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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 mechanical response of micro-twinned polycrystalline magnesium was studied through 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 agreeing with experimental results was also introduced to mimic the GB's barrier effect. The current simulation results show that TBs act as a strong obstacle to gliding dislocations, which contributes significantly to the hardening behavior of magnesium. On the other hand, the deformation accommodated by twinning plays a softening role. Therefore, the concave shape of the Mg stress-strain curve results from the competition between dislocation-TB induced hardening and twinning deformation induced softening. At low strain levels, twinning deformation induced softening dominates and a decreasing hardening rate is observed in Stage-I. In Stage-II, both the hardening and softening effects decline, but twinning deformation induced softening declines faster, which leads to an increasing hardening rate.

***Keywords**:* discrete dislocation dynamics; dislocation-twin boundary interaction; magnesium; hardening response

1. Introduction

With increasing demand to reduce carbon dioxide emission, many efforts are directed towards reducing the structural weight of fossil fuel powered vehicles in order to increase their fuel efficiency. As the lightest structural metal (one-third lighter than aluminum), magnesium (Mg) and its alloys has been attracting a lot of attentions in recent years for their potential utilizations in automotive, aerospace and defense applications [1]. However, at present, the wide utilization of Mg alloys as a structural material is still challenging due to their poor room temperature formability. Owing to its hexagonal closed packed (HCP) 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 dislocation-mediated plasticity, twinning plays an important role in its 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 roles in the overall mechanical behavior of HCP materials [2].

Due to the presence of deformation twinning, the overall mechanical response of Mg displays characteristics 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 curve of Mg displays a concave shape for both single crystals [3, 4] and polycrystals [4, 5], which is attributed to deformation twinning (i.e. tension twins). 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 twin nucleation and growth (mostly twinning-mediated plasticity), which accommodates most of the plastic deformation in this stage 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 (mostly dislocation-mediated plasticity) [6, 9]. In Stage-II, both dislocation slip and twinning are active and interact with each

other. However, the underlying mechanisms responsible for the increasing hardening rate are still debatable. Jiang et al. [6] examined the microstructure evolution during AZ31 deformation, and observed that in Stage-II intersections between primary and secondary $(10\bar{1}2)$ twins result in significant grain refinement and increasing hardening rate. These results are also in agreement with more recent observations [10]. On the contrary, Wang et al. [11] reported that during Stag-II the twin boundary (TB) barrier effect weakens as twins coalesce, which undermines the suggested effect of grain refinement. In addition, they suggested that the increasing hardening rate can be attributed to texture strengthening, since the twin is in a hard orientation with the *c*-axis nearly parallel to the loading axis. Furthermore, the work of Knezevic et al. [7] showed that twins consume the entire grains 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 the nucleation of compression twins in the tension-twinned grains attributes to the peak hardening rate reached at the end of Stage-II. Moreover, Barnett et al. [5] observed the formation of low angle boundaries arising from the glissile-to-sessile transition of dislocations induced by twinning shear [12, 13], which act as a source of strengthening. 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 [14]. All these results indicate that there is yet no clear consonance on the mechanisms responsible for the increasing strain hardening rate in Stage-II.

In the past two decades, several computational methods have been developed to understand the dislocation-related plastic behavior. Therein, discrete dislocation dynamics (DDD) is believed to be one of the most efficient methods to capture dislocation-mediated plasticity at the micro scale. To date, several two-dimensional [15, 16] and three-dimensional [17-20] DDD frameworks were proposed and used widely to study crystal size effects [21], grain size effects [22-24] and intermittent behavior [25]. In fact, previous DDD simulations mainly focused on the FCC and BCC materials, and recently more and more works on HCP materials, especially magnesium, are reported, in which the following important items were investigated:

dislocation junction formation and strength [26, 27], orientation influence on the grain size effects [24], micro/nano-pillar plasticity [28, 29], elastic anisotropy [30] and Peierls stress [31]. It can be seen that all previous DDD studies on HCP crystals are related to the single crystalline and polycrystalline samples, in which twinning deformation was not considered. Nevertheless, twinning plays an important and sometimes dominant role in the mechanical behavior of both single crystals and polycrystals. As a result, previous DDD simulations without twinning may lead to inaccurate predication of the mechanical behavior of HCP materials. This also indicates the importance and urgency of introducing dislocation-TB interaction model into DDD framework to study the deformation twinning.

As is aforementioned, the mechanical behavior of magnesium and its alloys is of great interest due to their numerous 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 it into the 3D-DDD code, ParaDiS [17]. A simple grain boundary (GB) model, which agrees with experimental results, is also implemented. Using this complex DDD framework, the mechanical behavior of micro-twinned polycrystalline magnesium is investigated. Specifically these simulations identify the influences of grain orientation, GBs, TBs and twin volume fraction on the overall response of Mg.

2. Computational Method

In this paper, a cubical simulation cell with periodic boundary conditions (PBCs) imposed along all three directions is employed, as shown in Fig. 1. All six surfaces of the cell are considered as representative GBs. A twin lamella having a thickness l_t is introduced at the center of the grain with size l_g as shown in Fig. 1. Thus, the twin volume fraction is given by $f_t = l_t / l_g$. In this work, only $(10\bar{1}2)$ tension twins are considered, as shown by the orientations of the grain and twin in Fig. 1. This simulation cell is actually a representative twinned grain in a bulk twinned

polycrystalline sample.

In metals, especially in Mg, there are at least three general sources of strain hardening: dislocations, GBs and TBs. In order to investigate their individual contributions, three simplified simulation cells are employed in addition to the twinned polycrystals in Fig. 1, namely single crystals (i.e. only dislocations), polycrystals (i.e. dislocations + GBs) and twinned crystals (i.e. dislocations + TBs), as shown in the insets of Fig. 3. Single crystal is a sample without any GBs and TBs, in which only dislocations operate. The 6 surfaces of the polycrystal are set to be GBs, in which TBs are still absent. This is a sample of both dislocations and GBs. In the twinned crystal, only TBs are presented to study the contribution of both dislocations and TBs. It should be noted that these simulation cells are simplified since twinning is typically observed in experimental bulk single and polycrystals. Nevertheless, these simulations provide new insights into the individual contributions of dislocations, GBs and TBs on the hardening behavior of Mg. In addition, the dislocation mechanisms and deformation modes for different loading orientations in each sample can be comparatively studied. Note the 3 simplified simulation cells (single, poly and twinned crystals) are used in Subsection 3.1, and twinned polycrystal is used in Subsection 3.2, which is identical to the experimental samples.

