Computational Materials Science 154 (2018) 147–151

Contents lists available at ScienceDirect

Computational Materials Science

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

An atomic perspective on twin transmission in magnesium

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ARTICLE INFO

Keywords:
Twinning
Twin transmission
Magnesium
Molecular dynamics

ABSTRACT

Twin transmission in magnesium is studied from an atomic perspective by molecular dynamics simulations. It is found that twin transmission tends to occur at grain boundaries with low misorientation angles and the geometric compatibility factor is useful for explaining the twin variant selection. Furthermore, this work contributes to understanding the essence of twin transmission. A stress concentration near the grain boundary is observed when the incoming twin impinges on the boundary, inducing twin nucleation in the neighboring grain accomplished by a pure-shuffle mechanism.

1. Introduction

Twinning is a vital deformation mechanism for hexagonal close-packed (hcp) metals such as Mg alloys due to the insufficient number of active slip systems at room temperature in these metals [1]. In recent years, twin transmission, a specific type of twinning event, which influences strain hardening, the development of localized shear bands and the formation of a yield plateau [2–5], has been widely investigated in Mg alloys [6–13].

Twin transmission is characterized by the observation of twins joined at the same region of the shared boundary in two adjacent grains. It is surmised that a twin in either grain induces the nucleation of a twin in the neighboring one [10,14]. Several studies of Mg alloys have shown that twin transmission tends to occur at low angle grain boundaries (GBs), while twin propagation is always blocked by high angle GBs [6–10]. A geometric compatibility parameter, $m' = \cos\psi\cos\kappa$, where $\psi(\kappa)$ is the angle between two twinning plane normals (two shear directions) of twin systems in neighboring grains, has been used to analyze twin transmission events [5,10,15,16]. It has been shown that most twin pairs have high values of m' and the transmitted twin variant is frequently the one which has the highest m' value correlating with the previously formed twin [10,15,16].

Some of these investigations proposed that twin transmission is associated with stress concentration at GBs [5,9,15]. For example, Guo et al. inferred that the occurrence of a new twin is induced by the impingement of the first formed twin on the GB because such impingement generates high stress concentration, and can be relieved via activating twinning in the neighboring grain [15]. However, such assumptions still lack direct evidence. More recently, with a crystal plasticity fast Fourier transform-based model, M. Arul Kumar et al. calculated the stress field in a neighboring grain produced by an impinging twin at a GB and studied whether the stress field can explain how and why twin transmission occurs in hcp metals [12]. By an integrated crystal plasticity-phase field model, Liu et al. simulated the twin transmit event and indicated that there is a stress concentration near the GB when the incoming twin impinges on the boundary [17]. Nevertheless, the simulation scale is too large to demonstrate the essential atomistic mechanism of twin transmission.

Focusing on the essence of twin transmission, the twin nucleation mechanism should be taken into consideration. Previous studies have proposed several scenarios for the heterogeneous nucleation of twins, including the pole mechanism [18] and the slip dislocation dissociation mechanism [19,20]. Using atomistic simulations, Wang et al. suggested twin nucleation most likely occurs at GBs via a pure-shuffle mechanism [21,22]. Nevertheless, there are still some debate with regards to twin nucleation [23,24]. Much work is required to provide an insight into twin transmission event.

In this work, as symmetric tilt grain boundaries (STGBs) are the simplest in all types of GBs, we simulate the interactions between a twin and STGBs with different tilt angles by molecular dynamics (MD) simulations. Moreover, we concentrate on the analysis of stress distribution and atomic shuffles to clarify the essence of twin transmission.

2. Methods

A bicrystal model is constructed to determine the structures of STGBs with different tilt angles [25]. As shown in Fig. 1a, the GB plane coincides with the x-z plane. The z-axis is the tilt axis and lies along the $[1\bar{2}10]$ direction. Periodic boundary conditions are used in the x and z directions and there are two fixed regions at the top and bottom in the y

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https://doi.org/10.1016/j.commatsci.2018.07.046
Received 21 June 2018; Received in revised form 23 July 2018; Accepted 24 July 2018

