On the Rapid Hardening and Exhaustion of Twinning in Magnesium Alloy

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Abstract —We numerically study the rapid hardening and possible role of exhaustion of twinning in magnesium alloys under twinning dominated conditions, based on the large strain elastic visco-plastic self-consistent model. It is found that upon the exhaustion of the tensile twinning, further deformation requires the material to activate Prismatic and Pyramidal slips, which have relative high critical resolved shear stress (CRSS). However, the stress level at the exhaustion of the tensile twinning is not high enough to activate Prismatic and Pyramidal slips. Consequently, the imposed strain increments must mainly be accommodated by elastic deformations, and the strain hardening rate becomes a large fraction of the elastic modulus. Therefore, it can be concluded that the rapid hardening is a composite response more associated with elasticity of a large volume fraction of the material, than the dislocation-dislocation interactions normally held responsible for strain hardening of metals.

Keywords: Twinning; Hardening; Polycrystal plasticity modeling; Magnesium alloys

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1. Introduction

Magnesium (Mg) and its alloys are of a hexagonal close-packed (HCP) crystallographic structure with low symmetry and, consequently, exhibit high anisotropy in mechanical behavior. Plastic deformation in HCP materials is accommodated by both slip and twinning. Twinning as an important plastic deformation mechanism in HCP materials has been extensively studied (see e.g. Arul Kumar et al. [1]; Balik et al. [2]; Barnett et al. [3, 4]; Ghaffari Tari et al. [5]; Guo et al. [6]; Jin et al. [7]; Kabirian et al. [8]; Kurukuri et al. [9]; Lynch et al. [10]; Mathis et al. [11]; McClelland et al. [12]; Niezgoda et al. [13]; Shi et al. [14]; Stanford et al. [15]; Steglich et al. [16]; Wang and Choo [17]; Wen et al. [18]; Wu et al. [19]; Xin et al. [20]). In Mg alloys, the most commonly observed twinning mode is the $\{10\bar{1}2\} \langle 10\bar{1}1 \rangle$ extension twinning. It is well known that conventionally rolled magnesium sheet exhibits a basal texture, in which the basal planes typically lie preferentially in the plane with its normal parallel to the normal direction (ND). When such a rolled Mg alloy sheet is under uniaxial compression along the rolling direction (RD) or the transverse direction (TD), plastic deformation is dominated by tensile twinning at small strains because the c -axes of many grains are in the direction of Poisson extension. It has been generally accepted that under twinning dominated conditions, the yielding and immediate post-yielding plasticity is governed largely by the twin nucleation, whereas plastic deformation at higher strains is governed by twin growth and dislocation slip. A region of particularly low work-hardening, or in some cases slight work-softening, can be clearly detected for the finer-grained samples (e.g., Ghaderi and Barnett [21]; Barnett et al. [22]). This Lüders-like plateau in the macroscopic stress strain curves implies that the freshly nucleated twins proceed without additional increase in the applied stress. In coarser grained samples, it has been observed by Barnett et al. [23] that there may be some strain hardening within the immediate

post-yield regime, presumably due to an increasing difficulty in twin nucleation with straining. After such a plateau-type region of low hardening, a steep increase in flow stress or a rapid hardening is also clearly observed. Depending on the initial texture, the hardening rate after the plateau in the macroscopic stress strain curve can attend a maximum value of one third of the elastic shear modulus (see Knezevic et al. [24]; Oppedal et al. [25]). It is this regime of rapid hardening which is of interest in the present paper.

It has been generally thought that the tensile twinning contributes to strain hardening through: (1) crystallographic lattice reoriented to a harder orientation (Lou et al. [26]), (2) the Basinski effect, i.e. a glissile-to-sessile transformation of dislocations already present in the region experiencing the twinning shear transformation (Basinski et al. [27]), and (3) a Hall-Petch-like effect resulted from grain refinement due to tensile twinning itself. However, Knezevic et al. [24] concluded that, based on their experiments on a rolled AZ31 alloy, these three mechanisms are unlikely to be high enough to explain the experimentally convinced rapid hardening. Instead, they postulated that (4) the thin contraction twins are very effective in strain hardening of the alloy by restricting the slip length associated with Pyramidal slip, i.e. another Hall-Petch-like effect. They demonstrated that this assumption is able to explain the key experimental features.

