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A new empirical equation for termination of twinning in magnesium alloys

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ABSTRACT

Since it is rare that a grain can be fully twinned, an empirical equation has been introduced in the current crystal plasticity models to terminate twinning within that grain. In the present paper, a new empirical equation for describing the termination of twinning in magnesium alloys is developed. The new description introduces only a single parameter, while the widely used empirical equation involves two parameters. It is demonstrated that it is easy to calibrate the single parameter and the proposed empirical equation is able to accurately simulate the experimentally observed rapid hardening associated with the twinning exhaustion.

Plastic deformation in Magnesium (Mg) and its alloys is accommodated by both slip and twinning. The most commonly observed twinning mode is the $\{10\bar{1}2\}<10\bar{1}1>$ extension twinning. Intensive research has been recently focused on the role of twinning in plastic deformation of Mg alloys (see [1–13]). Based upon acoustic emission data [1,3,4,12], it has been generally accepted that under twinning dominated conditions, the yielding and immediate post-yielding plasticity is governed largely by twin nucleation, whereas plastic deformation at higher strains is governed by twin growth and dislocation slip. After a region of low stress and low strain hardening, the material hardens rapidly resulting in an S-shaped flow curve. This is associated with two aspects: the radical texture evolution due to extensive extension twinning and the exhaustion of twinning as a strain accommodation mechanism. Therefore, to perform accurate deformation process modeling, it is important to develop constitutive models which properly account for reorientation due to twinning and twinning exhaustion. Different schemes for modeling the effect of twinning have been proposed, including the widely used predominant twin reorientation (PTR) scheme (Tomé et al. [14]) and the recently developed twinning and de-twinning (TDT) model (Wang et al. [15,16]).

In both the PTR and TDT models, a threshold twin volume fraction is defined to terminate twinning because it is rare that a grain can be fully twinned. Correspondingly, the models introduce two statistical variables: accumulated twin fraction V_{acc} and effective twinned fraction V_{eff}, with V_{acc} and V_{eff} being respectively the weighted volume fraction of the twinned region and volume fraction of grain in which twinning is exhausted. The threshold volume fraction V_{th} is defined as

$$V_{th} = \min\left(1.0, A_1 + A_2 \frac{V_{eff}}{Vacc}\right) \tag{1}$$

where A_1 and A_2 are two parameters. It has been demonstrated that the above equation is able to simulate experimental flow curves for Mg alloys by carefully calibrating the two parameters. However, it has been noticed that values of the fitted A_1 and A_2adopt a wide range of values, are difficult to be determined, and have no clear connection with a physical process. It is important to point out that the PTR model considers only the twin variant with the maximum Schmid factor (SF), while the TDT model considers all possible twin variants. Furthermore, the TDT model considers a twin as a new grain. The orientation of the new grain is initially related to that of the parent through the crystallographic twin relation, and the volume fraction associated with the new grain is updated at the end of the first straining step in which the twin variant is activated. Therefore, even considering only the $\{10\bar{1}2\}$ extension twinning mode, a parent grain could potentially become seven grains (parent plus six twins). In the PTR model, the number of grains remains fixed throughout the simulation, which gives it a computational advantage, though there is a compromise in the fidelity of the results.

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After carefully reviewing recent crystal plasticity based modeling of plastic deformations of Mg alloys, a new empirical equation to terminate twinning is proposed. For a given grain g, assume that f_g^α is the twin volume fraction of extension twinning system $\alpha(\alpha=1,6)$, and $V_{th,g}^\alpha$ is its threshold value. Consequently, twinning is terminated by $f_g^\alpha = V_{th,g}^\alpha$ or $\sum_\alpha f_g^\alpha = 1$, where the latter condition corresponds to the point where the entire parent grain has been consumed. We define $V_{th,g}^\alpha$ as

$$V_{th,g}^{\alpha} = \begin{cases} A\left(\dfrac{m_g^\alpha}{m_g^{\alpha_{\max}}}\right)^5 & \alpha \neq \alpha_{\max} \\ A + \dfrac{m_g^{\alpha_{\max}}}{0.5}\dfrac{\overline{V}_{eff}}{V_{acc}} & \alpha = \alpha_{\max} \end{cases} \tag{2}$$

Here, m_g^α denotes the Schmid Factor (SF) of twinning system α at the beginning of loading, $\alpha_{\max}$ is the twinning system with the maximum value of the SF, $m_g^{\alpha_{\max}}$. Same as in Eq. (1) V_{acc} is the accumulated twin fraction in the aggregate and is written as $V_{acc} = \sum_g (w_g \sum_\alpha f_g^\alpha)$, with w_g being the weight or volume fraction of the grain g in the aggregate. In Eq. (2) $\overline{V}_{eff}$ is the effective twinned fraction defined by $\overline{V}_{eff} = \sum_g (w_g \sum_\alpha f_g^{\alpha,T})$, with $\int_g^{a,T}$ denoting the twin volume fraction of the twinningsystem α in which twinning has been terminated. It is noted that in Eq. (1) used in the PTR and TDT approaches, $V_{eff} = \sum_g w_g$ for those grains in which twinning has been terminated. This implies that if $\sum_\alpha f_g^{\alpha,T} = 1$ is assumed, $\overline{V}_{eff}$ in Eq. (1) reduces to Veff in Eq. (1).

