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The role of twinning deformation on the hardening response of polycrystalline magnesium from discrete dislocation dynamics simulations

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Abstract—The deformation of micro-twinned polycrystalline magnesium (Mg) was studied using three-dimensional discrete dislocation dynamics (DDD). A systematic interaction model between dislocations and $\{10\bar{1}2\}$ tension twin boundaries (TBs) was proposed and introduced into the DDD framework. In addition, a nominal grain boundary (GB) model based on experimental results was also introduced to mimic the GB's barrier effect. The current simulations show that tension TBs act as strong obstacles to gliding dislocations, and contribute significantly to the overall hardening response, while twin growth results in a softening effect. Therefore, the Mg concave stress–strain curve can be explained in terms of the competition between TB induced hardening and twin growth induced softening. At low strain levels, twin growth induced softening dominates and a decreasing hardening rate is observed in Stage-I. In Stage-II, the TB induced hardening dominates, which leads to an increasing hardening rate.

Keywords: Discrete dislocation dynamics; Dislocations; Twinning; Magnesium; Hardening

1. Introduction

With the increasing demand to reduce carbon dioxide emission, many efforts are directed toward reducing the structural weight of fossil fuel powered vehicles to increase their fuel efficiency. As the lightest structural metal (one-third lighter than aluminum), magnesium (Mg) and its alloys have been attracting a lot of attention in recent years for their potential use in automotive, aerospace and defense applications [1]. However, at present, the wide use of Mg alloys as a structural material is still challenging due to their poor room temperature formability. Owing to its hexagonal closed packed (hcp) lattice structure and low crystal symmetry, Mg cannot maintain sufficient independent slip modes to accommodate arbitrary deformation in polycrystalline materials at room temperature. Consequently, in addition to dislocations, twinning plays an important role in their plastic deformation. Therefore, it is vital to grasp a full understanding of the combined effects of dislocations, twinning, and their mutual interactions to address their role on the overall mechanical behavior of hcp materials [2].

Due to deformation twinning, the deformation of Mg and its alloys displays characteristics that are different than those commonly observed in face centered cubic (fcc) and body centered cubic (bcc) crystals. One common characteristic is that the true stress–strain curves of both single crystals [3,4] and polycrystalline [4,5] Mg display a concave shape. In addition, the stress–strain curve can be characterized by three distinct stages. In Stage-I a decreasing hardening rate is observed, followed by Stage-II with an increasing hardening rate, and finally a decreasing hardening rate in Stage-III [4,5]. Stage-I is generally associated with twinning-mediated plasticity in the form of twin nucleation and growth, leading to a decreasing hardening rate [6–8]. On the other hand, the progressive decrease in the work hardening rate in Stage-III is a result of post-saturation in the twin volume fraction leading to predominant dislocation-mediated plasticity [6,9]. In Stage-II, both dislocation slip and twinning are active and interact; however, the underlying mechanisms associated with the increasing hardening rate are still debated.

Jiang et al. [6] examined the microstructure evolution during AZ31 deformation, and observed that in Stage-II intersections between primary and secondary $\{10\bar{1}2\}$ tension twins result in significant grain refinement and subsequently an increasing hardening rate. On the contrary, Wang et al. [10] reported that the barrier effect of tension twin boundaries (TBs) weakens as twins coalesce during Stage-II, which undermines the suggested contribution from grain refinement. In addition, they suggested that the increasing hardening rate can be attributed to texture induced hardening. This is a result of the tension twin hard

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orientation, since its c-axis is nearly parallel to the loading axis. Knezevic et al. [7] showed that tension twins consume the entire grain before the end of Stage-II, and all the aforementioned twinning mechanisms cannot explain the peak strain hardening rate at the end of Stage-II. Instead, they suggested that this peak strain hardening rate may be attributed to the nucleation of compression twins in the tension twinned grains. Barnett et al. [5] observed the formation of low angle boundaries arising from the glissile-to-sessile transition of dislocations induced by twinning shear [11,12], which can also act as a source of hardening. Finally, de-twinning as a result of strong interactions between dislocations and twins was also suggested to contribute to the observed increasing strain hardening rate in Stage-II [13]. These conflicting proposed mechanisms indicate that there is no clear consonance yet regarding the mechanisms responsible for the increasing strain hardening rate in Stage-II.