It is here hypothesized that the rapid hardening effect is induced by (5) the exhaustion of twinning. It can be rationalized that the tensile twinning reorients the material in the twinned region into a hard orientation. Further plastic deformation in the material inside the twin has to activate Pyramidal slip, which has much higher critical resolved shear stress (CRSS) comparing to tensile twinning. In short, the proposed mechanism is a natural consequence of item (1) above. However, the details presented here have not been systematically presented elsewhere, and it will

be shown that there are specific, temporal problems with each of the previously proposed explanations (2)-(4). Regarding item (2), additional evidence has recently been produced to indicate that the Basinski effect does occur (Wang and Agnew [28]), however, it can only be held indirectly responsible for the present effect, as we will discuss later in the paper. Regarding item (3) the microstructure is most refined by twinning at early stages (where the strain hardening rate is low). By the time the strain hardening rate is high, the twins have largely consumed the grains and the refinement is no longer significant. Regarding item (4), it is suggested that compression twinning is mainly significant at later stages in the deformation (c.f. Oppedal et al. [25]), where strain hardening is slowing and/or localization is underway.

The purpose of this work is therefore to numerically investigate the rapid hardening induced by hypothesis (5), the exhaustion of twinning in Mg alloys. All the simulations reported in this paper are based on the large strain Elastic-Viscoplastic Self-Consistent (EVPSC) model developed by Wang et al. [29]. The EVPSC model has been successfully used to study effects of basal texture (Wang et al. [30]), formability of AZ31 sheet (Wang et al. [31]), lattice strain evolution in Mg alloys and steel (Wang et al. [32, 33]; Lee et al. [34]) and large strain behaviour of Zr alloys (Qiao et al. [35]). Wang et al. [36, 37] also developed a new constitutive model of Twinning and De-Twinning (TDT) for HCP materials. The TDT model has been implemented into the EVPSC framework. The EVPSC-TDT model has been applied to study inelastic deformation in Mg alloys during unloading (Wang et al. [38]), the Swift effect under free-end torsion (Guo et al. [39]), and lattice strain evolution associated with twinning and detwinning under cyclic loadings (Wu et al. [40]; Qiao et al. [41]; Wang et al. [42]).

2. The EVPSC-TDT model

The EVPSC model is a completely general elastic visco-plastic, fully anisotropic, self-consistent polycrystal model, applicable to large strains and to any crystal summary. The TDT model is a new physics-based crystal plasticity model of twinning and detwinning for HCP materials. In this section, we very briefly recapitulate the EVPSC-TDT model, mainly for the purpose of definition and notation. For details we refer readers to Wang et al. [29, 36, 37].

The plastic deformation of a crystal is assumed to be due to crystallographic slip and twinning on crystallographic system (s^α, n^α) , with s^α and n^α being respectively the slip/twinning direction and the normal of the slip/twinning plane for system α . For Mg alloys, we usually consider Basal $\langle a \rangle$ ($\{0001\} \langle 11\bar{2}0 \rangle$), Prismatic $\langle a \rangle$ ($\{10\bar{1}0\} \langle 11\bar{2}0 \rangle$) and Pyramidal $\langle c+a \rangle$ ($\{\bar{1}\bar{1}22\} \langle \bar{1}\bar{1}23 \rangle$ slip systems, and the $\{10\bar{1}2\} \langle \bar{1}011 \rangle$ extension twin system.

