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Initiation, evolution, and saturation of coupled grain boundary motion in nanocrystalline materials

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ABSTRACT

Coupled grain boundary (GB) motion in sheared nanocrystalline materials composed of Ni, Al, or Cu is investigated by atomistic simulation methods, and the effects of grain size and temperature are evaluated. Due to the pinning effect of triple junctions, saturation of coupled GB motion is observed in all the nanocrystals except Cu. The two components of coupled GB motion, normal migration (NM) and tangential motion (TM), initiate and saturate at nearly equivalent nominal shear strains. Accompanied with coupled GB motion, massive dislocations and stacking faults are found to form within some grains, and the elementary structure units in the observed GBs transform from in-order to out-of-order. Compared with nanocrystalline Ni, the coupled GB motion in nanocrystalline Al has a reduced shear strain threshold and saturated NM displacement. The effects of grain size and temperature are similar in both NM and TM, so that their influence on coupled GB motion is slight.

1. Introduction

Grain size has a significant effect on the deformation behavior of nanocrystalline materials. In general, the deformation of a polycrystalline material is dominated by dislocations for grain sizes of hundreds of microns, but mediated by grain boundaries (GBs) for grain sizes of a few nanometers [1–3]. Accordingly, GBs play a key role in determining the mechanical properties and deformation behaviors of nanocrystalline materials, which are remarkably different from their coarse-grained counterparts.

An extraordinary deformation behavior involving grain growth has been observed in both experimental studies [4–6] and atomistic simulations [7,8]. Recently, numerous investigations have been conducted to reveal the mechanism of grain growth in nanocrystals [9–12], and some elaborate experiments were also employed for clarifying the role of shear stress as the driving force for mechanically induced GB migration and grain growth [13]. It was found that grain growth generally scales with the applied stress.

Moreover, GBs are mobile during deformation, rather than acting as stationary obstacles, so that deformation involving grain growth is always accompanied by GB motion. However, both experiments and theoretical predictions have presented an interesting complexity regarding GB motion [14,15]. In a bicrystal or nanocrystal, normal GB migration (NM) perpendicular to the GB plane is often coupled to tangential motion (TM) parallel to the GB plane. The coupling factor characterizing coupled GB motion is defined as the ratio of TM to NM. For a bicrystal, this ratio can be geometrically related to the GB misorientation angle according to a theoretical model [14]. However, the predictions of this model are slightly larger than experimental results when applied to a nanocrystalline material [16]. This is possibly because GB motion in a nanocrystal is easily affected by triple junctions and intragranular defects [17,18]. Triple junctions always act as obstacles to GB motion, while intragranular defects not only change the local stress distribution, but also interact with the GBs. In contrast to the sustained NM occurring in a bicrystal, NM in a nanocrystal becomes saturated due to the pinning effect of triple junctions and the impact from dislocations [17,18]. However, the saturation behavior of coupled GB motion in nanocrystals has not been carefully studied yet. A more comprehensive study is required to uncover the mechanisms underlying this phenomenon.

Grain growth is widespread in nanocrystals, but rare in coarse-grained materials [2]. This indicates that grain growth is a grain-size related process. Therefore, it can be safely assumed that GB motion also depends on the grain size. In addition, grain growth was found to dominate the plastic deformation of gradient nanograined Cu [19], but no grain growth was observed in gradient-structured interstitial free steel [20]. These conflicting results seemingly imply that the phenomenon of grain growth is multitudinous.

The present study focuses on coupled GB motion in metal nanocrystals. A series of face-centered-cubic (FCC) models respectively composed of nanocrystalline Ni, Al, and Cu with $\Sigma 9\langle 1\,1\,0\rangle$

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{2 2 1} symmetric tilt GBs are respectively constructed as the objects of observation. Their shear responses are evaluated by atomistic simulation methods, and the initiation, evolution, and saturation processes of coupled GB motion are subjected to careful analysis. Finally, the effects of grain size, material, and temperature are discussed.

2. Models and computational method

A series of quasi-three-dimensional FCC nanocrystalline models with idealized $[1\bar{1}0]$ texture were constructed. The nanocrystalline Ni, Cu, and Al models all have the same grain orientations, and have a horizontal $\Sigma9\langle1\,1\,0\rangle\{2\,2\,1\}$ symmetric tilt GB with a misorientation angle of 38.94° [21] and two component grains lying in the middle of the models. This GB was considered as the observation object. The remaining grains were oriented randomly. Among these models, the nanocrystalline Ni models were constructed with grain sizes of 10 nm, 20 nm, 30 nm, 40 nm, and 70 nm to evaluate the effect of grain size on the coupled GB motion. Their outline dimensions are 2 nm along the $\langle1\,1\,0\rangle$ texture direction, and vary respectively from 16.5 nm × 16.5 nm to 115.5 nm × 115.5 nm in the plane perpendicular to the texture direction when the grain sizes increase from 10 nm to 70 nm. The nanocrystalline Cu and Al models were constructed with grain sizes of 30 nm for comparison with the coupled GB motion of the nanocrystalline Ni model having an equivalent grain size. In addition, a bicrystal model with a $\Sigma9\langle1\,1\,0\rangle\{2\,2\,1\}$ symmetric tilt GB was also constructed as a reference for comparison.