All current simulations were conducted using the 3D-DDD simulation code, ParaDis [17]. All the possible dislocations and slip planes of 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 both $\langle a \rangle$ dislocations and $\boldsymbol{b}_t$ twinning dislocations on $(10\bar{1}2)$ twinning planes are possible slip systems. Thus, these dislocations are also accounted for in the current simulations. The experimentally measured Peierls stresses for dislocations on the basal (0.52 MPa [32]), prismatic (39.2 MPa [33]), and pyramidal planes (105 MPa [34]) were introduced into the code. These values are also in good agreement with recent molecular dynamics (MD) predictions [35-37]. Basic Mg parameters used in the current simulations include: shear modulus, G = 17 GPa; Poission ratio, ν = 0.29; magnitude of <*a*> dislocation Burgers vector, b = 0.325 *nm*; axial ratio, *c/a* = 1.6236; and mass density, ρ = 1738

kg/m^3.

Most DDD simulations typically adopted a linear dislocation mobility law. However, recent MD simulations of the dislocation mobility in magnesium [36] suggest that at low stress levels the dislocation velocity increases linearly with the applied stress. At higher stresses the velocity also increases linearly but with a much smaller slope. Thus, in the current simulations a bi-linear law for the dislocation mobility that is fitted to these MD results is employed. The drag coefficients and transition velocities for the stress-velocity curve are listed in Table A1, in appendix A. To avoid any divergence in the iterative algorithm, a spline curve was used near the transition velocity to smoothen the bi-linear curve. The upper limit to the dislocation velocity was set as the shear wave velocity, $\sqrt{G/\rho}$. Furthermore, as a first approximation, the dislocation mobility and Peierls stress on the twinning plane were set to equal those for pyramidal plane, since their precise values have not been reported in literature yet.

Uniaxial strain-controlled loading (compressive or tensile) with a constant strain rate of $\dot{\varepsilon} = 5000/\mathrm{s}$ was imposed in the current simulations. Due to the configuration symmetry along the x and z axes with respect to the twin lamella, the loading axis is limited within the yz plane. As a result, four representative loading directions denoted by y, z, yz, and $y\bar{z}$, are considered. Loadings along the y and z directions are realized by imposing a strain rate $\dot{\varepsilon}_y = \dot{\varepsilon}$ and $\dot{\varepsilon}_z = \dot{\varepsilon}$, in the y and z directions, respectively. The yz loading is a uniaxial loading that is 45º from either the y or z axis, and is achieved by imposing a strain rate tensor:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\varepsilon}\begin{bmatrix} -\nu & 0 & 0 \\ 0 & (1-\nu)/2 & (1+\nu)/2 \\ 0 & (1+\nu)/2 & (1-\nu)/2 \end{bmatrix} \tag{1}$$

Similarly, the $y\bar{z}$ loading is 45º from the y axis and 135º from the z axis, and is achieved by imposing the following strain rate tensor:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\varepsilon}\begin{bmatrix} -\nu & 0 & 0 \\ 0 & (1-\nu)/2 & -(1+\nu)/2 \\ 0 & -(1+\nu)/2 & (1-\nu)/2 \end{bmatrix} \tag{2}$$

Initially, Frank-Read (FR) dislocation sources were randomly distributed within

the simulation cell. The initial dislocation source density in all simulations was chosen as ρ_{src} = 5×10^{12} m^{-2}, and the FR source length was l_{src} = 0.26 μm. While dislocation slip on various slip planes is possible in HCP crystals as listed in Table 1, $\langle a \rangle$ dislocations on basal, prismatic and pyramidal I planes as well as $\langle c+a \rangle$ dislocations on pyramidal II planes play a predominant role in dislocation mediated plasticity in Mg [38, 39]. Therefore, in the current simulations all dislocation sources were initially assigned on these specific four slip planes, which also agree with previous studies [24, 40, 41]. To account for possible statistical variations due to the random distribution of dislocation sources, each simulation was repeated three times with different initial distributions.

2.1 Dislocation-twin boundary interaction model

Twinning and dislocation-mediated slip both play important roles in the deformation of Mg and its alloys. Thus, it is crucial to account for the contribution of dislocation interactions with TBs. To accurately model these interactions in DDD we first derive a set of physically based rules for these interactions from experimental observations and/or MD simulations. Price [42] first studied these interactions in Zinc and showed that an $<a_1>$ dislocation, which intersects the TB in a screw character, can transmit through the TB without any remnants on the TB. On the other hand, $<a_2>$ and $<a_3>$ dislocations in the matrix can only be transmitted mutually through the TB by forming a $<c>$ dislocation in the twinned crystal, while leaving two twinning dislocations on the TB. Yoo and Wei [43] subsequently developed a set of dislocation-TB interaction scenarios for $<a>$ and $<c+a>$ dislocations based on geometric considerations of the HCP crystal structure. Electron microscope observations have shown good agreement with the Yoo and Wei model [43-46]. Furthermore, Yoo [47] performed a detailed analysis and proposed twenty six distinct types of interactions between three dislocation families and four most familiar twin boundaries in HCP crystals. In addition to these experimental observations, recently, MD simulations showed that the dislocation-TB interactions are also dependent on the applied loading. Under different applied stress directions, $<a_1>$ dislocations on the basal plane in the matrix can be transmitted to the basal plane in the twin, the

prismatic plane in the twin, or the prismatic plane in the matrix [48, 49]. In addition, no residual dislocation is left on the TB, which agrees well with the experimental observations. However, $<a_2>$ and $<a_3>$ dislocations form some steps on TB after absorbed [50, 51]. The subsequent motion of these steps along the TB leads to TB migration, which supports the twin growth mechanism by twinning dislocations [50].