Following Asaro and Needleman [43], the grain level plastic strain rate consists of the shear rate $\dot{\gamma}^\alpha$ on slip/twinning system α as

$$d^p = \sum_{\alpha} \dot{\gamma}^\alpha P^\alpha \quad (1)$$

where $P^\alpha = (s^\alpha n^\alpha + n^\alpha s^\alpha)/2$ is the Schmid tensor. For both slip and twinning, the resolved shear stress $\tau^\alpha = \sigma : P^\alpha$ is the driving force for shear rate $\dot{\gamma}^\alpha$. For slip,

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \tau^\alpha / \tau_{cr}^\alpha \right|^{\frac{1}{m}} \text{sgn}(\tau^\alpha) \quad (2)$$

For twinning,

$$\dot{\gamma}^\alpha = \begin{cases} \dot{\gamma}_0 \left| \tau^\alpha / \tau_{cr}^\alpha \right|^{\frac{1}{m}} & \tau^\alpha > 0 \\ 0 & \tau^\alpha \leq 0 \end{cases} \quad (3)$$

where $\dot{\gamma}_0$ is a reference shear rate, τ_{cr}^α is the critical resolved shear stress (CRSS), and m is the strain rate sensitivity. The key assumption of the TDT model is that a grain has four potential operations associated with twinning and detwinning (Wang et al. [36]). Operation A is twin nucleation and initiates a twin band or ‘child’. Operation B is a propagation of the child into the parent. Operations A and B increase the twin volume fraction and thus correspond to twinning. Operation C is a propagation of the parent into the child. Operation D splits the twin band and decreases the twin volume fraction through re-twinning. Operations C and D decrease the twin volume fraction and thus correspond to detwinning. The TDT model treats new twin band (child) as a new grain.

For both slip and twinning, the evolution of CRSS, τ_{cr}^α , is given by:

$$\dot{\tau}_{cr}^\alpha = \frac{d\hat{\tau}^\alpha}{d\Gamma} \sum_{\chi} h^{\alpha\chi} |\dot{\gamma}^\chi| \quad (4)$$

where $\Gamma = \sum_{\beta} \int |\dot{\gamma}^\beta| dt$ is the accumulated shear strain in the grain, and $h^{\alpha\chi}$ are the latent hardening coupling coefficients, which empirically account for the obstacles on system α associated with the activity of system χ . $\hat{\tau}^\alpha$ is the threshold stress and is characterized by:

$$\hat{\tau}^\alpha = \tau_0^\alpha + (\tau_1^\alpha + h_1^\alpha \Gamma) (1 - \exp(-\frac{h_0^\alpha}{\tau_1^\alpha} \Gamma)) \quad (5)$$

Here, τ_0 , h_0 , h_1 , and $\tau_0 + \tau_1$ are the initial CRSS, the initial hardening rate, the asymptotic hardening rate, and the back-extrapolated CRSS, respectively.

Because it is rare that a grain can be fully twinned, a threshold twin volume fraction is defined in the model to terminate twinning. Consequently, the TDT model introduces two statistical variables: accumulated twin fraction, v^{acc} , and effective twinned fraction, v^{eff} . More specifically, v^{acc} and v^{eff} are the weighted volume fraction of the twinned region and volume

fraction of twin terminated grains, respectively. The threshold volume fraction, v^{th} , is defined as

$$V^{th} = \min\left(1.0, A_1 + A_2 \frac{V^{eff}}{V^{acc}}\right), \text{ where } A_1 \text{ and } A_2 \text{ are two material constants.}$$

Although it is not employed in the present work, a single parameter version of the TDT model has already been developed (Qiao et al. [44]). Incidentally, it is natural to ask, “Why would twinning become exhausted prior to completely consuming the grains?” Though a complete answer is beyond the scope of the present paper, since the results hinge so critically on this notion of twin exhaustion, it merits some comment. One hypothesis, which is presently under evaluation by some of the authors, is that the twin boundaries accumulate debris, in the context of sweeping the surrounding dislocated crystals (Wang and Agnew [28]). It is suggested that this accumulation of debris could render further twin boundary motion difficult.

