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Modelling the role of slips and twins in magnesium alloys under cyclic shear

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ABSTRACT

Magnesium alloys under cyclic shear show different deformation behaviour from that under cyclic tension–compression, for example, symmetry vs. asymmetry of stress–strain curves. Using the Twinning–DeTwinning (TDT) model, we studied the role of different deformation mechanisms, slip systems, twinning and detwinning, in shear deformation behaviour of magnesium alloys. The results indicate that the nearly symmetrical shear stress-shear strain curve unlike the asymmetrical stress–strain curve under cyclic tension–compression is ascribed to the dominated prismatic slips and the simultaneous activation of deformation twinning and detwinning under reverse shear. The typical shear texture observed in experiments is ascribed to the activation of extension twin that induces the extension strain along normal direction of the shear plane under simple shear.

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1. Introduction

Magnesium (Mg) alloys are the lightest structural materials but have poor formability at room temperature because of insufficient available deformation mechanisms. Modelling deformation behaviour of Mg alloys under different loading conditions will provide insights into fabricating structural components. Under complex strain paths, such as cyclic tension–compression and strain path changes, detwinning is activated and induces the characteristic phenomena: unsymmetrical hysteresis loops of stress strain curves [1–7], inelasticity during unloading [7–10], and the low yield stress upon load reversals [10,12], etc. Employing the Twinning–DeTwinning (TDT) models [12–15], these characters have been correctly captured and understood in terms of the activity of twinning and detwinning.

Magnesium alloys under cyclic shear show different deformation behaviour from that under cyclic tension–compression, for example, symmetry vs. asymmetry of stress–strain curves [6,16,17]. Lou et al. [1] and Zhang et al. [17] conducted cyclic shear and torsion of magnesium alloys and found that the unsymmetrical hysteresis loops of the stress strain curves during cyclic tension–compression were not apparent under cyclic shear/torsion even at large deformation. Zhang et al. [18] experimentally observed that simple shear could improve the ductility of magnesium alloys and ascribed this to the activity of deformation twinning. In addition, twinning also results in a plastic deformation perpendicular to the shear plane during shear or torsion of Mg alloys [1,20–28]. Zhang et al. [18] also observed that the basal pole in the (0002) pole figure tends to rotate 45° away from the RD after simple shearing along the RD. They ascribed this to the high activity of prismatic slip systems as suggested by Kang et al. [28]. According to these experimental observations, the difference in deformation behaviour of Mg alloys between cyclic shear and compression–tension loadings has been qualitatively ascribed to the change in the relative activity of slip systems, twinning and detwinning [2,18]. However, the quantitative study is rare to explore the role of different deformation mechanisms in deformation behaviour of Mg alloys under cyclic shear. This is because of the lack in modelling tools that incorporate both twinning and detwinning mechanisms. The Twinning and DeTwinning (TDT) model [13,15] has been examined for Mg alloys under different loadings and is able to capture the role of both twinning and detwinning in plastic deformation [13]. The purpose of this work is to examine the role of different deformation mechanisms in the cyclic shear of magnesium alloys. Mechanical behaviour of AZ31B sheet is simulated using the TDT model under cyclic shear loading, including stress strain curve, activity of deformation mechanisms, and evolution of twin volume fraction and texture.

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2. Deformation mechanisms under shear deformation

Magnesium alloy sheets exhibit strong basal texture with *c*-axis nearly perpendicular to the sheet plane while *a*-axis randomly distributed in the sheet plane (Fig. 1). Each grain is subjected to pure shear, i.e., the non-zero stress components of each grain are $\sigma_{12} = \sigma_{21} = \sigma$ (where τ is the applied shear stress; 1 refers to rolling direction (RD), 2 refers to transverse direction (TD), and 3 refers to normal direction (ND)).