Accordingly, in the current study the systematic interaction scenarios of Yoo [47] between different dislocations (i.e. $\langle a \rangle$, $\langle c \rangle$ and $\langle c+a \rangle$) and the $(10\bar{1}2)$ TB were introduced into the DDD framework. It should be noted that in Yoo's model some peculiar dislocation reactions were proposed. In particular, $\langle c+a \rangle$ and $\langle c \rangle$ incident dislocations were proposed to be transmitted as $[5\bar{7}2\bar{3}]/6$ and $[\bar{1}100]$, respectively. These high lattice index dislocations would not be stable because of their high Peierls stresses and core energies, and should dissociate into more common dislocations having Burgers vectors with low lattice indexes. Our MD simulations show that a $[\bar{1}100]$ dislocation dissociates into two $<a>$ dislocations ($[\bar{1}100] \rightarrow [\bar{1}2\bar{1}0]/3 + [\bar{2}110]/3 = < a_2 > - < a_1 >$). Furthermore, through simple geometric calculations it can be shown that $[5\bar{7}2\bar{3}]/6$ can be decomposed into 1.5 $<a>$ and 0.5 $<c+a>$ dislocations (i.e. $[5\bar{7}2\bar{3}]/6 \rightarrow [1\bar{2}10]/2 + [2\bar{1}\bar{1}\bar{3}]/6 = 1.5 < a > + 0.5 < c + a >$). Thus, in the current simulations, these transmitted dislocations with low lattice index are defined instead.

In the current simulations, three rules are specified to identify the reaction outcome of a dislocation-TB interaction, in terms of twinning dislocations on the TB as well as Burgers vectors and slip planes of the transmitted dislocations in the twin. In general, the dislocation transmission reaction across a TB can be expressed as follows

$$\boldsymbol{b}_i \rightarrow \sum_{j=1}^{n} \boldsymbol{b}_{rj} + k\boldsymbol{b}_t \tag{3}$$

where $\boldsymbol{b}_i$ is the incident dislocation in the matrix, $\boldsymbol{b}_{rj}$ is the *j*th resulting dislocation in the twin, and $\boldsymbol{b}_t$ is the twinning dislocation on the TB. In particular, these rules are based on (a) geometric constraints, (b) maximum power dissipation, and (c) energy minimization. The geometric constraints guarantee that the number of

twinning dislocations is smallest. This geometric rule is used to predict the resulting dislocations and twinning dislocations, similar to that proposed by Yoo [47]. According to this rule, the general dislocation decomposition is listed in Table A2 in Appendix A, in which all the possible incident dislocations from any slip planes, as listed in Table 1, are considered. All the resulting dislocations and slip planes have low lattice index. The resulting slip planes were chosen to be tilt planes with respect to the incident plane. Thus, if a tilt plan does not exist the dislocation is not allowed to penetrate (i.e. twisted boundaries are impenetrable). This geometric rule is analogous to that proposed for dislocation-GB interaction from previous DDD simulations of FCC polycrystals [15, 22, 25].

While for most incident dislocations this geometric rule is sufficient to identify the transmitted dislocation plane, this is not the case for incident $<a_1>$ dislocations, which intersect the TB in a screw configuration. Here, six potential tilt planes in the twin exist. Serra et.al [48] showed based on MD simulations that depending on the characteristics of the applied load a matrix $<a_1>$ dislocation on a basal plane can be transmitted to the twin basal plane, twin prismatic plane or reflected back into the matrix on a prismatic plane. Generally, the slip plane with the largest resolved shear stress was usually selected as the resulting slip plane. Since in HCP crystals the Peierls stresses and mobility laws are strongly dependent on the slip system under confederation, thus, to account for all these factors, the most favorable plane is chosen to be the one that would result in the largest power dissipation [17]:

$$P = \sum \boldsymbol{F}_j \boldsymbol{V}_j \tag{4}$$

where $\boldsymbol{F}_j$ and $\boldsymbol{V}_j$ are the stress and velocity of the jth transmitted dislocation.

Finally, to account for the barrier strength of the TB, dislocation transmission is performed only if the energy associated with the incident dislocation is larger than or equal to the energy associated with the transmitted dislocations and twinning dislocations. Thus, the critical resolved shear stress τ_c acting on the incident dislocation should obey the following energy minimization equation

$$\tau_c {b_i}^2 + \alpha_i G_i {b_i}^2 \geq \sum_{j=1}^{n} \alpha_{rj} G_{rj} {b_{rj}}^2 + k\alpha_t G_t {b_t}^2 + k\gamma_{\mathrm{TB}} b_t, \qquad (5)$$

where $\gamma_{\mathrm{TB}} = 113\mathrm{mJ/m^2}$ is the TB energy [52], α and G are the corresponding self-energy parameter of dislocations and shear modulus associated with the slip planes [53].

2.2 Dislocation-grain boundary interaction model

Using the representative grain model with PBCs in all three directions, as shown in Fig. 1, the orientation of each grain in the bulk materials is identical, which corresponds to a strong basal texture in polycrystalline Mg. However, the misorientation between the *a*-axes in neighboring grains is not accounted for here. Nevertheless, in the current simulations, the GB is introduced as an artificial interface/barrier to dislocation motion. Dislocations trapped at the GB can be transmitted into neighboring grains if the shear stress on the dislocation exceeds the GB strength. This approximation was successfully adopted by DDD simulations of polycrystalline materials [24, 54]. The GB transmission strength is largely governed by the misorientation angle, θ_{mis}, which can be approximated as $\tau_{GB} = 2Gsin^2(0.5\theta_{mis})$ [15, 22, 25]. The effect of the misorientation angle on the stress-strain response from our DDD simulations in the absent of twinning is shown in Fig. 2. In these simulations the grain size was l_g = 0.81 μm, and a compressive loading along the *y*-axis was imposed, which produces a predominant basal slip deformation. An experimental stress-strain curve of a 0.8 μm grained Mg alloy under a similar loading condition [55] is also shown. It is clear by comparing the DDD simulations with this experimental result that a misorientation angle of $\theta_{mis} = 15°$ (i.e. GB strength $\tau_{GB} =$ 580 MPa) agrees well with this experimental result, and thus in all subsequent simulations this misorientation angle is chosen.