Coupling the single crystal plasticity outlined above to the aggregate response is accomplished using self-consistent approaches based upon the Eshelby inclusion formalism (Eshelby [45]). Various self-consistent schemes have been proposed. Wang et al. [46] have evaluated several self-consistent approaches by studying the large strain behaviour of magnesium alloy AZ31B sheet under tension and compression along different directions. It has been demonstrated that, of the approaches examined, the Affine self-consistent scheme gives the best overall performance. Therefore, the EVPSC-TDT model the Affine self-consistent scheme is employed in the present study.

3. Results and Discussion

In the present paper, we consider rolled Mg alloy sheets under in-plane uniaxial tension and compression. In all the simulations, a strain rate, $D_{11} = \dot{\epsilon} = 5 \times 10^{-3} s^{-1}$, is prescribed in the loading direction, and the macroscopic stress components are enforced to be zero, except for the

stress $\sigma_{11} = \sigma$ along the loading direction. In all the figures shown in the present paper, stress σ and strain ε are presented in their absolute values, and stress is in unit of MPa.

As mentioned previously, the present work focuses on the rapid hardening observed in Mg alloy sheets under in-plane compression. We consider two AZ31B sheets: one with very strong basal texture and the other with strong basal texture. In order to assess effects of initial texture on the rapid hardening, we also consider two extreme cases: one with ideal basal texture [i.e. a single crystal with Euler angles $(30^\circ, 0^\circ, 0^\circ)$] and a random texture. Fig. 1 shows the initial textures represented in terms of the $\{0002\}$ pole figure. The sheet with strong basal texture (texture 3 in Fig. 1) has been studied experimentally by Jain and Agnew [47] and numerically by Wang et al. [46] based on the EVPSC model with the Predominant Twin Reorientation (PTR) scheme proposed by Tomé et al. [48], while the sheet with very strong basal texture (texture 2 in Fig. 1) has been investigated experimentally by Wu et al. [49] and numerically by Wang et al. [37] based on the EVPSC-TDT model.

In all the simulations reported in the present paper, the reference slip/twinning rate, $\dot{\gamma}_0$, and the rate sensitivity, m , are prescribed to be the same for all slip/twinning systems: $\dot{\gamma}_0 = 0.001\text{s}^{-1}$ and $m = 0.05$, respectively. The room temperature elastic constants of magnesium single crystal $C_{11} = 58.0$, $C_{12} = 25.0$, $C_{13} = 20.8$, $C_{33} = 61.2$ and $C_{44} = 16.6$ (units of GPa) are used. The set of CRSSs and hardening parameters for each plastic deformation mode are estimated by fitting numerical simulations of uniaxial tension and compression along the RD to the corresponding experimental flow curves for the sheet with very strong basal texture reported by Jain and Agnew [47]. The uniaxial tension and compression true stress and true strain curves along the RD are presented in Fig. 2. The macroscopic yield stresses for uniaxial compression and tension are around 100 MPa and 165 MPa, respectively, showing the strong

tension/compression asymmetry associated with twinning. The maximum stresses in tension and compression are 275 MPa and 400 MPa, respectively. Under uniaxial compression, after a low stress plateau in the stress and strain curve, the Mg sheet hardens dramatically resulting in the characteristic S-shape of the compressive flow curve. It is clear that the EVPSC-TDT model fits the experimental curves quite well. Table 1 lists the values of the material parameters obtained from these simulations. These parameters are used in all of the subsequent simulations. It should be emphasised that the main purpose of this paper is to assess the influence of the twinning on the rapid hardening, and that the overall results and conclusions are not particularly dependent on the above values of the material parameters. It is also worth mentioning that we repeated the simulations by assuming isotropic elasticity with a Young's modulus of $E = 45$ GPa and Poisson's ratio of $\nu = 0.33$. It was found that the predicted flow curves based on the isotropic elasticity assumption were almost the same as those shown in the Fig. 2. This could be easily understood because Mg crystals exhibit a nearly isotropic elasticity. For more efficiently interpreting results, it is appropriate to apply the isotropic elasticity assumption to all the simulations reported in the present paper.

