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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.

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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 behaviour. 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 $\{10\overline{1}2\} < 10\overline{1}1$ > 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

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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 worksoftening, 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 plateautype 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.







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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 feathers.

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

 $(s^{\alpha}, \mathbf{n}^{\alpha})$, with s^{α} and \mathbf{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 $\langle a \rangle (\{0001\}\langle 11\overline{2}0 \rangle)$, Prismatic $\langle a \rangle (\{10\overline{1}0\}\langle 11\overline{2}0 \rangle)$ and Pyramidal $\langle c + a \rangle (\{\overline{1}122\}\langle \overline{1}123 \rangle$ slip systems, and the $\{10\overline{1}2\}\langle \overline{1}011 \rangle$ extension twin system.

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

$$\boldsymbol{d}^{p} = \sum_{\alpha} \dot{\gamma}^{\alpha} \boldsymbol{P}^{\alpha} \tag{1}$$

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,

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

For twinning,

$$\dot{\gamma}^{\alpha} = \begin{cases} \dot{\gamma}_{0} |\tau^{\alpha} / \tau^{\alpha}_{cr}|^{\frac{1}{m}} & \tau^{\alpha} > 0\\ 0 & \tau^{\alpha} \le 0 \end{cases}$$
(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 through re-twinning. 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:

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

where $\Gamma = \sum\limits_{eta} \int \lvert \dot{\gamma}^lpha
vert \mathrm{d}t$ 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:

$$\widehat{\tau}^{\alpha} = \tau_0^{\alpha} + \left(\tau_1^{\alpha} + h_1^{\alpha}\Gamma\right) \left(1 - \exp\left(-\frac{h_0^{\alpha}}{\tau_1^{\alpha}}\Gamma\right)\right)$$
(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 $V^{th} = \min\left(1.0, A_1 + A_2 \frac{V^{eff}}{V^{acc}}\right)$, where A_1 and A_2 are two material constants. Although it is not employed in the present work, a single

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