3. Results and Discussions

3.1 Hardening behavior of single crystals, polycrystals and twinned crystals

In this subsection, three simplified simulation cells are employed to study the

individual contributions of dislocations, GBs and TBs on the hardening behavior of Mg, which are single crystals, polycrystals and twinned crystals as shown in the insets of Fig. 3. All the simulation cells have an edge-length l_g = 1.3 μm. Figure 3 also shows the stress-strain responses under different loading orientations from the three simulation cells. Figure 4 shows the contours of the effective plastic strain at the end of those simulations. From these contours the slip traces are clearly identified. It is clear that the single crystal responses (black curves in Fig. 3) for loadings along both the y and z axes are identical. These two loading directions make angles 46.85° and 43.15° with respect to the basal plane, respectively, leading to predominant basal slip since the Schmid factor is maximum on these planes, as shown in Fig. 4(a). The low yield stress for these two loading orientations are mainly governed by the low Peierls stress and high dislocation mobility on the basal plane. On the other hand, loadings along the yz and $y\bar{z}$ directions lead to higher yield points. The yz direction is almost perpendicular to the c-axis, and plasticity is mediated by prismatic $\langle a \rangle$ dislocation slip (see Fig. 4(b)). Furthermore, the $y\bar{z}$ loading is 1.85° away from the c-axis, which leads to predominant $\langle c+a \rangle$ slip on pyramidal II planes (see Fig. 4(c)). As expected, the yield stress for loading along the $y\bar{z}$ direction is the highest since pyramidal slip is the hardest slip mode. It is also clear from Fig. 3 that regardless of the loading direction, all results exhibit weak strain hardening response in the absence of GBs or TBs up to ~1% strain.

Figure 3 also shows the predicted stress-strain responses of polycrystals loaded in three different orientations (red curves). These simulations show that GBs lead to a significant rise in the crystal strength as compared to single crystal simulations. In particular, the yield strength increases by 208% for y and z loadings (basal slip), by 70% for yz loading (prismatic slip), and by 19% for $y\bar{z}$ loading (pyramidal slip). It is clear from the contour maps in Figs. 4(d)-(f) that the deformation modes are similar to those in single crystal simulations, but with fewer slip traces due to the GB's barrier effect. In addition, the higher strain hardening rates are observed in all simulations with GBs (i.e. 15.5 GPa for basal, 8.2 GPa for prismatic and 5.4 GPa for pyramidal slips). Note that these hardening rates are mean values from 3 realizations with

different initial dislocation distributions. The orientation dependence of the hardening rate is a result of the anisotropy in slip modes and Peierls stresses in Mg. Since the basal slip orientation is a single slip orientation (Fig. 4(d)), many dislocations pile up at the GBs, which lead to a strong back stress and a high strain hardening rate. For the prismatic and pyramidal slip orientations (Figs. 4(e)-(f)), plasticity is mediated by multi-slip, resulting in small dislocation pileups and low strain hardening rates.

Finally, the twinned crystals response is shown by the blue curves in Fig. 3. The simulation cell has edge-length $l_g = 1.3$ μm, and the twin lamella of thickness $l_t = l_g/2$ is located at the center of the simulation cell. For these simulations, only two unique loading directions exist. The y and z loading directions share the same response and deformation modes in the matrix and twinned regions, while yz and $y\bar{z}$ loading directions share another one. The hardening rates for the y and yz loading directions are 20.4 GPa and 26.6 GPa, respectively, for deformation up to 0.8% strain. These rates are significantly higher than those observed from the GB simulations. Fig. 4(g) shows the contours of the effective plastic strain at the end of the simulations in a twinned simulation cell loaded along the y direction. Dislocation slip is predominant on basal planes in both the matrix and twin. Some slip traces are observed to be fully blocked in the twin or matrix, which is consistent with the high hardening rate observed in Fig. 3. On the other hand, some traces are connected across the TB, forming a long zigzag trace from basal planes in the matrix to basal planes in the twin. These observations are in excellent agreement with experimental observations [43, 44]. Furthermore, Fig. 4(h) shows a different deformation response during loading along the yz direction. Plasticity here is confined in the matrix since the twin is in a much harder orientation (pyramidal slip) as compared to the softer orientation of the matrix (prismatic slip).

As discussed above, there are at least three sources contributing to strain hardening in Mg crystals, including dislocation forest hardening, GB strengthening, and TB hardening. The single crystal simulations, discussed in Fig. 3, indicate a minor contribution from dislocation forest hardening for the given initial dislocation density and strain levels reached. On the other hand, GBs and tension TBs clearly act

as strong barriers to dislocation glide, leading to a more significant hardening. Furthermore, TBs obviously provide the most important contribution to hardening response.