Figure 3 shows the predicted stress and strain curves of the four initial textures under uniaxial compression along the RD. The result for texture 3 and its comparison with the corresponding experimental result have been represented in Fig. 2. The most striking observation from Fig. 3 is that the maximum stress increases with increasing basal texture. The difference in the maximum stress between the various initial textures seems to relate to the difference in the rapid hardening between the initial textures. The stronger the basal texture, the more rapid the strain hardening. It is found that the rapid hardening starts at around a strain of 0.04 for all the

initial textures considered. It should be noted that the shear strain of 0.1289 associated with tensile twinning and the value of $A_1 = 0.60$ correspond to a maximum axial strain of about 0.04.

The effects of initial texture and tensile twinning on the rapid hardening are more clearly exhibited in Fig. 4, which shows the normalized hardening rate ($\frac{d\sigma/d\varepsilon}{E}$) as a function of axial strain ε . It is found that in the case of ideal basal texture (texture 1) the work hardening rate can rapidly increase to a value close to E . The predicted maximum hardening rates, during the rapid hardening stage, are $0.4E$, $0.3E$ and $0.1E$ for the very strong basal texture (texture 2), strong basal texture (texture 3) and random texture (texture 4), respectively. For a comparison, the experimental hardening rate for the strong basal texture (texture 3) is also included. It is found that the EVPSC-TDT model accurately describes the rapid hardening. Fig. 4 also strongly suggests that the maximum hardening rate is proportional to the sharpness of the basal texture (see Fig. 1). On the other hand, it could be rationalized that the basal texture intensity will affect the fraction of orientations favoring the tensile twinning and thus eventually influences the hardening rate in the rapid hardening stage. The intensity is calculated as the ratio of the number of grains with a maximum orientational difference to the ideal basal orientation of less than 15° , to the total number of grains. The ideal grain orientation (texture 1) corresponds to perfect alignment of the basal pole with the ND. The calculated basal texture intensities are 5%, 36% and 68% respectively for texture 4 (random texture), texture 3 (strong basal texture) and texture 2 (very strong basal texture), while 100% for texture 1 (ideal basal orientation). The results shown in Fig. 4 imply that the maximum hardening rate is proportional to the basal intensity and there is a nonlinear relationship between the volume fraction of grains which are prone to undergo twinning and the maximum hardening rate. A question then arises: how initial texture and tensile twinning induce the rapid hardening shown in Figs. 3 and 4?

Figure 5 presents relative activities of slip/twinning for the four initial textures under uniaxial compression along the RD. For the sheet with strong basal texture (texture 3), it is found that at strains $|\varepsilon| < 0.04$, plasticity is accommodated by tensile twinning and Basal slip. When the tensile twinning activity is dramatically reduced, at a strain $\varepsilon \approx -0.04$, the Basal slip and Prismatic slip activities significantly increase until $\varepsilon \approx -0.055$. After that, the activity of Prismatic slip decreases slowly with increasing strain, while the activities of Basal slip and Pyramidal slip increases steadily. For the random texture, Basal slip is the most important contributor, and the predicted activities in Prismatic slip and Pyramidal slip are low throughout the deformation process. The predicted activity of tensile twinning is significant and contributes about 17% of the plastic deformation at strains $|\varepsilon| < 0.04$. After that, its activity decreases and it becomes essentially inactive at strains $|\varepsilon| > 0.10$. For the ideal basal texture, the tensile twinning dominates the plastic deformation with very little activity of Basal slip at small strains. When the tensile twinning activity dramatically reduces, at a strain $\varepsilon \approx -0.04$, the Basal slip activity rapidly increases and almost vertically jumps to nearly 100%. Shortly after the peak, the EVPSC-TDT model predicts that the activity of Basal slip decreases rapidly to a very low level. Meanwhile, the Prismatic slip increases its activity dramatically to around 80% and then decreases quickly to about 50%. During the rapid decrease of the activity in Prismatic slip, the activity of Pyramidal slip increases significantly up to about 42%. At large strains, the single crystal deforms mainly through the Prismatic and Pyramidal slips with little contribution of Basal slip. The predicted activities for the sheet with very strong basal texture (texture 2) are found to be between those for the sheet with strong basal texture (texture 3) and the ideal basal texture (texture 1). The predicted activity levels have been validated by previous studies of internal strain (Wu et al.

