Acta Materialia 131 (2017) 400–409

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Size and rate dependent grain boundary motion mediated by disconnection nucleation

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ARTICLE INFO

Article history:
Received 19 January 2017
Received in revised form
7 April 2017
Accepted 7 April 2017
Available online 8 April 2017

Keywords:
Grain boundary motion
Disconnection
Molecular dynamics simulations

ABSTRACT

The synthetic driving force method is a widely-used technique in molecular dynamics simulations to investigate the migration of grain boundaries. Its physical essence, however, has been under debate for quite some time for generating the driving force by artificially introducing some energy into the crystals. In this study, the elementary process governing the grain boundary motion under the driven motion method was explored by applying a varying synthetic driving force that increases from zero at a constant rate, which is in contrast to a constant driving force that is usually applied in past studies. With this method, it was found that a rate-controlling process, i.e., disconnection nucleation that has been reported before to dominate the physical grain boundary motion coupled to an applied shear, also operated for grain boundary motion caused by the synthetic driving force. Furthermore, the disconnection nucleation mediated process was also found to cause a strong size dependence and transitions of grain boundary motion modes at different temperatures. It is hoped that with this study, the synthetic driving force method in studying grain boundary motion can be used with more confidence in its physical essence and a universal mechanism can be proposed to explain grain boundary motion in materials despite how it is caused.

1. Introduction

Grain boundary (GB) motion is fundamental to the microstructural evolution in almost every class of polycrystalline materials during processing and service. A quantitative description of the kinetic process of GB motion under various thermal and loading conditions is thus desired, which has attracted dramatic attention in recent years by using both experimental [1–4] and computational approaches [5–7].

To date one the most well studied types of GB motion is that coupled to an applied shear [8–15]. For shear coupled GB motion, the vertical velocity of the GB is proportional to the applied horizontal shear velocity via a simple relation:

$$v_{\perp} = \beta v_{\parallel}, \tag{1}$$

where $v_{\perp}$ is the vertical velocity of the GB, $v_{\parallel}$ is the horizontal velocity due to the applied shear, and β is the shear coupling factor which is mainly related to the GB structure [8]. Past experimental, theoretical and computational studies on shear-coupled GB motion have shown excellent agreement with each other [8–10,13]. However, this method cannot be easily applied to extract the intrinsic mobility of individual GBs, which is normally defined by a simple relation between the GB velocity and the applied driving force:

$$v = MP, \tag{2}$$

where v is the GB velocity, P is the applied driving force, and M is the GB mobility [1]. For example, many GBs under shear coupling were found to move in a stick-slip or stop-and-go fashion from molecular dynamics (MD) simulations [8,16], and the GB velocity in this fashion does not scale linearly with the applied shear stress as described in Equation (2). Instead, the GB velocity strongly depends on how fast the external shear loading is applied and the shear coupling factor in those MD simulations. Nevertheless, shear coupled GB motion has been used as an important reference to validate other computational methods for extracting the intrinsic GB mobility.

One such method is the synthetic driving force method (SDFM)

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http://dx.doi.org/10.1016/j.actamat.2017.04.018
1359-6454/

that was first proposed by Janssens et al. [5] and further developed by many others [17–22], including the most recent one by Ulomek et al. [18] known as the energy conserving orientational (ECO) driving force method. Although the SDFM and its variants are effective in driving the GB motion at a constant velocity under a constant driving force, thus ideal for extracting the GB mobility as defined in Equation (2), the "physical" essence of the SDFM has been long debated. Therefore, many efforts [17,21,23–25] have been made trying to justify if the GB motion driven by the synthetic force is indeed physical. For example, Homer et al. [21] have studied shear coupling in GB motion by applying the SDFM and reported similar observations as predicted by applying a shear directly. Mendelev et al. [23] have proposed a benchmark study to compare the GB mobility extracted from various computational methods and essentially proved that the SDFM is physical for predicting the same GB mobility as from other well-known "physical" methods, e.g., the interface random walk [6] and the biaxial strain methods [7]. In a recent MD study by Coleman et al. [17], the GB motion driven by the SDFM and that by an external shear loading was also found to be dominated by the same fundamental mechanisms.