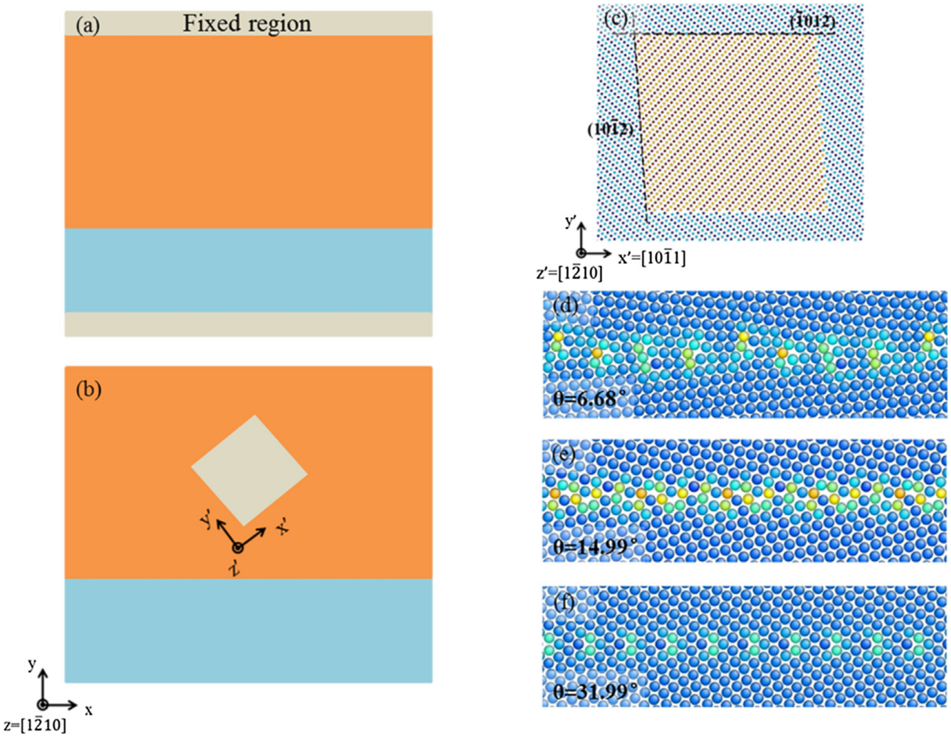

Fig. 1. The atomistic simulation cells. (a) Volume containing a STGB. (b) Simulation area containing a twin nucleus and a STGB. (c) Illustration of the twin nucleus. The x′-axis and z′-axis are parallel to the [101̄1] and [12̄10] direction respectively. The two conjugate twinning planes are labeled by two dashed lines. Different colors represent different planes parallel to basal planes. (d–f) Atomic structures of the representative STGBs. Atoms are colored according to their potential energies.

direction. The x dimension varies with the tilt angle θ (the corresponding misorientation angle of GB is 2θ) to satisfy the periodic boundary conditions, but is not less than 45 nm. The height of the bicrystal in the y direction is 45 nm and the thickness of the fixed regions along y is 1.5 nm. The z dimension is 1.6 nm, which is five times the lattice constant. The model is relaxed by MD using an embedded atom method (EAM) for Mg [26], which has been proven to be able to reproduce a set of experimentally measured properties accurately and has been widely used in previous studies. A twin nucleus is then inserted in the upper grain of the relaxed bicrystal model illustrated in Fig. 1b. The twin nucleus is bordered by (1̄012) and (101̄2) twinning planes by imitating the method proposed by Xu et al. [27] shown in Fig. 1c. Periodic boundary conditions are applied in the x and z directions and the grains are terminated at free surfaces in the y direction. Note that as the twinned region is not stable, it will shrink and disappear during the energy minimization. Therefore, a proper value of shear strain ($\gamma_{x'y'}$) parallel to the (1̄012) planes in the [101̄1] direction is applied in advance to stabilize the nucleus [27]. The interactions between the twin and the STGBs with different tilt angles are investigated and three representative cases are presented. The structures of the typical STGBs with tilt angles 6.68°, 14.99° and 31.99° (corresponding to the (1̄013) twinning boundary), whose formation energies are close to those in the reference [25], are illustrated in Fig. 1d–f. The simulations are performed by LAMMPS [28] and the atomic configurations are visualized using AtomEye [29].

3. Results

To simulate the twin-GB interactions, an increasing shear strain ($\varepsilon_{x'y'}$) parallel to the (1̄012) twinning planes along the [101̄1] direction was applied to the volume at a constant temperature close to 0 K. This low temperature was chosen to avoid perturbations caused by other thermally activated processes. The interactions between the twin and the STGB with a tilt angle of 6.68° are shown in Fig. 2. In the initial stage, as illustrated in Fig. 2a, the twinning nucleus is bordered by conjugate {1̄012} twinning planes and prismatic/basal (PB) interfaces [27]. As the deformation increases, the twin grows and impinges on the GB (Fig. 2b). Subsequently, a (1̄012) twin embryo nucleates near the interaction site in the bottom grain and expands further shown in Fig. 2c–d. That is, twin transmission occurs at the low angle GB. Fig. 2e–f show the structure of the new twin. It is clear that the twin is surrounded by (1̄012) coherent twinning boundaries (CTBs), PBs and a boundary associated with the original STGB.

In contrast to the case of low angle STGB, twin transmission does not occur at the STGBs with higher misorientation angles shown in Fig. 3. When the tilt angle of STGB is 14.99°, as illustrated in Fig. 3a–c, twin propagation is blocked by the GB and several basal dislocations are produced via the twin-GB interactions. Fig. 3d–f show the interactions of the twin with the CTB ($\theta = 31.99°$). The CTB still acts as a barrier to twin propagation and the twinned region just extends along it.

4. Discussion

As shown above, twin transmission occurs at the low angle GB, while the high angle GBs act as barriers to twin propagation. These results agree with previous studies [6–10]. To provide an insight into the twin transmission, further analyses of this GB twinning event are shown in Fig. 4. The stress ($\tau_{x'y'}$) distribution near the GB with a tilt angle of 6.68° before and after twin transmission is illustrated in Fig. 4a. A high stress concentration (in red color) is observed near the GB when the twin impinges on the boundary and is relieved via the nucleation and growth of twin in the neighboring grain. Since the tilt angle of the GB is quite low, the nucleated (1̄012) twin in the bottom grain and the original (1̄012) twin in the upper grain have close orientations, which is favorable for local strain accommodation. As mentioned earlier, a geometric compatibility factor m' can be employed to assess the efficiency of strain accommodation between two twins [10,15]. The nucleated (1̄012) [101̄1] twin has the highest m' of 0.947 among the six potential twin variants in the bottom grain with the incoming (1̄012) twin shown in Fig. 4b. Therefore, it can efficiently accommodate the