[40]) and texture evolution (Wang et al. [50]), during deformation of Mg alloy polycrystals with texture strengths similar to texture 2 or texture 3.

From Fig. 5, it becomes clear that at small strains the stronger the basal texture the more active the tensile twinning. Consequently, the twin volume fraction increases with increasing basal texture. At large strains, the activity of Basal slip decreases with increasing the basal texture. Dramatic changes in relative activities in slip/twinning are found at a strain $\varepsilon \approx -0.04$, where the tensile twinning is nearly exhausted. Notably, the EVPSC-TDT model predictions of twin volume fraction have been experimentally validated for a number of different Mg alloys and textures (Wang et al. [37, 50]; Wu et al. [19]).

It is believed by many that the rapid hardening is due to the exhaustion of twinning and the activation of the Pyramidal slip, since the CRSS of the latter is much higher than the basal slip and tensile twinning. However, comparing Fig. 3 with Fig. 4 shows that the Pyramidal slip is not activated until after the rapid hardening occurred. In other words, the strain interval from the moment of rapid hardening occurs to the activation of the Pyramidal slip is short but noticeable. On the other hand, it is noticed that during the rapid hardening the hardening rate can reach a value which approaches E , in the case of the ideal basal texture under uniaxial compression. Such a high hardening rate cannot be explained solely by the activation of Pyramidal slip. Rather, slip activation would lead to a lowering of the observed hardening rate. Thus, this extremely high hardening rate must, to some extent, be associated with elastic deformation. The necessary condition for verifying this hypothesis is that during the rapid hardening the plastic strain rate must be relatively small and the elastic strain rate is of a significant portion of the imposed/applied strain rate.

Figure 6 shows the normalized macroscopic plastic strain rate $\frac{D_{11}^p}{D_{11}}$ (dashed lines), and normalized macroscopic elastic strain rate $\frac{D_{11}^e}{D_{11}}$ (solid lines) along the RD. Note that $D_{11} = \dot{\varepsilon} = 5 \times 10^{-3} s^{-1}$ is the applied strain rate under uniaxial compression along the RD. At the initial elastic-plastic transition, the normalized elastic strain rate decreases and plastic strain rate increases rapidly. After the initial macroscopic yield stress and at strains $|\varepsilon| < 0.04$, the imposed deformation is essentially accommodated by the plastic deformation and the elastic strain rate is very small. During the rapid hardening, the normalized elastic strain rate increases dramatically, while the plastic strain rate decreases quickly. For the ideal basal texture (texture 1), the normalized elastic strain rate approaches one. This implies that the deformation is nearly entirely elastic. The changes in the normalized elastic and plastic strain rates decrease with decreasing the basal texture. However, even in the sheet with a random texture (texture 4) the normalized elastic strain rate is appreciable. The predicted maximum normalized elastic strain rates are 0.4, 0.3 and 0.1 for the very strong basal texture (texture 2), strong basal texture (texture 3) and random texture (texture 4), respectively. It is interesting to note that the trend of the predicted normalized hardening rate shown in Fig. 4 seems to follow the normalized elastic strain rate exhibited in Fig. 6.