In order to identify the hardening source associated with TBs, the dislocation configurations from the twinned crystal simulations in both loading directions are shown in Fig. 5. For simulations with loading along the *y* direction, it is observed that many parallel dislocations pile up against the TB as shown in Fig. 5(a) by straight dislocations (red in the matrix and green in the twin). In this case, all the piled up dislocations in the matrix and twin are only basal $<a_2>$ and $<a_3>$ dislocations, since the Schmid factor of $<a_1>$ is 0. According to the dislocation-TB interaction model shown in Table A2, these dislocations should decompose as follows

$$< a_2 > \text{ or } < a_3 > \rightarrow \ 0.5 < c + a > + \boldsymbol{b_t} \tag{6}$$

Thus, when the first dislocation (incident dislocation $\boldsymbol{b_i}$) arrives at the TB, it decomposes into one half $<c+a>$ dislocation (residual dislocation $\boldsymbol{b_r}$) and a twinning dislocation ($\boldsymbol{b_t}$), as shown in Fig. 5(a1). This decomposition is identical to that reported by MD simulations [49-51] and predicted experimentally [43, 44]. While the Schmid factor on the TB is zero, the twinning dislocation is observed to glide away on the TB, as shown in Fig. 5(a2), due to the repulsive force between the residual dislocation and twinning dislocation. This may provide a mechanism for twin growth in the crystal [50, 51]. However, the one half $<c+a>$ dislocation is a sessile dislocation that will remain on the TB. This residual dislocation will also have a repulsive interaction with subsequent incident dislocations, which would contribute to the dislocation pileup near the TB (see Fig. 5(a2)). With the increasing applied stress and number of pileup dislocations, the shear stress acting on the new leading incident dislocation in the pileup increases remarkably, and overcomes the repulsive interaction with the residual dislocation on the TB. Thus, the new incident dislocation would reach the TB and then decompose into another one half $<c+a>$ dislocation and a twinning dislocation. Therefore, an integrated $<c+a>$ can subsequently be emitted into the twinned crystal from the TB, as shown in Fig. 5(a3). This is consistent with the experimental observations [44, 45]. As further dislocations reach the TB, the same

decomposition processes would repeat. Finally, it should be noted that while dislocation transmission across TB is observed in the current simulations, it occurs only at high local stress levels due to heavy dislocation pileups, as shown in Fig. 5(a4). This is the reason for the strong barrier effect of the TB.

On the other hand, during loading along the *yz* direction two dense dislocation networks are observed on the TBs (see Fig. 5(b)). Figure 5(b1) shows that the network consists of two intersecting sets of parallel straight dislocations, in addition to curved dislocations. As stated previously, during loading along the yz direction, plasticity is accommodated by prismatic slip in the matrix. According to equation (6), the straight dislocations are half <*c*+*a*> residual dislocations, as an output from incident prismatic <*a*> dislocations. The angle between the intersecting sets is 45.7°, which is the angle between the intersection lines of two prismatic planes on the TB. Furthermore, the curved dislocations are twinning dislocations, which are glissile on the TB since the Schmid factor is nonzero for this orientation. Because few dislocation pileups are observed in Fig. 5(b), dislocation transmission events across the TB in this loading orientation are rare.

As shown in Fig 4(g), loading along the *y* direction is a single slip orientation since plasticity is accommodated by basal slip only. Thus, plasticity is confined to distinct planes and many dislocation pileups would be expected at the TBs (see Fig. 5(a)). On the other hand, loading along the *yz* direction leads to multi-slip deformation on prismatic planes. Subsequently, the contour of plastic strain in the matrix is uniform, as seen in Fig. 4(h), and few dislocation pileups are expected at the TBs (Fig. 5(b)). It should be noted that prismatic slip during *yz* loading induces a higher hardening rate than basal slip during *y* loading, which seems contradictory to the previous hardening mechanism of polycrystals. In fact, this is a result of the hard orientation (pyramidal slip) of the twin with respect to the *yz* loading axis, in which almost no plastic deformation is seen (Fig. 4(h)). Also note that such hardening behavior holds true only at low stress levels, at which twin is hard to plastically deform. Section 3.2 will show that such mechanism is invalid for high stresses, since the twin would play an important role in the overall plastic behavior. Furthermore, in

the *yz* loading the Schmid factor on the TB plane is high, leading to the glide of many twinning dislocations, which would contribute greatly to TB migration and twin growth [50, 51]. In other words, compressive loading along the yz direction is a favorable orientation for twin growth, in agreement with experiments oriented for compressive loading perpendicular to the *c*-axis [6, 8].

The three popular hardening mechanisms that are usually attributed to cause the twinning-related hardening in magnesium are: (a) Hall-Petch strengthening due to grain refinement by the evolving twins [9, 56, 57]; (b) Basinski mechanism: glissile-to-sessile transformation of dislocations due to the twinning shear [12, 13]; and (c) texture hardening induced by the hard orientation in the twins [11, 13]. The current DDD simulation results of the twinned crystals provide direct evidences of these mechanisms. In Figs. 5(a) and (b), many sessile residual dislocations remain on the TB, which agrees well with the Basinski mechanism. The TBs act as strong obstacles to dislocations, and induce grain refinement hardening. In addition, the absence of plasticity in the twinned region (see Fig. 4(h)) clearly demonstrates the hardening induced by the lattice orientation of the twins.

3.2 Hardening behavior of twinned polycrystals

To identify the collective contribution of dislocations, GBs and TBs on the hardening behavior of magnesium, in this subsection, the mechanical behavior of twinned polycrystals is investigated. This crystal is identical to the experimental samples. In the following simulations the grain size is kept constant at l_g = 1.3 μm and the twin size, l_t, is varied to address the effect of twin volume fraction. Tension twinning has been reported experimentally to be facilitated by compression perpendicular to the *c*-axis, or tension parallel to the *c*-axis [6, 8]. These correspond to the current yz compressive loading and $y\bar{z}$ tensile loading, respectively. The engineering stress-strain responses for different twin volume fractions ($f_t = l_t / l_g$) under yz compressive loading are shown in Fig. 6. The case of f_t = 0.0 corresponds to an untwinned polycrystal, while f_t = 1.0 corresponds to a fully twinned polycrystal. It is observed that the yield stress increases with increasing twin volume fraction, until it reaches a peak value at f_t = 0.7. The inset in Fig. 6 shows that dislocation activity in

