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Generation of nanoscale deformation twins at locally distorted grain boundaries in nanomaterials

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ABSTRACT

Special mechanisms for formation of nanoscale deformation twins at grain boundaries (GBs) in nanocrystalline and ultrafine-grained materials are suggested and theoretically described. Within our description, nanoscale deformation twins are generated at locally distorted GBs that contain local, deformation-distorted fragments being rich in GB dislocations produced by preceding deformation processes. The twin formation mechanisms represent (i) the successive events of partial dislocation emission from GBs; (ii) the cooperative emission of partial dislocations from GBs; and (iii) the multiplane nanoscale shear generated at GBs. The energy and stress characteristics of the nanoscale twin formation through these special mechanisms in nanocrystalline nickel (Ni), copper (Cu) and silicon carbide (3C-SiC) are calculated and analyzed. Competition between the twin formation mechanisms in nanomaterials is discussed.

1. Introduction

Specific deformation mechanisms/modes effectively operate in nanocrystalline and ultrafine-grained bulk materials, ultrathin films and nanowires, strongly influencing the outstanding mechanical properties of these solids with external and/or internal nanoscale geometries; see, e.g., (Valiev and Langdon, 2006; Kawasaki and Langdon, 2007; Koch et al., 2007; Farrokh and Khan, 2009; Pande and Cooper, 2009; Abdolrahim et al., 2010; Bobylev et al., 2010; Sha et al., 2011; Abdolrahim et al., 2012; Branicio, 2012; Fang et al., 2012; Valiev et al., 2012; Wang et al., 2012; Zhu et al., 2012; Zhu and Lu, 2012; Branicio et al., 2013; Choi et al., 2013; Estrin and Vinogradov, 2013; Feng et al., 2013a,b; Kumar et al., 2013; Xu et al., 2013; Zhang et al., 2013; Abdolrahim et al., 2014; Shao et al., 2014). For instance, lattice dislocation slip in nanocrystalline and ultrafine-grained bulk and thin-film materials (hereinafter called nanomaterials) shows dramatic behavioral deviations from its conventional counterpart in coarse-grained polycrystals. Also, specific GB deformation modes highly contribute to plastic flow in nanocrystalline materials with finest grains in wide temperature intervals and carry superplasticity in nanomaterials at elevated temperatures; see, e.g., book (Koch et al., 2007) and reviews (Kawasaki and Langdon, 2007; Pande and Cooper, 2009; Zhu et al., 2012). Besides, following numerous experimental data, computer simulations and theoretical models, nanoscale twin deformation effectively operates in nanomaterials with various chemical compositions and

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structures; see, e.g., original research papers (Chen et al., 2003; Liao et al., 2003; Wang et al., 2005; Wu et al., 2006; Zhu et al., 2008; Zhu et al., 2009a,b; Ovid'ko, 2011; Wu et al., 2011; Ovid'ko and Skiba, 2014) and a review (Zhu et al., 2012). In doing so, in contrast to coarse-grained polycrystals where deformation twins are typically generated within grain interiors, in nanomaterials under mechanical load, twins are often generated at GBs; see (Zhu et al., 2012) and references therein. In order to explain this experimentally documented fact indicative of specific deformation behavior of nanomaterials, it was suggested that nanoscale deformation twinning occurs through successive emission of partial dislocations from GBs (Zhu et al., 2008, 2009a,b, 2012). According to this explanation scheme, partial dislocations should either pre-exist at GBs on every slip plane or be resulted from transformations of pre-existent GB dislocations located on every slip plane to form a single twin through dislocation emission from the GB. However, it is practically impossible to have pre-existent GB dislocations or partial ones at a GB on every slip plane in real materials (Zhu et al., 2009a, b). In order to avoid the discussed discrepancy, Zhu with co-workers (Zhu et al., 2009a,b) suggested that multiplication of partial dislocations can occur through dislocation reactions and cross-slip processes in deformed nanomaterials. As a result of such defect transformations, partial dislocations are capable of existing at a GB on every slip plane, in which case their successive emission events provide a twin to grow continuously (Zhu et al., 2009a,b). However, within this explanation, each dislocation reaction transforms a partial dislocation into two dislocations: a full dislocation and another partial dislocation. As a corollary, the dislocation reactions in question are characterized by very large energy barriers being of the order of the full dislocation energy. Such reactions can come into play, if only a very high level of the applied stress is operative in a specimen. Therefore, multiplication of partial dislocations is hardly typical in nanomaterials in wide ranges of their deformation parameters. This motivates search for new alternative explanations of twin generation at GBs in mechanically loaded nanomaterials. The main aim of this paper is to suggest and theoretically describe new physical mechanisms for formation of nanoscale deformation twins at GBs. Within our approach briefly described earlier (Ovid'ko and Skiba, 2014), nanoscale deformation twins are generated at locally distorted GBs that contain local, deformation-distorted fragments with GB dislocations located on every slip plane and produced by preceding deformation processes. The twin formation mechanisms represent (i) the successive events of partial dislocation emission from GBs; (ii) the cooperative emission of partial dislocations from GBs; and (iii) the multiplane nanoscale shear generated at GBs.