Figure 7 shows the predicted normalized hardening rate $\frac{d\sigma/d\varepsilon}{E}$ (thin black solid lines) and normalized elastic strain rate $\frac{D_{11}^e}{D_{11}}$ (thick red dashed lines) as a function of the applied axial strain. It is clear that the $(\frac{d\sigma/d\varepsilon}{E} \sim \varepsilon)$ and $(\frac{D_{11}^e}{D_{11}} \sim \varepsilon)$ curves are almost on top each other for all

the four initial textures considered. The relationship between the hardening rate and elastic strain rate can be easily understood by applying classical plasticity to analyze one-dimensional elastic-plastic behaviour. Assume that σ and ε are the true stress and true strain along the loading direction, and that $\dot{\varepsilon}_e$ and $\dot{\varepsilon}_p$ are the elastic and plastic strain rate, respectively. The elastic constitutive model gives

$$\dot{\sigma} = E\dot{\varepsilon}_e \quad (6)$$

The hardening rate can be written as

$$\frac{d\sigma}{d\varepsilon} = \frac{d\sigma}{dt} \frac{dt}{d\varepsilon} = \frac{\dot{\sigma}}{\dot{\varepsilon}} = \frac{E\dot{\varepsilon}_e}{\dot{\varepsilon}} \quad (7)$$

Thus

$$\frac{d\sigma/d\varepsilon}{E} = \frac{\dot{\varepsilon}_e}{\dot{\varepsilon}} \quad (8)$$

The results shown in Fig. 7 strongly suggest that the rapid hardening is associated with the elastic straining.

To further verify the hypothesis that the rapid hardening is associated with elastic straining, Fig. 8 presents the predicted relative activities of slip/twinning modes in the matrix and twinned regions for the ideal basal texture. Note that the total relative activities were already shown in Fig. 5. The relative activity of twinning in the matrix is due to Operation A (the twin nucleation and formation of a twin band), while the relative activity of twinning in the twinned region is from Operation B (a propagation of the twin into the matrix). From Fig. 8, it is clear that, after the rapid hardening and at relatively large strains, the plastic deformation in the matrix is dominated by the Prismatic slip, which has the second highest CRSS (75 MPa) among all the plastic deformation modes considered. The plastic deformation in the twinned region is mainly accommodated by the Pyramidal slip, which has the highest CRSS (140 MPa), with a little help

from the Basal slip. A careful observation indicates that the Prismatic slip is initiated in the matrix before the Pyramidal slip is activated in the twinned region (see Fig. 5).

From the numerical results presented above, it is observed that, for an Mg alloy sheet with a typical basal texture under in-plane uniaxial compression, the c -axes of a considerable number of grains must undergo extension. Therefore, tensile twinning makes a significant contribution to initial yielding and the plateau in the macroscopic stress strain curve immediate post-yielding. During this deformation stage, the easily activated Basal slip also accommodates plastic deformation. The relative activities of Prismatic and Pyramidal slips are almost zero or very small. Upon the exhaustion of the tensile twinning, further deformation of the sheet requires the activation of Prismatic and Pyramidal slip modes, which have relative high CRSS. However, the stress level at the exhaustion of the tensile twinning is not high enough to activate Prismatic and Pyramidal slips. Thus, the imposed strain increments must be accommodated by elastic deformations. *In other words, after the exhaustion of the tensile twinning and before the activation of Prismatic and Pyramidal slips, the grain behaves like an elastic inclusion.* The overall hardening of the polycrystal is proportional to the volume fraction of such elastic inclusions (see e.g. Taya et al. [51]).

