Morozov et al., 2010) has

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* Corresponding author. Tel.: +86 731 89822841; fax: +86 731 88822330.
E-mail addresses: fangqh1327@tom.com, fangqh1327@hnu.edu.cn (Q.H. Fang).

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been suggested describing NRD occurring through cooperative GB sliding and GB dislocation climb in nanocrystalline materials. However, the cooperative GB sliding and GB dislocation climb process is typically slow at low and ambient temperature, because its rate is controlled by GB diffusion carrying GB dislocation climb. Therefore, the model (Fang et al., 2012; Feng et al., 2013b; Morozov et al., 2010) is questionable in explanation of the experimentally documented (Cheng et al., 2010, 2013; Cui et al., 2009; Ke et al., 1995; Liu et al., 2011; Shan et al., 2008) fast grain rotations occurring near advancing crack tips in nanocrystalline materials with finest grains at room temperature. Then, Ovid'ko and Sheinerman (2012) suggested and theoretically described a special micromechanism of NRD near crack tips in nanocrystalline materials with finest grains at room temperature. The fast NRD micromechanism occurring through the collective events of nanoscale ideal shear is responsible for the fast grain rotations near crack tips. They calculated the conditions for realization of NRD through ideal shear events, and found that such rotational deformation can effectively occur near the tip of a blunt crack rather than a sharp crack. They also found that the NRD can enhance the fracture toughness of NC materials, and it is the easiest to occur in finest grains, which is highly consistent with the experimental observations (Cheng et al., 2010; Ke et al., 1995; Shan et al., 2008).

On the other hand, it is well known that dislocation emission from a crack tip is one of the most fundamental processes for understanding the crack blunting in NC and ultrafine-grained materials (Rice and Thomson, 1974). Once dislocations are emitted in many crystals, they move out of the crack tip area, leaving behind a dislocation-free zone. An internal back stress due to the dislocations emitted from crack tip accommodates the stress intensity due to the applied load, causing an increase fracture toughness of materials (Thomson, 1986). So, the critical stress intensity factor (SIF) for dislocation emission for a sharp crack has been widely analyzed in previous studies (Huang et al., 1995; Tsai and Lee, 1997; Zhang and Qian, 2000, 1996). In addition, a few works reported on dislocation emission from a V-shape crack (Chen and Lee, 2000; Zhang et al., 1995). However, the real crack in a material is always of finite length and the radius of curvature of the crack tip is never small enough to be zero, having a curvature radius of several Burgers vectors due to the removal of atoms via diffusion, or mechanical and chemical erosions (Chen et al., 2003; Wang and Li, 2003). Therefore, the interaction between dislocations and blunt cracks had received much attention during the last several years (Fang et al., 2009; Fischer and Beltz, 2001; Huang and Li, 2004; Qian et al., 2002).

Recently, Ovid'ko and Sheinerman (2010) investigated the effects of grain size and blunting of cracks on the fracture toughness of NC materials in a typical situation where crack blunting and growth processes are controlled by dislocation emission from crack tips. According to their description, edge dislocations emitted from cracks are stopped at GBs, resulting in blunting of cracks. Both crack blunting and the stress field of the arrested dislocations hamper further dislocation emission from cracks in NC materials. As a result, grain size reduction causes NC materials to show a brittle behavior. Based on the above description, Fang et al. (2012) described the effect of the special rotational deformation on the emission criterion of dislocations from a crack tip in NC materials. Within their discussion, the special rotational deformation can suppress the dislocation emission from the crack tip. While the special rotational deformation is stronger, the edge dislocation emission from the crack tip is more difficult. However, in the study of Feng et al. (2013a), they found the cooperative GB sliding and migration can promote the dislocation emission from the crack tip, which causes effective blunting of the crack thus suppresses its growth and improves the toughness of NC materials. Therefore, there is great interest in identifying the special deformation –NRD occurring through ideal shear events near an elliptical blunt crack tip effects on dislocation emission and crack growth in NC materials.

In the present paper, we study the influence of the special NRD on the criterion for dislocation emission from an elliptical blunt crack in NC solids. The NRD occur through generation of walls of nanodisturbances, their transformations into lattice dislocation dipoles and formation of dislocation dipole walls with associated nanoscale rotations of crystal lattice near blunt crack tips in NC materials. Here, using the complex variable method, the impact of the stresses produced by the NRD on the dislocation emission from the elliptical blunt crack tip is investigated. The grain size dependent criterion for dislocation emission is derived. The critical stress intensity factors (SIFs) (caused by applied loadings) for the dislocation emission increase with increasing of grain size due to the influence of NRD. In addition, the emission of dislocations from crack tip becomes more difficult comparing with the case without considering NRD, which indicates that NRD releases, in part, the high stresses near the crack tip area and thereby enhances the critical SIFs (caused by applied loadings) for dislocation emission.

2. Modeling

The model of the problem to be studied is shown in Fig. 1. Consider a deformed NC specimen consisting nanoscale grains divided by GBs and containing an elliptically blunted crack. The specimen is assumed to be elastic and isotropic, whose shear modulus is μ and Poisson ratio is v. It is subjected to remote mode I loadings and mode II loadings. A two-dimensional (2D) section of a typical fragment of the solid is schematically shown in Fig. 1(a). For simplicity, we assume that the defect structure of the solid is the same along the coordinate axis z perpendicular to the xy plane. This assumption will allow us to restrict our consideration to a 2D grain structure which definitely reflects the key aspects of the problem.

The collective events of ideal shear near a blunt crack tip and the high local stresses near the blunt crack tip can initiate nanoscale rotational deformation (NRD) in a nanoscale grain adjacent to the tip (Fig. 1(a)). Within our model, NRD occurs through the generation and evolution of walls of GB dislocation dipoles by means of nanoscale ideal shears (Fig. 2(a)–(c)). More precisely, nanoscale ideal shears simultaneously occur under the shear stress τ in several (n) parallel slip planes (Fig. 2(b)–(c)). Such shears are characterized by a tiny shear magnitude s and produce a wall of n generalized stacking faults having nanoscopic sizes (Fig. 2(b)). In the theory of crystals, a generalized stacking fault is defined as a planar defect resulting from a cut of a perfect crystal across a single plane into two parts which are then subjected to a relative displacement by an arbitrary vector s (lying in the cut plane) and rejoined (Ovid'ko and Sheinerman, 2012, 2011).

The generalized stacking faults are bounded by 'non-crystallographic' partial dislocations located at GBs (which are called nanodisturbances) and characterized by non-quantized (non-crystallographic) Burgers vectors $\pm s$ with quite a small magnitude $s < b_r$, where b_r is the magnitude of the Burgers vector of a perfect dislocation (Fig. 2(b)). At the following stage of deformation, the magnitude s continuously increases, and generalized stacking faults evolve in parallel with growth of s. Finally, s reaches the magnitude b_r, in which case generalized stacking faults disappear and conventional dipoles of perfect dislocations are formed at GBs (Fig. 2(c)).

According to the estimates in the work of Ovid'ko and Sheinerman (2012), NRD can be initiated by high local stresses near the tip of a blunt crack, in contrast to a flat crack. In this context, we will focus our consideration on the NRD occurring near the tip of an elliptical blunt crack in a NC solid (Fig. 1).