the matrix contributes mostly to the overall plastic deformation. Subsequently an increasing twin fraction results in reducing the grain volume, which would in turn result in an increase in the yield stress of the crystal. Furthermore, the case of $f_t = 1.0$ indicates that the yield stress for the twin orientation is about 350 MPa. Thus, once the yield stress exceeds 350 MPa when the volume fraction increases beyond $f_t = 0.5$, dislocation activity in the twin begins to contribute to the overall plastic deformation. For $f_t > 0.7$, the overall plastic deformation is mainly accommodated by dislocation activity in the twin, since fewer dislocation sources would exist in the smaller matrix region. Therefore, the yield stress decreases with further increase in the twin volume fraction. In the fully twinned grain with $f_t = 1.0$, the *c*-axis is rotated close to the *yz* compressive loading direction, which is an orientation that would promote compression twinning. Knezevic et al. [7] observed compression twins and double twins in various individual grains, which are always in a thin band shape with low fraction and suggested to contribute to the peak hardening rate in stage II. To model this, here we introduced a nominal compressive twin with a volume fraction of 0.05 in the center of the fully twinned grain, and these TBs are assumed to be impenetrable to dislocations. To keep the notation consistent, this case is denoted by $f_t = 1.05$. Fig. 6 shows that the volume fraction of $f_t = 1.05$ produces the highest yield stress, which confirms the important role of compression twins after saturation of tension twinning.

Figure 7 shows the hardening rate due to dislocation slip, θ_s, as a function of twin volume fraction. These hardening rates were computed from a linear fit of the stress-strain curve beyond a plastic strain of $\varepsilon_p = -0.05\%$. It is clear that the hardening rate increases before $f_t = 0.3$, and then decreases between $f_t = 0.3$~1.0. Subsequently, the hardening rate increases again at a volume fraction of $f_t = 1.05$. It should be noted that only dislocation-mediated plasticity is modeled in the current DDD framework. Under actual experimental conditions, plastic deformation is mediated by both dislocations and twinning, with twinning playing a major role especially at low strain levels. Thus, the contribution of twinning plasticity must be taken into account. Accordingly, the overall hardening rate, θ, can be decomposed into a contribution from dislocation slip and a contribution from twinning, such that θ

would be given by:

$$\theta = \frac{d\sigma}{d\varepsilon} = \frac{d\left(E\left(\varepsilon - \varepsilon_{slip}^{p} - \varepsilon_{twin}^{p}\right)\right)}{d\varepsilon}$$

$$= \frac{d(E(\varepsilon - \varepsilon_{slip}^{p}))}{d\varepsilon} - \frac{d(E\varepsilon_{twin}^{p})}{d\varepsilon} = \theta_s - \theta_t \quad (7)$$

where θ_s is the hardening rate induced only by dislocation slip, which is plotted in Fig. 7. On the other hand, θ_t is the hardening rate induced only by twinning and can be computed based on the twin volume fraction [8] such that

$$\theta_t = \frac{d(E\varepsilon_{twin}^{p})}{d\varepsilon} = E\bar{m}\gamma_{twin}\frac{df_t}{d\varepsilon} \quad (8)$$

where $\bar{m}$ and γ_{twin} represent the average Schmid factor of the twin variants and characteristic twinning shear, respectively. For the $(10\bar{1}2)$ twinning in Mg and its alloys, γ_{twin} = 0.13, and $\bar{m}$ = 0.437 for yz compressive loading and 0.499 for y$\bar{z}$ tensile loading [8]. In order to calculate $df_t/d\varepsilon$, the twin volume fraction reported experimentally by 6 different groups [6-8, 10, 58-60] for AZ31 is plotted in Fig. 8 as a function of the applied strain. A parabola function of the form $f_t = -42.0\varepsilon^2 + 13.6\varepsilon - 0.083$ gives the best fit to these experimental data, and subsequently θ_t is computed by equation (8). It is clear that the twinning-induced θ_t continuously decreases with increasing twin volume fraction. The total hardening rate $\theta = \theta_s - \theta_t$ is also shown in Fig. 7. Two stages can be identified: a) decreasing hardening rate below a twin volume fraction of 0.1; and b) increasing hardening rate above 0.1. These two stages mimic the experimentally identified stages I and II [6-8, 59]. Furthermore, for the volume fraction of $f_t = 1.05$, the highest hardening rate is achieved. This indicates that the compression twins in the fully tension-twinned grains are responsible for the peak hardening rate in stage II, which agrees well with experimental results [7]. Note the total hardening rate is mainly negative, which agrees with experiments showing a negative hardening rate for small grain sizes (~3 μm) at room temperature [5]. Nevertheless, the overall hardening rates are still lower than those experimentally measured, which is possibly a result of different initial conditions. In experiments, AZ31 polycrystals are usually in an annealed condition with a low initial dislocation density [7, 8, 59] and having a high density of second

phase particles [28], thus the dislocation-mediated hardening rate θ_s, and the overall θ is expected to be higher than those from the current DDD simulations.

The stress-strain responses of $y\bar{z}$ tensile loading are plotted in Fig. 9. The yield stress displays a different character from that of *yz* compressive loading. With increasing twin volume fraction up to 0.2, the yield stress is observed to increase. For a volume fraction between 0.2 and 1.0, the yield stress continuously decreases. This can be explained as following. Under $y\bar{z}$ tensile loading, the grain *c*-axis is close to the loading direction, which results in a hard deformation mode. Below $f_t = 0.2$, the plastic deformation is mainly mediated by dislocations activity in the grain. Thus, an increasing twin volume fraction confines the grain volume and leads to an increasing yield stress. With the increasing twin fraction above 0.2, the plastic deformation is gradually dominated by the twin, which is in a soft orientation, as shown by the inset in Fig. 9. As a result, the yield stress decreases with increasing twin fraction. In fact, Figs. 6 and 9 are very similar, only with the inverse twin volume fractions. This comes from the exchange of the grain and twin orientations with respect to the two loading directions. That is to say, the main deformation mechanisms are identical under these two loading paths.