Finally, it is worth mentioning that for a rolled magnesium sheet under cyclic loading (compression and then tension) along the RD, tensile twinning and de-twinning are activated in the initial compression and subsequent tension, respectively. More specifically, the initial loading in compression activates twinning. During the compressive unloading and tensile-reloading process detwinning dominates the response. Rapid hardening occurs again during the tensile straining, once the detwinning operation is complete (see e.g., Wu et al. [40] and Wang et al. [50]). Fig. 9 shows the measured and calculated stress and strain curves of an AZ31B sheet

with very strong basal texture under cyclic loading along the RD (Fig. 9a), and the normalized hardening rate and elastic strain rate as functions of accumulated strain (Fig. 9b). The experimental data are taken from Wu et al. [40], and the values of the hardening parameters are from Guo et al. [39]. Both the first rapid hardening during the initial compression (upon the exhaustion of the tensile twinning) and the second rapid hardening regime which occurs during the tensile straining (once the detwinning operation is complete, i.e., exhausted) are associated with the elastic straining.

4. Conclusions

Using the EVPSC-TDT model, we have numerically studied the relationship between the exhaustion of twinning and the observed rapid hardening in magnesium alloys under twinning dominated conditions. It has been found that upon the exhaustion of the tensile twinning, further deformation of the material requires activation of Prismatic and Pyramidal slip modes, which have relative high CRSS. However, the stress level at the exhaustion of the tensile twinning is not high enough to activate Prismatic and Pyramidal slips. It has been numerically demonstrated that, in the strain (or time) interval from the exhaustion of twinning to the activation of Prismatic and Pyramidal slip modes, the imposed strain increments are mainly accommodated by elastic deformations. Since the rapid hardening occurs during the same interval, it has been concluded that the rapid hardening is associated with elasticity.

Acknowledgement

P.D. Wu and H. Qiao were supported by the Natural Sciences and Engineering Research Council of Canada (NSERC). X.Q. Guo was supported by the National Basic Research Program of China (2007CB209400) and the 111 Project of China (B07028). S.R. Agnew would like to thank the National Science Foundation of the U.S.A., grant number CMMI 1235259.

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Figure Captions

- Figure 1. Initial textures presented in terms of the $\{0001\}$ pole figure. Textures 1-4 are, from left to right, an ideal orientation with Euler angles $(30^\circ, 0^\circ, 0^\circ)$, a very strong basal texture of AZ31B from Wu et al. [49], a strong basal texture of AZ31B from Jain and Agnew [47] and a random texture.
- Figure 2. Measured (symbols) and calculated (solid lines) stress and strain curves under uniaxial compression and tension along the RD. The initial texture (texture 3 in Fig. 1) and experimental stress and strain data are from Jain and Agnew [47].
- Figure 3. Calculated effect of initial texture on stress and strain curve under uniaxial compression along the RD.
- Figure 4. Calculated effect of initial texture on work hardening rate under uniaxial compression along the RD. The experimental data (open circles) for texture 3 are from Jain and Agnew [47].
- Figure 5. Calculated effect of initial texture on relative activities of the slip modes and tensile twinning under uniaxial compression along the RD.
- Figure 6. Calculated effect of initial texture on normalized plastic strain rate (dashed lines) and elastic strain rate (solid lines) under uniaxial compression along the RD.
- Figure 7. Calculated normalized hardening rate (thin black solid lines) and normalized elastic strain rate (thick red dashed lines) under uniaxial compression along the RD.
- Figure 8. Calculated relative activities of the slip modes and tensile twinning in the matrix and twins for the ideal basal texture. Note that the total of the relative activities were presented in Figure 5.
- Figure 9. Measured and calculated stress and strain curves of an AZ31B sheet with very strong basal texture under cyclic loading along the RD (a), and the normalized hardening rate and elastic strain rate as functions of accumulated strain (b). The experimental data are taken from Wu et al. [40], and the values of the hardening parameters are from Guo et al. [39].

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Table 1. List of values of the hardening parameters involved in the EVPSC-TDT model.

Mode	τ_0 (MPa)	τ_1 (MPa)	h_0 (MPa)	h_1 (MPa)	$h^{a\beta}$	A_1	A_2
Basal	10	1	500	0	4		
Prismatic	75	50	450	0	4		
Pyramidal	140	65	2500	0	2		
Extension twin	42	0	0	0	4	0.60	0.0