In the past two decades, several computational methods have been developed to characterize dislocation-mediated plasticity. Of those, discrete dislocation dynamics (DDD) is one of the most efficient methods to capture dislocation-mediated plasticity at the micro scale. To date, several two-dimensional [14,15] and three-dimensional [16–19] DDD methods were proposed and used widely to study crystal size effects (e.g. [20–22]), grain size effects (e.g. [23–25]) and intermittency behavior (e.g. [26]). While most previous DDD studies have focused on fcc and bcc crystals, more recently several studies have been performed on hcp crystals. In particular DDD simulations of hcp materials have focused on dislocation junction formation and strength [27,28], orientation influence on the grain size effects [25], micro/nano-pillar plasticity [29,30], elastic anisotropy [31], and the role of plastic anisotropy on microcracking [32]. It should be noted that in these studies deformation twinning was not considered. Nevertheless, twinning plays an important and sometimes dominant role in the mechanical behavior of both single crystalline and polycrystalline Mg. As a result, DDD simulations not accounting for twinning may lead to inaccurate predictions of the mechanical behavior of hcp materials. This also indicates the importance and urgency of developing a dislocation–TB interaction model within the framework of DDD to account for deformation twinning.

As aforementioned, the deformation of Mg and its alloys is of great interest due to their numerous potential applications in industry. However, the mechanisms associated with their hardening response, mainly in Stage-II, are not well characterized. In order to address this, we propose a systematic interaction model between dislocations and $\{10\bar{1}2\}$ TBs, and integrate this model into 3D-DDD simulations. A simple grain boundary (GB) model, which agrees with experimental results, is also implemented. Using this complex DDD framework, the deformation of micro-twinned polycrystalline Mg is investigated. Specifically these simulations identify the influences of grain orientation, GBs, TBs and twin volume fraction on the deformation of Mg polycrystals.

2. Computational methods

In the following simulations, a cubic simulation cell is employed to model a representative grain in a bulk material, as shown schematically in Fig. 1(a), where periodic boundary conditions (PBCs) are imposed along all three directions. A twin lamella having a thickness l_t is introduced at the center of the grain with size l_g. Thus, the twin volume fraction is given by $f_t = l_t/l_g$. Here, only $\{10\bar{1}2\}$ tension twins are considered, as shown by the relative orientations of the grain and twin in Fig. 1(a). It has been shown experimentally that the number of twins per grain is proportional to the square of grain size, and the probability of having more than one twin per grain decreases considerably for grains having diameters less than 40 μm [33]. Thus, given the grain sizes modeled here, the current proposed simulation cell can be considered as a representative twinned grain in a bulk Mg polycrystal with grain size below 40 μm.

In Mg polycrystals, strain hardening can be attributed to three microstructural features: dislocations, GBs and TBs. In order to investigate their individual contributions, three additional simplified cubic simulation cells are considered, as shown in Fig. 1. In one case, only dislocations are accounted for in a single crystal cubic simulation cell with PBCs along all three directions. In another case, the contribution of GBs is accounted for in a polycrystal simulation cell in the absence of TBs. In this case, the six surfaces of the simulation cell are considered as representative GBs with PBCs along all three directions. Finally, the effect of TBs is accounted for in a twinned crystal simulation cell in the absence of GBs. Here, a twin lamella is inserted in the middle of the simulation cell and PBCs are employed along all three directions. It should be noted that these simulation cells are idealized, since twinning is typically observed experimentally in bulk single crystals and polycrystals. Nevertheless, these simulations can provide new insights into the individual contributions of dislocations, GBs and TBs on the hardening response of Mg.

In metals, screw dislocation cross-slip is an important mechanism for strain hardening [34] and creep behavior [35]. Therefore, a general cross-slip mechanism is utilized in the current simulations. Cross-slip of a screw dislocation is possible when more than one slip system share the same Burgers vector [36]. In particular $\langle a \rangle$ dislocations can cross-slip between basal, prismatic and pyramidal I planes, $\langle c \rangle$ dislocations between prismatic slip planes, and $\langle c + a \rangle$ dislocations between prismatic, pyramidal I and pyramidal II planes. Further details about the cross-slip mechanism used here can be found elsewhere [36].

In fully tension-twinned grains, compressive loading parallel to the c-axis, or tensile loading perpendicular to the c-axis, would promote compression twinning [7]. These compression twins appear always in a thin band shape with low volume fraction [7]. To model this effect, in a small number of simulations we also introduce a nominal compressive twin with a volume fraction of 0.05 in the center of the fully twinned grain. These compression TBs are assumed to be impenetrable to dislocations.

All current simulations were conducted using the 3D-DDD simulation code, ParaDiS [16]. All possible dislocation Burgers vectors and slip planes in hcp crystals, which are listed in Table 1, were accounted for in these simulations. It should be noted that according to the hcp lattice structure, slip of $\langle a \rangle$ dislocations and dislocations with Burgers vector $\boldsymbol{b}_t$ (i.e. twinning dislocations) on the $\{10\bar{1}2\}$ twinning planes are also possible. Thus, these dislocations are accounted for in the current simulations as well. The experimentally measured Peierls stresses for dislocations on the basal (0.52 MPa [37]), prismatic