2. Mechanisms for formation of nanoscale deformation twin at locally distorted grain boundaries in nanomaterials: Geometric features

Within our description, nanoscale deformation twins are generated at locally distorted GBs, that is, GBs containing local fragments being rich in GB dislocations produced by preceding deformation processes. For instance, such local GB fragments can be formed due to either splitting of extrinsic lattice dislocations trapped at GBs (Fig. 1) or GB deformation processes involving slip and climb of GB dislocations (Fig. 2). The splitting of extrinsic dislocations at high-angle GBs is a well experimentally documented process (Lojkowski and Fecht, 2000) resulting at its initial stage in formation of several closely located GB dislocations (Fig. 1a and b). These dislocations and pre-existent GB dislocations can form a nano-sized wall of GB dislocations located on every slip plane (Fig. 1). In a rather typical situation, the extrinsic dislocation that undergoes the splitting transformation at a GB represents a head dislocation of a pile-up configuration stopped by the GB (Fig. 1). In this case, after the splitting of the head dislocation of the pile-up, its second dislocation can reach the GB where this extrinsic dislocation splits into new GB dislocations. Both pre-existent GB dislocations and the GB dislocations resulted from the splitting transformations of the extrinsic dislocations are capable of forming a nano-sized wall of GB dislocations located on every (or almost every) slip plane (Fig. 1). Their transformations followed by emission of partial dislocations into adjacent grain produce nanoscale deformation twins (for details, see below).

Another scenario for formation of local deformation-distorted fragments of GBs is related to GB deformation processes as follows (Ovid'ko and Skiba, 2014). First, a nanostructured specimen is deformed by GB sliding that produces pile-ups of GB dislocations stopped by triple junctions of GBs (Fig. 2a and b). These dislocations under the applied stress climb along GBs adjacent to triple junctions (Fig. 2b–f). Since the rate of GB dislocation slip is much larger than that of diffusion-controlled climb of GB dislocations, the combined slip and climb of GB dislocations typically result in dense, wall-like configurations of climbing GB dislocations that can exist on every (or almost every) slip plane (Fig. 2c–f).

We now discuss generation of nanoscale twins at locally deformation-distorted GBs by the following three mechanisms: (i) the cooperative emission of partial dislocations from GBs; (ii) the successive events of partial dislocation emission from GBs; and (iii) the multiplane nanoscale shear generated at GBs. The former two mechanisms are realized through splitting of the GB dislocations located at local deformation-distorted GB fragments into immobile GB dislocations and mobile partial dislocations (Figs. 3 and 4). The mobile dislocations move either successively (Fig. 3) or cooperatively (Fig. 4) on every slip plane within a nanoscale region where a nanoscale twin is thereby generated.

Note that the splitting transformation of each GB dislocation at a local deformation-distorted GB fragment into another GB dislocation and a partial dislocation (Figs. 3 and 4) is specified by an energy barrier being around the energy of a partial dislocation. This barrier is lower than that (being around the energy of a full dislocation) for multiplication of partial dislocations, the dislocation reaction considered by Zhu et al. (2009a, 2009b). In these circumstances, the splitting transformation (Figs. 3 and 4) is more energetically favored, as compared to the multiplication reaction.