The activity of different deformation mechanisms can be predicted according to Schmidt factor analysis. For a grain oriented as shown in Fig. 1a, the three basal slip systems are described as the slip direction $\boldsymbol{s}^{\alpha} = (\cos\phi,\ \sin\phi,\ 0)$ with $\phi = \theta$, $\theta + 60°$, $\theta + 120°$ and the same normal direction $\boldsymbol{n}^{\alpha} = (0,\ 0,\ 1)$. Therefore basal slip systems will not be activated because the resolved shear stress $\tau^{\alpha} = \boldsymbol{s}^{\alpha} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{n}^{\alpha}$ is equal to zero. For the three prismatic slip systems, $\boldsymbol{s}^{\alpha} = (\cos\phi, \sin\phi, 0)$ and $\boldsymbol{n}^{\alpha} = (-\sin\phi, \cos\phi, 0)$, the resolved shear stress is equal to $\tau^{\alpha} = \tau\cos 2\phi$ with respect to $\phi = \theta$, $\theta + 60°$, $\theta + 120°$. The pyramidal slip systems are rarely activated and thus are not considered here because of its low mobility. For six extension twins, $\boldsymbol{s}^{\alpha} = \left(\frac{\sqrt{3}a}{\rho}\sin\phi,\ -\frac{\sqrt{3}a}{\rho}\cos\phi,\ \frac{c}{\rho}\right)$ and $\boldsymbol{n}^{\alpha} = \left(-\frac{c}{\rho}\sin\phi,\ \frac{c}{\rho}\cos\phi,\ \frac{\sqrt{3}a}{\rho}\right)$ with respect to $\phi = \theta$, $\theta + 60°$, $\theta + 120°$, $\theta + 180°$, $\theta + 240°$, $\theta + 300°$, the resolved shear stress is equal to $\tau^{\alpha} = \frac{\sqrt{3}a}{\rho}\tau\sin 2\phi \approx \frac{1}{2}\tau\sin 2\phi$, where $\rho = \sqrt{3a^2 + c^2}$. The factor τ^{α}/τ is plotted in Fig. 1b as a function of 2θ. Unlike unidirectional twinning in Mg, gliding dislocations can be activated regardless of the sign of τ^{α}/τ, the absolute value of τ^{α}/τ is plotted in Fig. 1b for prismatic slip systems. The shadows indicate the ranges of τ^{α}/τ under pure shear. The range of the factor τ^{α}/τ associated with prismatic slip systems with highest possibility of activation is from 0.866 to 1, while that for extension twins is from 0.25 to 0.5 and −0.5 to −0.25. During cyclic shear, shear stress reversal does not change the activity of prismatic slip systems but changes the activity of twinning. Twinning only takes place in a grain where the resolved shear stress is positive and detwinning only takes place in a twinned grain where the resolved shear stress is negative. Therefore the activity of extension twin will be nearly doubled upon shear stress reversal. Of course, their relative activities among prismatic slip systems, twinning, and detwinning depend on their critical resolved shear stresses (CRSSs).

3. TDT model

TDT model [13,15] has been developed to deal with twinning and detwinning deformation mechanisms according to deformation physics including twin nucleation, twin growth, twin shrinkage and re-twinning that retain the glide of twinning dislocations (TDs). TDs including their characteristics and mobility have been studied and characterized at atomic scale by using high resolution transmission electron microscopy and molecular dynamics simulations [29–35]. Under a loading that enables twinning, twin nucleation (TN) creates a fresh twin in a grain and the grain is then split into an untwinned domain (matrix) and a twinned domain (twin). The nucleated twin grows according to Eqs. (1) and (2) under the resolved shear stress associated with TDs. With respect to the resolved shear stress computed in the matrix and in the twin, the migration of twin boundaries results matrix reduction (MR) and twin propagation (TP), respectively. Detwinning can be accomplished through two mechanisms, twin shrinkage and re-twinning. Twin shrinkage is the reverse mechanism of twin growth and re-twinning (RT) corresponds to twin nucleation in a twin. Again, with respect to the resolved shear stress computed in the matrix and in the twin, twin shrinkage includes matrix propagation (MP) and twin reduction (TR), respectively. TDT model has been implemented into the elastic viscoplastic self-consistent (EVPSC) model [35], named as EVPSC-TDT that has been successfully employed in modelling plastic deformation of magnesium alloys under different loadings [13,22,23,36–42]. Associated with each operation, the shear rates are expressed as:

$$\dot{\gamma}_I^{\alpha} = \begin{cases} \dot{\gamma}_0\left|\tau^{\alpha}/\tau_{cr}^{\alpha}\right|^{1/m} & \tau^{\alpha} > 0 \\ 0 & \tau^{\alpha} \le 0 \end{cases} \quad \text{if} \quad I = TN,\ TP,\ MP,\ RT \tag{1}$$

$$\dot{\gamma}_I^{\alpha} = \begin{cases} -\dot{\gamma}_0\left|\tau^{\alpha}/\tau_{cr}^{\alpha}\right|^{1/m} & \tau^{\alpha} < 0 \\ 0 & \tau^{\alpha} \ge 0 \end{cases} \quad \text{if} \quad I = MR,\ TR \tag{2}$$

where $\dot{\gamma}_0$ and m are constants of the reference shear rate and the rate sensitivity, and τ^{α} and τ_{cr}^{α} are the resolved shear stress and the threshold shear stress, respectively. The evolution of the threshold shear stress for each slip or twinning system is described by the extended Voce-hardening law as

$$\hat{\tau}^{\alpha} = \tau_0^{\alpha} + \left(\tau_1^{\alpha} + \theta_1^{\alpha}\Gamma\right)\left(1 - \exp\left(-\theta_0^{\alpha}\Gamma/\tau_1^{\alpha}\right)\right) \tag{3}$$

Here τ_0^{α}, τ_1^{α}, θ_0^{α} and θ_1^{α} are the associated hardening parameters, and $\Gamma = \sum_{\alpha}\int\dot{\gamma}^{\alpha}dt$ is the accumulated shear strain.

The twin volume fractions associated with twin nucleation and re-twinning are small, the net evolution of the twin volume fraction f^{α} is mainly due to twin growth (MR and TP) and twin shrinkage (MP and TR):

$$\dot{f}^{\alpha} = \left(1 - \sum_{\beta} f^{\beta}\right)\left(\left|\dot{\gamma}_{MR}^{\alpha}\right| - \left|\dot{\gamma}_{MP}^{\alpha}\right|\right)/\gamma^{tw} + f^{\alpha}\left(\left|\dot{\gamma}_{TP}^{\alpha}\right| - \left|\dot{\gamma}_{TR}^{\alpha}\right|\right)/\gamma^{tw} \tag{4}$$

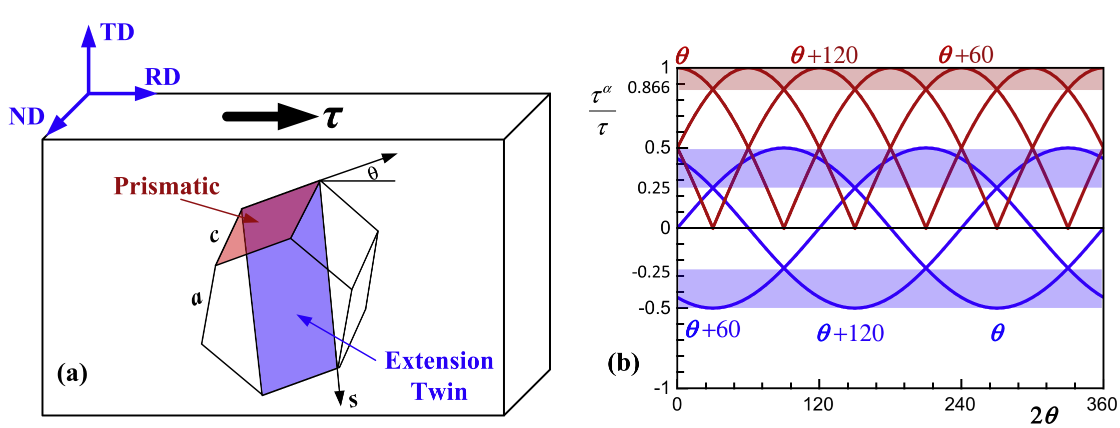

Fig. 1. (a) Schematic of magnesium alloy sheets under shear, showing orientation of grains with respect to shear; (b) the factor τ^{α}/τ as a function of 2θ with respect to prismatic slip systems (red) and twinning systems (blue). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)