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Energetics of point defect interacting with grain boundaries undergone plastic deformations

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ABSTRACT

Grain boundaries (GBs) in the polycrystalline and nanocrystalline materials are usually at their non-equilibrated states due to the plastic deformations. Thus, the point defect sink efficiencies of non-equilibrated GBs may be different from those of equilibrated counterparts, which may influence the irradiation tolerance of materials. In this paper, we firstly performed the shear responses of four copper symmetric tilt grain boundaries (GBs). The plastic deformation modes of four GBs include GB sliding, shear-coupling and complex mechanism due to atom-shuffling, partial dislocation nucleation and local GB dissociations. We then study the energetics of point defects interacting with a series of GB configurations undergone plastic deformations. It is found that the plastic deformation dominated by the sliding and shear-coupling has no effect on the point defect sink efficiency of GB in comparison with initial GB states. However, sink efficiencies of GB configurations produced from the complex deformation mode are generally intensified, for both vacancy and self-interstitial atom. In addition, the residual stress in the crystals due to the dislocation nucleating from GB affects the point defect concentration in the crystals. On the other hand, complex deformation mechanism drives GBs to higher energy states with highly disordered structures. As a result, the distribution of lower point defect formation energies extends a larger distance from GB, which may therefore favor GB absorbing the point defects nearby.

1. Introduction

It has long been known to us that the material strength and ductility are strongly affected by changing grain size as described by Hall–Petch and inverse Hall–Petch relations (Chokshi et al., 1989; Dunstan and Bushby, 2014; Hall, 1951; Lim et al., 2011; Padmanabhan et al., 2007; Pande and Cooper, 2009; Petch, 1953; Tang et al., 2013), which correlate the grain size to strength. As grain size refines to the submicron and nanometer scale, structures of grain boundaries (GBs) within materials are remarkably altered as compared to their initial states. Their structures contain highly disordered regions, steps, ledges and other complex dislocation content (Meyers et al., 2006). As a result, the properties of the resulting GBs, such as average energy (Tucker and McDowell, 2011), excess volume (Tucker and McDowell, 2011), GB migration and slide (Frolov,

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2014) and other mechanical responses (Fensin et al., 2012a,b; Hasnaoui et al., 2002) would be different from their initial counterparts (Sauvage et al., 2012).

Both experimental and modeling studies show GBs generally act as sinks for the point defects produced from irradiation (Beyerlein et al., 2015; Dollar and Gleiter, 1985; Gleiter, 1979; Han et al., 2012; King and Smith, 1980; Siegel et al., 1980). Thus, GB may impart irradiation resistance properties to polycrystalline materials (Han et al., 2013; Misra et al., 2007; Misra and Thilly, 2010). For this reason, understanding the point defect sink efficiency of GBs is of great importance for the design of materials with irradiation resistance and understanding the properties of such materials (Li et al., 2012; Misra and Thilly, 2010; Singh and Zinkle, 1993; Xiao et al., 2015a,b). Extensive studies have been carried out to understand the possible factors that determine the sink efficiency of GBs (Demkowicz et al., 2011b; King and Smith, 1981; Millett et al., 2009; Zhang et al., 2012). To evaluate the point defect sink efficiency of GBs, many efforts have been invested into GBs of different materials, such as Cu (Bai et al., 2012; Han et al., 2012; Suzuki and Mishin, 2003a,b), W (Bristowe et al., 1980), Fe (Bristowe et al., 1980; Chen et al., 2013) and Au (Hahn and Gleiter, 1981; Siegel et al., 1980) etc. It has also been pointed out that material irradiation tolerance may be enhanced via increasing the GB fraction within materials (Singh, 1974). To do that, we may resort to ultrafine-grained (UFG) and nanocrystalline (NC) materials. For that reason, we may raise a question, i.e., how does the point defect sink efficiency of GBs undergone plastic deformations vary compared to initial states of them? In this study, we will attempt to answer it.

The sink efficiency of a GB is usually characterized by the defect-free zone (DFZ) width existing on both sides of GB (Adamson et al., 1980; Dollar and Gleiter, 1985; Han et al., 2012; Siegel et al., 1980; Singh et al., 1986). Experiments have revealed that DFZ width is generally dependent on not only the GB character such as misorientation angle and GB planes (Han et al., 2012), but also some other information pertaining to GB type such as low angle vs. high angle (Dollar and Gleiter, 1985; Siegel et al., 1980), Σ value (Han et al., 2012; Siegel et al., 1980) etc. For instance, Siegel et al. (1980) observed that the sink efficiency of both small and non-special large-angle GB was found to be high in polycrystalline Au. They also found that the sink efficiency of small angle GBs is somewhat smaller than the large-angle GBs.