Some recent studies from both in-situ TEM analysis [2,9,26] and MD simulations [4,16,27–29] reveal that the elementary process in shear coupled GB motion is correlated to the nucleation and motion of disconnections. If the GB motion driven by the SDFM shares the same physical essence as the shear coupled GB motion, e.g., as proposed by Coleman et al. [17], it is natural to suspect if disconnections are also fundamental to the GB motion caused by a synthetic driving force. Disconnections are interfacial line defects in crystals with both dislocation and step nature [8,29–31]. As similar to dislocation nucleation in crystals, disconnection nucleation is also a thermally activated process, which suggests that GB motion driven by the SDFM could be strongly size- and rate-dependent. Due to the intrinsic limitations of atomistic simulations, MD studies on GB motion normally focus on relatively small GBs while applying periodic boundary conditions. However, the GB motion may strongly depend on the size of the simulation cell. For example, Race et al. [25] have revealed that the GB mobility has a strong and complex dependence on the system size by using the SDFM and proposed that a large enough system size, or the so-called "meso-scale", should be used for MD studies on the motion of flat GBs to ensure the physical kinetic process to be activated. The idea of "meso-scale" has later been employed by Hadian et al. [32] so that the key process, i.e., the nucleation of islands, can be observed during the migration of flat GBs by using the SDFM. Humberson and Holm [33] have also systematically investigated the dependence of the mobility of a Σ3 [111] {11 8 5} GB on its size in the plane of the GB and found that the larger the size of the GB plane, the higher the GB mobility. Nevertheless, the dependence of GB mobility on its vertical size in the direction perpendicular to the GB plane, or the grain size, has not been discussed before. On the other hand, no rate-dependency has been considered before; usually a constant driving force is directly applied to the GB when the SDFM is used [5,17,34]. Furthermore, since disconnection nucleation requires a threshold stress (or a critical stress) to be reached during the shear coupled GB motion, which is the cause for the widely observed "stick-and-slip" behavior at low temperatures [8,16], it suggests that a threshold driving force should also exist when using the SDFM below which no GB motion can be caused at low temperatures. This is partly supported by the findings by Olmsted et al. [35] that a sufficient driving force is needed to move a GB below the roughing temperature.

In order to explore the fundamental process of GB motion caused by the SDFM and further validate the physical essence of this method in extracting GB mobility, the following fundamental questions will be addressed in this study: (1) Is there a well-defined threshold driving force to initiate the GB motion? (2) Is disconnection nucleation and motion also the elementary process of GB motion under a synthetic driving force? (3) Is the GB motion under a synthetic driving force rate- and size-dependent? It is hoped that with this study, the SDFM can be used more appropriately and confidently in investigating GB motion in the future.

2. Methodology

As shown in Fig. 1(a), a bicrystal model containing two identical GBs was constructed. The symmetric tilt Σ5 (210) GB in Cu was used as the main model system in this study, which has been reported to show strong shear coupling under both an applied shear [8] and a synthetic driving force [21]. However, two other GBs, a coherent Σ3 (111) twin boundary and a twist (111) 38.21° GB with no shear coupling were also studied and discussed. The atomic configurations of the three types of GBs are shown in Fig. 1 (b)-(d). It is noted that the Σ5 (210) GB has a kite structure, while the coherent Σ3 (111) GB and the twist (111) 38.21° GBs have a single and two-atomic layer structure, respectively. The synthetic driving force was added in the two grains in such a way that the two identical GBs would move towards each other. Specifically, as shown in Fig. 1(a), an extra energy of $-\Delta E/2$ or $\Delta E/2$ was added to the atom belonging to Grain 1 or Grain 2 depending on their crystal orientation so that the overall energy of the whole crystal is not significantly changed. The atoms at the vicinity of the GB would have an extra energy close to 0 based on the original formalism developed by Janssens et al. [5]. More discussion regarding how the artificial energy should be added has been included in a later section. It has been pointed out by Olmsted et al. [35] that a correction may be applied to reflect the actual thermodynamic driving force on the GB. For the GBs and temperature range that have been studied in this work, it was found that P can be calculated as $P = \Delta E/\Omega$ with no need of correction, where Ω is the volume of a single atom. For Cu [36] with a lattice constant of $a = 0.364\ nm$, the conversion is $P = \Delta E \cdot \frac{13.3 GPa}{eV}$. In the following, ΔE will be sometimes referred to as the driving force (P) without further explanation.

All simulations were performed by using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [37] with an embedded atom method potential for Cu [36]. The time-step was 5 fs as similar to previous studies [19]. Periodic boundary conditions were applied along x-, y-, and z-directions if not otherwise specified. For the Σ5(210) GB, the lengths of the simulation cell along x- and y-directions were fixed at $L_x = 14.5$ nm and $L_y = 2.5$ nm respectively, while the length along z-direction varied from $L_z = 4.8–28.8$ nm. As defined in Fig. 1(a), d_z is used to represent the varying grain size of the bicrystal model. The size of the simulation cell with the Σ3(111) GB and the twist (111) GB was fixed at $L_x = 10.6$ nm, $L_y = 2.0$ nm, $L_z = 10.0$ nm and $L_x = 8.3$ nm, $L_y = 2.7$ nm, $L_z = 10.0$ nm, respectively. Before a synthetic driving force was applied, all models were relaxed at zero pressure and the target temperature for 25 ps under the isothermal–isobaric ensemble (NPT). Zero pressure under the same thermal ensemble (NPT) was also used for all simulations during the GB motion under an applied synthetic driving force, if not otherwise specified, to minimize the possible influence from shear stress. In order to investigate the possible rate dependence, the driving force in terms of ΔE was increased in a stepwise fashion from 0 eV as shown in the inset of Fig. 2. Accordingly, the incremental rate can be calculated as $\dot{E} = \frac{\delta E}{2\delta t}$ and the applied driving force at any specific time t can be calculated as $\Delta E = 2\dot{E}t$. The average displacement of the GB plane (ΔGB) was calculated by tracking the overall change of the added artificial energy in the whole system as similar to a previous study [20]. The visualization of the atomistic structures of all models was done