Molecular dynamics (MD) simulations were performed using LAMMPS [22] with embedded atom method potentials for Ni [23], Al [23], and Cu [24]. Periodic boundary conditions were imposed in the X $[1\,1\,4]$ and Z $[\bar{1}\,1\,0]$ directions, while the boundaries were free in the Y $[2\,2\,\bar{1}]$ direction. Before application of a shear strain, the models were relaxed at 300 K for 100 ps to obtain equilibrium configurations. Subsequently, the models were slowly adjusted to the desired temperature and relaxed for another 100 ps. The simulation temperature employed was 10 K, unless otherwise stated. Two slabs that were 2 nm in thickness were fixed at the top and bottom of each model. The shear strain was applied by deforming the model as a whole in the X direction at a strain rate of $2 \times 10^8\ s^{-1}$. The canonical ensemble (NVT) with a constant number of atoms, volume, and temperature was employed to trace the atomic trajectories. The MD integration step was 1.0 fs.

The common neighbor analysis method was employed to identify the crystalline structures during the visualization [25]. Atoms were colored according to their profiles in the atomic configurations. In what follows, FCC atoms are marked blue, hexagonal close packed (HCP) atoms are marked light blue, and the remainder are marked red. Visualization of the atomistic simulation data was performed by the three-dimensional visualization software OVITO [26].

3. Characteristics of coupled GB motion in nanocrystalline Ni

The location coordinates of the middle point of the observed GB during deformation were captured, and the respective normal and tangential displacements d_n and d_t of the GB were obtained. The NM displacement versus nominal shear strain curve of the nanocrystalline Ni model with a grain size of 30 nm is plotted in Fig. 1. An examination of Fig. 1 indicates that the NM displacement curve can be obviously separated into three stages. During Stage I, the GB does not migrate until experiencing a nominal shear strain of about 1.00%, which is denoted as the threshold shear strain for NM. When the nominal shear strain exceeds this threshold value, the GB begins to migrate stably during Stage II, and the NM

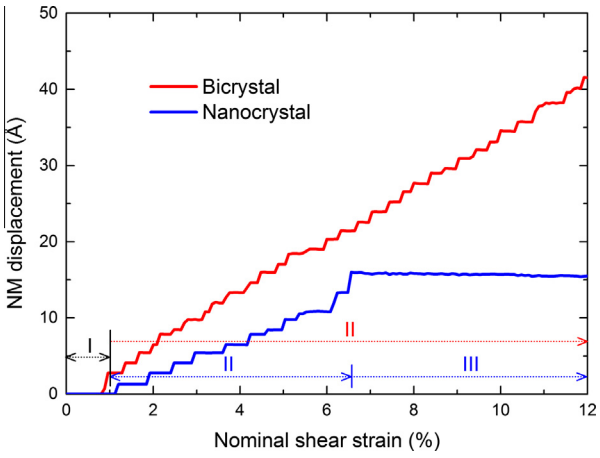

Fig. 1. NM displacement versus nominal shear strain curves of a Ni bicrystal and nanocrystal.

displacement curve exhibits a stepped character denoted as stick–slip [21], where the term "stick" corresponds to the shear strain applied to the nanocrystal, while the term "slip" is related to the resulting NM displacement. Moreover, most of the slip events represent very similar displacements. After the nominal shear strain reaches about 6.60%, the NM progresses into Stage III, where the GB motion is saturated. GB motion in a sheared bicrystal has been observed [14,21]. Therefore, the NM displacement versus nominal shear strain curve of a Ni bicrystal is also plotted in Fig. 1 for comparison. As shown in the figure, GB motion saturation is not observed in the case of a bicrystal, so that the curve exhibits only two stages. Stage I occurs until attaining a threshold shear strain of slightly less than 1.00%, after which the GB motion in Stage II corresponds to a stick–slip character similar to that observed in the nanocrystal.

To analyze the underlying mechanism of GB motion saturation in the nanocrystal, the nanocrystal configurations at nominal shear strains of 0%, 6.80%, and 12.00%, corresponding to the three stages, are shown in Fig. 2(a)–(c), respectively. The horizontal and vertical marker lines represent the geometrical symmetry centers, and are drawn to track the NM and TM displacements. The observed GB is initially located at the center of the nanocrystal model, and lies along the horizontal marker line, as shown in Fig. 2(a). With increasing nominal shear strain, the atoms in the model are progressively relocated so that both the horizontal and vertical marker lines are spatially altered. Fig. 2(b) shows that the observed GB is obviously separated from the horizontal marker line, but its two ends are pinned by triple junctions. Therefore, the GB becomes distorted as a result of shear deformation, indicating the occurrence of uneven NM. While the NM displacement increases with increasing shear deformation, it eventually reaches saturation because of the pinning effect of the triple junctions, as shown in Fig. 2(c). A slight unpinning effect of the triple junctions is observed owing to the dislocation activities near the triple junctions. This suggests that the triple junctions are relatively immobile compared to the GB [18]. However, slight unpinning does not significantly affect the distorted GB shape and the onset of NM saturation. Due to the restricted deformation between neighboring grains, massive dislocations and stacking faults are formed within some grains, which is in accordance with experimental evidence [27]. In addition, it is also observed in Fig. 2(b) that the vertical marker line inclines abruptly between the observed GB and the horizontal marker line. This shows that NM is accompanied by TM. The coupled GB motion can be further confirmed by the distribution of the von Mises local shear strain invariant shown in Fig. 2(d). In addition to the dislocation and stacking fault regions, the area over which the GB motion occurs exhibits a larger shear strain invariant.