It is important to point out that the popular empirical equation, Eq. (1), is applied at the grain level, while the proposed new empirical equation is at the twinning system level. According to the proposed empirical formulation, for a given grain g, twinning system α is terminated when $f_g^\alpha = V_{th,g}^\alpha$. However, the other twinning systems in the grain can be still active if $\sum_\alpha f_g^\alpha < 1$. Therefore, for a given grain, while twinning exhaustion is a sudden event according to Eq. (1), twinning exhaustion described by Eq. (2) is a gradual process, which more closely approximates what is observed physically. It is also important to note that since the proposed new empirical equation is at the twinning system level, the new empirical equation can be applied only to the TDT model.

For the twinning system having the maximum SF, $(\frac{m_g^{\alpha_{\max}}}{0.5})$ is used in Eq. (2). This is rationalized that the threshold volume fraction should scale with the SF. It is important to note that the term $(\frac{m_g^\alpha}{m_g^{\alpha_{\max}}})^5$ is used in Eq. (2) for the twinning systems other than the one with the maximum SF. This implies that a twinning system with a very low SF should not still be active at large strains. It is also important to mention that in the early stage of the development of the proposed empirical Eq. (2), the power of $(\frac{m_g^\alpha}{m_g^{\alpha_{\max}}})$ was a free parameter. We have carried out a detailed parametrical study to assess effects of the power on the calculated stress-strain response and twin volume fraction. For example, for an extruded AZ31 cylinder under uniaxial compression along the extrusion direction (this material will be studied in Fig. 2), it was found that at small strains the power has a negligible effect. At strains larger than 0.06, the predicted twin volume fraction decreases with increasing the power, while the predicted stress-strain curve is not very sensitive to the power. This implies that a high power will significantly reduce the non-maximum system contribution. It is noted that Pei et al. [17] investigated activities of the extension twin variants in a commercially available AZ31 sheet under uniaxial compression along the RD. They found that at a strain of 5% approximately 30% of the examined grains contain twins corresponding to twin variants with the third or lower ranked SF. This figure increases to 40% for samples deformed to 10% compression. Probabilistic meaningful statistics, such as the one reported by Beyerlein et al. [18] for Mg, show results consistent with those reported by Pei et al. [17]. Eq. (2) suppresses twin variants with very low SF but allows the other twin variants, those with their SFs not being significantly lower than the highest SF, to be active at large strains. Surprisingly, fixing the value of the power at 5 and employing A as a fitting parameter, Eq. (2), could accurately simulate the mechanical behaviour of all the Mg alloys examined.

The proposed new empirical equation, Eq. (2), has been implemented in the elastic visco-plastic self-consistent (EVPSC) model (Wang et al. [19]), with the recently developed twinning and detwinning (TDT) description (Wang et al. [15,16]). In addition, it has been shown that, among the popular self-consistent schemes examined, the Affine self-consistent scheme gives the best overall performance for Mg alloys (Wang et al. [20]), while both the Affine and M_{eff} schemes are suitable for Zr alloys (Qiao et al. [21]). Therefore, the Affine self-consistent scheme is applied in the present study.

The proposed empirical equation is validated by applying it to (1) three typical wrought Mg alloys: a rolled AZ31B plate, an extruded AZ31 cylinder and an extruded ZK60 sheet; and to (2) a cast Mg alloy AZ80. The three Mg alloys have previously been studied based on the EVPSC-TDT model, with Eq. (1) being used for termination of twinning. On the other hand, the behaviour of cast Mg alloy AZ80 has been studied previously using the VPSC-PTR model by Jain et al. [22]. In all the simulations reported in the present paper, we consider slip in the Basal $\{0001\}\langle 11\bar{2}0\rangle$, Prismatic $\{10\bar{1}0\}\langle 11\bar{2}0\rangle$, and Pyramidal $\{\bar{1}\bar{1}22\}\langle\bar{1}\bar{1}23\rangle$ slip systems, and twinning in the $\{10\bar{1}2\}\langle\bar{1}011\rangle$ extension twinning system.

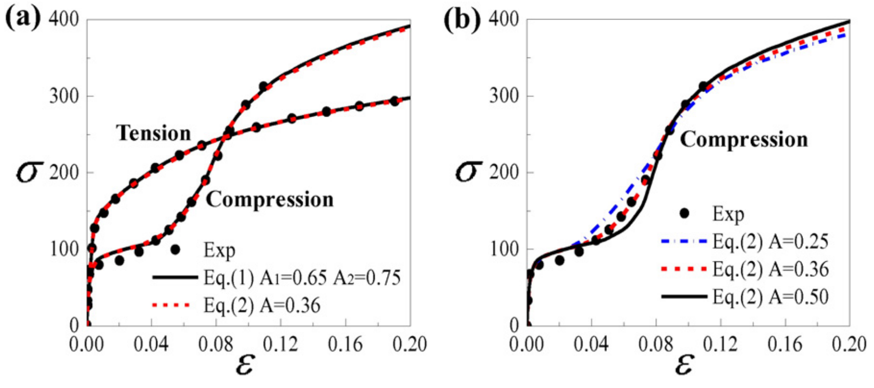

Fig. 1. Measured (symbols) and simulated (solid lines are based on Eq. (1) with $A_1 = 0.65$ and $A_2 = 0.75$, and dashed lines are according to Eq. (2) with $A = 0.36$) true stress and true strain curves under uniaxial tension and compression along the RD (a), and predicted effect of parameter A on flow curve of uniaxial compression along the RD (b) for a H24-temper AZ31B sheet. The experimental data are taken from Guo et al. [23].