The answer to the different sink efficiencies of GBs with different characters may be given through revealing the mechanisms of point defect-GB interactions (Kolluri and Demkowicz, 2010, 2012; Kolluri et al., 2013). Advances in experiments supply information related to the changes in macroscopic GB properties, but cannot enable us to understand the microscopic mechanisms regarding point defect-GB interactions (Tschopp et al., 2012). Thus, we may resort to atomistic simulations. Atomistic simulations incorporating a large number of GBs can shed light on how GB character affects the point defects-related properties of polycrystalline and monocrystalline materials and what mechanisms are in the point defect-GB interactions. For example, Samaras et al. (2002, 2003a, b) performed atomistic simulations in the nanocrystalline Ni and showed the GBs acting as sinks for self-interstitial atoms after collision cascade event. Millett et al. (2008, 2009) used atomistic simulations of the 2D columnar nanocrystalline Mo and studied the GB acts as a sink for point defects and a source for vacancies.

The aforementioned atomistic simulations incorporated a large number of GBs, in which some other factors such as the size of grains and triple junctions present us from ascertaining the mechanisms of point defects interacting with an individual GB. Therefore, bicrystalline simulations as an efficient approach can be employed to investigate the mechanisms of point defect interacting with an individual GB. For example, the collision cascade simulations in which GB structure evolvement and absorption of point defects after the initial primary knock-on atom event were analyzed have been often performed in the bicrystalline model (Bai et al., 2010; Demkowicz et al., 2011a; Perez-Perez and Smith, 2000, 2001; Zhang et al., 2012). In addition, there are also some studies on the point defect diffusion in GBs concerning the diffusivities and diffusion mechanisms of point defects (Kwok et al., 1981, 1983, 1984a,b; Nomura et al., 1991; Sorensen et al., 2000; Suzuki and Mishin, 2003a). Another commonly used method is to analyze how the point defect formation energies distributes at different atomic sites within GBs. With this method, vacancy and SIA formation energies are calculated at all potential sites within a given width of slab centered on the GB (Yu et al., 2016; Yu and Demkowicz, 2015). Although it doesn't involve the point defect diffusivities within GB using this method, general information of the interaction energies of point defects with GBs and the distributions of point defect formation energies within GB can be obtained (Bai et al., 2012; Suzuki and Mishin, 2003a, b; Tschopp et al., 2012; Yu and Demkowicz, 2015). We can see that, although enormous efforts had been invested into point defect sink efficiency of GBs, detailed information of such topic with regard to GBs undergone plastic deformation has not been achieved yet. This is important because the understanding of sink efficiency of plastically deformed GB may shed lights on how the plastic deformations of GBs influence the irradiation tolerance of materials.

In this study, we attempt to investigate the energetics of point defects interacting with plastically deformed GBs to reveal the point defect sink efficiencies of GBs undergone the plastic deformations. This study targets four copper symmetric tilt grain boundaries (STGBs) with tilt axis <110>, i.e., $\sum$9-(114), $\sum$9-(221), $\sum$11-(113) and $\sum$11-(332). These four GBs are selected in this study due to two main reasons. One is that GB misorientations such as $\sum$9 and $\sum$11are usually observed in the polycrystalline materials and GBs tend to have GB plane with smaller indexes (Randle, 1998). On the other hand, it will be shown that four GBs under shear on the GB plane exhibit three representative predominant plastic deformation behaviors connecting to the GBs in the polycrystalline materials during the plastic deformations (Barai and Weng, 2009; Berbenni et al., 2013; Cahn et al., 2006; Peron-Luhrs et al., 2014; Prieto-Depedro et al., 2015; Sansoz and Molinari, 2004, 2005; Taupin et al., 2014; Wan and Wang, 2009, 2010). In the following, we firstly perform the mechanical behavior simulations of four GBs by applying shear loadings in the four different directions at 0 K and 300 K. Then, some representative GB configurations undergone plastic deformations are selected for the further study of average energies of them and point defect formation