The dislocation induced hardening rate, θ_s, for $y\bar{z}$ tensile loading from the current DDD simulations is shown in Fig. 10. Similar trends to the *yz* compressive loading are observed. It is observed that θ_s increases below $f_t = 0.4$, and decreases beyond 0.4. The experimentally measured variation of twin volume fraction as a function of strain for $y\bar{z}$ tensile loading is shown in Fig. 8. The twin volume fraction increases slowly at low and high strain stages, but quickly at intermediate strains, which is different than that for *yz* compressive loading. This is a result of the different activated twin variants [8]. A cubic equation of the form $f_t = -1650.6\varepsilon^3 + 303.4\varepsilon^2 - 4.9\varepsilon + 0.00817$ provides the best fit for the experimental data. As shown in Fig. 10, θ_t calculated from experiments increases below $f_t = 0.4$, and decreases after 0.4. Although θ_t is different from that of yz compressive loading, the overall hardening rate θ displays two distinct stages, which are identical to *yz* compressive loading and experimental observations [8, 59]. Again, the twin volume fraction of

$f_t = 1.05$ yields the peak hardening rate in stage II, and agrees well with experimental results [7].

It is clear that both the *yz* compressive and $y\bar{z}$ tensile loadings show a two-stage hardening rate curve, as shown in Figs. 7 and 10, in agreement to experimental observations. As aforementioned, three mechanisms are usually attributed to explain this hardening behavior in magnesium: (a) Hall-Petch strengthening due to grain refinement by the evolving twins [9, 56, 57]; (b) Basinski mechanism: glissile-to-sessile transformation of dislocations due to the twinning shear [12, 13]; and (c) texture hardening induced by the hard orientation in the twins [11, 13]. In addition, the current DDD simulations demonstrated that (d) compression twining in fully tension-twinned grains is yet another mechanism [7]. In fact, mechanism (c) plays a minor role in the hardening behavior. In Fig. 6 for *yz* compressive loading, the case of $f_t = 1.0$ displays the weakest hardening, indicating the twin orientation with a hard deformation mode can increase the yield stress significantly, but contributes less to increasing the hardening rate. This is true at least for high stress levels (> 350 MPa) or twin fractions (> 0.5), since the twin plastically deforms and its hardening effect diminishes. At low stress levels (< 350 MPa) or twin volume fractions less than 0.5, the twin hard orientation does contribute to hardening, as shown in Section 3.1, but its role in the overall behavior is limited by the low twin volume fraction. Furthermore, during $y\bar{z}$ tensile loading a similar hardening curve is still seen in Fig. 10, however, tension twining plays a softening role. Thus, regardless of the hardening or softening contribution twinning plays, its influence on the resulting hardening behavior is minor.

On the other hand, as observed in Fig. 5, many sessile residual dislocations are observed on the TB, which provides direct evidences of mechanism (b) (i.e. the Basinski mechanism). Due to the residual dislocations on the TB, subsequent dislocations pile up against the TB, resulting in mechanism (a) (i.e. Hall-Petch effect due to the grain refinement by twins). In fact, the mechanism (d) also operates through the grain refinement in fully tension-twinned grains by compression twins. Accordingly, mechanisms (a), (b) and (d) are a similar mechanism, i.e. Hall-Petch

effect induced by TB barrier. Therefore, based on the current DDD simulations, the hardening behavior due to dislocation slip, θ_s, is only a consequence of the TB's barrier effect.

From this viewpoint, it is possible to develop a unified understanding of the observations from both the *yz* compressive and $y\bar{z}$ tensile loading cases. Since TBs act as barriers to gliding dislocations, the best grain refinement with 3 equal-sized grains is achieved at f_t = 1/3. That is why the hardening rate θ_s from current DDD simulations reaches its highest value at f_t = 0.3 for *yz* compressive loading and f_t = 0.4 for $y\bar{z}$ tensile loading, as shown in Figs. 7 and 10. The overall hardening rate θ depends on θ_s induced by TB barrier effect and θ_t induced by twinning deformation (i.e. $\theta = \theta_s - \theta_t$). In Figs. 7 and 10, θ_t is always positive, indicating that twinning deformation always leads to a softening effect. On the other hand, θ_s is also positive and TB always produces hardening. As a result, a competition exists between dislocation-TB induced hardening and twinning deformation induced softening. Below the twin volume fraction of 0.1 for *yz* compressive loading, or 0.2 for $y\bar{z}$ tensile loading, twinning deformation induced softening dominates, and thus a decreasing overall hardening rate is observed in stage I. In stage II, both the hardening and softening effects decline, but softening effect declines faster and results in an increasing hardening rate.

4. Conclusions

In this work, a systematic interaction model between dislocations and $(10\bar{1}2)$ TBs was proposed. In this model all the possible incident dislocations were taken into account, as shown in Table A2. In order to mimic the GB strengthening, a nominal GB model agreeing with experimental results was used. Both the TB and GB models were introduced into the DDD framework to study the mechanical behavior of a representative twinned Mg grain. The TB was shown to be a strong obstacle to dislocation glide, and play a dominant role in the hardening behavior. On the other hand, previous experimental results show that the plastic deformation induced by

twinning acts as a softening role. Therefore, a competition exists between dislocation-TB induced hardening and twinning deformation induced softening, which is responsible to the concave shape of the stress-strain curve. At low strain levels, twinning deformation induced softening dominates, leading to a decreasing hardening rate in Stage-I. In Stage-II, both the hardening and softening effects decline, but the softening declines faster and leads to an increasing hardening rate.

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References

[1] Luo AA. Journal of Magnesium and Alloys 2013;1:2.
[2] Christian JW, Mahajan S. Progress in Materials Science 1995;39:1.
[3] Prasad KE, Rajesh K, Ramamurty U. Acta Mater. 2014;65:316.
[4] Kelley EW, Hosford WF. Technical report 1967.
[5] Barnett MR, Keshavarz Z, Beer AG, Atwell D. Acta Mater. 2004;52:5093.
[6] Jiang L, Jonas JJ, Luo AA, Sachdev AK, Godet S. Materials Science and Engineering: A 2007;445–446:302.
[7] Knezevic M, Levinson A, Harris R, Mishra RK, Doherty RD, Kalidindi SR. Acta Materialia 2010;58:6230.
[8] Hong S-G, Park SH, Lee CS. Acta Materialia 2010;58:5873.
[9] Salem AA, Kalidindi SR, Doherty RD. Acta Materialia 2003;51:4225.
[10] Lou C, Zhang X, Duan G, Tu J, Liu Q. Journal of Materials Science & Technology 2014;30:41.
[11] Wang B, Xin R, Huang G, Liu Q. Materials Science and Engineering: A 2012;534:588.
[12] Basinski ZS, Szczerba MS, Niewczas M, Embury JD, Basinski SJ. Revue de Metallurgie. Cahiers D'Informations Techniques 1997;94:1037.
[13] Salem AA, Kalidindi SR, Doherty RD, Semiatin SL. Metallurgical and Materials Transactions A 2006;37:259.
[14] Sarker D, Chen DL. Scripta Materialia 2012;67:165.

[15] Fan H, Li Z, Huang M, Zhang X. Int. J. Solids. Struct. 2011;48:1754.
[16] Van der Giessen E, Needleman A. Modelling Simul. Mater. Sci. Eng. 1995;3:689.
[17] Arsenlis A, Cai W, Tang M, Rhee M, Oppelstrup T, Hommes G, Pierce TG, Bulatov VV. Model. Simul. Mater. Sci. Eng. 2007;15:553.
[18] Zbib HM, Rhee M, Hirth JP. International Journal of Mechanical Sciences 1998;40:113.
[19] Kubin LP, Canova G, Condat M, Devincre B, Pontikis V, Brechet Y. Solid State Phenom. 1992; 23 & 24:455.
[20] El-Awady JA, Bulent Biner S, Ghoniem NM. Journal of the Mechanics and Physics of Solids 2008;56:2019.
[21] Fan H, Li Z, Huang M. Scripta Mater. 2012;67:225.
[22] Li Z, Hou C, Huang M, Ouyang C. Comp. Mater. Sci. 2009;46:1124.
[23] Huang M, Li Z, Tong J. International Journal of Plasticity 2014;61:112.
[24] Fan H, Aubry S, Arsenlis A, El-Awady JA. submitted 2014.
[25] Fan H, Li Z, Huang M. Scripta Mater. 2012;66:813.
[26] Wu CC, Chung PW, Aubry S, Munday LB, Arsenlis A. Acta Mater. 2013;61:3422.
[27] Monnet G, Devincre B, Kubin LP. Acta Materialia 2004;52:4317.
[28] Aitken Z, Fan H, El-Awady JA, Greer JR. submitted 2014.
[29] Kim GS. PhD thesis 2011;University of Grenoble.
[30] Capolungo L, Beyerlein IJ, QWang Z. Modelling and Simulation in Materials Science and Engineering 2010;18:085002.
[31] Olarnrithinun S, Chakravarthy SS, Curtin WA. J. Mech. Phys. Solids 2013;61:1391.
[32] Conrad H, Robertson WD. Trans.Met.Soc.AIME 1957;209:503.
[33] Reed-Hill RE, Robertson WD. Acta Metall. 1957;5:717.
[34] Staroselsky A, Anand L. Int. J. Plast. 2003;19:1843.
[35] Tang Y, El-Awady JA. Materials Science and Engineering: A 2014;618:424.
[36] Groh S, Marin EB, Horstemeyer MF, Bammann DJ. Model. Simul. Mater. Sci. Eng. 2009;17:075009.
[37] Yasi JA, Nogaret T, Trinkle DR, Qi Y, L. G. Hector J, Curtin WA. Modelling and Simulation in Materials Science and Engineering 2009;17:055012.
[38] Tang Y, El-Awady JA. Acta Mater. 2014;71:319.
[39] Agnew SR, Duygulu Ö. Int. J. Plast. 2005;21:1161.
[40] Zhang J, Joshi SP. J. Mech. Phys. Solids 2012;60:945.
[41] Zhang J, Ramesh KT, Joshi SP. Model. Simul. Mater. Sci. Eng. 2014;22:075003.
[42] Price PB. Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences 1961;260:251.
[43] Hyong Yoo M, Wei C-T. Philosophical Magazine 1966;14:573.
[44] Tomsett DI, Bevis M. Philosophical Magazine 1969;19:129.
[45] Dickson JI, Robin C. Materials Science and Engineering 1973;11:299.
[46] Lay S, Nouet G. Philosophical Magazine A 1994;70:1027.
[47] Yoo MH. Transactions of the Metallurgical Society of AIME 1969;245:1841.
[48] Serra A, Bacon DJ. Acta Metallurgica et Materialia 1995;43:4465.
[49] Yuasa M, Masunaga K, Mabuchi M, Chino Y. Philosophical Magazine 2013;94:285.
[50] Serra A, Bacon DJ. Philosophical Magazine A 1996;73:333.
[51] Wang J, Beyerlein IJ, Tomé CN. International Journal of Plasticity 2014;56:156.

[52] Wang Y, Chen LQ, Liu ZK, Mathaudhu SN. Scripta Materialia 2010;62:646.
[53] Tromans D. International Journal of Research and Reviews in Applied Sciences 2011;6:462.
[54] Zhou C, LeSar R. Int. J. Plast. 2011;30-31:185.
[55] Li B, Joshi S, Azevedo K, Ma E, Ramesh KT, Figueiredo RB, Langdon TG. Materials Science and Engineering: A 2009;517:24.
[56] Asgari S, El-Danaf E, Kalidindi S, Doherty R. Metallurgical and Materials Transactions A 1997;28:1781.
[57] Xin Y, Wang M, Zeng Z, Nie M, Liu Q. Scripta Materialia 2012;66:25.
[58] Yang HJ, Yin SM, Huang CX, Zhang ZF, Wu SD, Li SX, Liu YD. Advanced Engineering Materials 2008;10:955.
[59] Park JH, Kim HL, Jung JE, Chang YW. Metals and Materials International 2013;19:389.
[60] Levinson AJ. PHD thesis 2012.