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MODELLING OF PLASTIC DEFORMATION IN MAGNESIUM

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ABSTRACT: In the present contribution, a viscoplastic rate-dependent constitutive model based on Schmid's law has been used to designate the activity level of pure magnesium deformation systems. A crystal plasticity model in the framework of finite elements was used to investigate the deformation systems on the scale of single- and polycrystals. Twinning has been modelled by coupling between finite shear and subsequent lattice rotation. It is shown for pure magnesium, that twinning can affect the slip systems activities and therefore changes the hardening mode within the crystal as a result of crystal reorientation. Furthermore, the twinning evolution during in plane and through-thickness deformation of pure Mg polycrystal rolled plate reveals that tensile {10-12} and compression {10-11} twinning have different effects on the mechanical response.

KEYWORDS: Crystal Plasticity, Magnesium, Twinning, Reorientation

1 INTRODUCTION

To model the macroscopic mechanical response of magnesium, it is essential to understand the behaviour of its micromechanical deformation systems. Pioneering research on magnesium revealed that basal $\langle a \rangle$ and prismatic $\langle a \rangle$ slip systems are active on close packed plane [1-2]. Wonsiewicz and Backofen conducted channel die tests on pure magnesium single crystals [3]. They showed that contraction along the c-axis was accommodated by twinning on {10-11} followed by twinning on {10-12} which results in a small amount of shear and reorients basal planes. Then larger strains are accommodated by basal deformation inside the twinned volume. Furthermore, extension of the c-axis activates twinning on {10-12}. Later investigations on magnesium single crystals by uniaxial loading of its c-axis, raised evidences about activity of pyramidal slip system $\langle a+c \rangle$, [4]. Those authors observed that $\langle a+c \rangle$ pyramidal system induces shear strain along the c-axis in room temperature up to 0.03 macroscopic strains [4]. Recently Clausen et al, have used an extended version of elasto-plastic self consistent method to account for activation, reorientation and stress relaxation associated with twinning in magnesium [5]. The present authors use a crystal plasticity model in the framework of finite elements to investigate the deformation systems on the scale of single- and polycrystals. Twinning has been modelled by coupling between finite shear and subsequent lattice rotation. The key contribution of this approach is using the geometrical effect of twinning to describe macroscopic hardening in magnesium.

2 CONSTITUTIVE MODELLING OF PLASTIC DEFORMATION

It is well known that both elastic and plastic macro-scale deformation in metals are related to stretching of atomic structure and dislocation movements. It has been assumed that total deformation gradient follows a multiplicative decomposition to elastic F^e and plastic F^p deformation gradients [6].

$$F = F^e \cdot F^p \quad (1)$$

The net dislocation motion of $i^{(th)}$ dislocation system toward its vector $\pm s^i$ on plane m^i is considered as shear strain γ^i and the plastic velocity gradient is given by [7]:

$$L^p = \dot{F}^p \cdot F^{-p} = \sum_{i=1} \dot{\gamma}^i (s^i \otimes m^i) \quad (2)$$

According to Schmid's Law, the plastic shear strain rate $\dot{\gamma}^i$ depends on the applied resolved shear stress τ_{RS}^i and the activity of each deformation system can be modelled in a rate-dependent visco-plastic form, [7]:

$$\dot{\gamma}^i = \dot{\gamma}_0^i \left| \frac{\tau_{RS}^i}{\tau_Y^i} \right|^n \text{sign}(\tau_{RS}^i) \quad (3)$$

where $\dot{\gamma}_0^i$, n and τ_Y^i are reference shear strain rate, strain rate sensitivity exponent and current dislocation strength, respectively, which is able to represent isotropic hardening.

As twinning has polar character, Eqs. (4) for twinning systems has been modified:

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$$\dot{\gamma}^{\text{Twin}} = \dot{\gamma}_0^i \left| \frac{\tau_{\text{RS}}^{\text{Twin}}}{\tau_Y^{\text{Twin}}} \right|^n, \quad \tau_{\text{RS}}^{\text{Twin}} > 0$$

$$\dot{\gamma}^{\text{Twin}} = 0, \quad \tau_{\text{RS}}^{\text{Twin}} \leq 0 \quad (4)$$

By considering a linear form of latent hardening:

$$\tau_Y^i = \tau_0^i + \int_0^t h(\bar{\gamma}) (\dot{\gamma}^i + q_{ij} \sum_{i \neq j} \dot{\gamma}^j) dt \quad (5)$$

with τ_0^i as critical resolved shear stress and scalar values q_{ij} which correspond to slip interactions. Isotropic hardening evolutions for different slip systems are controlled by linear and exponential decay type hardening functions ($h(\bar{\gamma})$).

$$\bar{\gamma} = \sum_i \int_0^t |\dot{\gamma}^i| dt \quad (6)$$

$$h_1^i(\bar{\gamma}) = h_0^i \quad (7a)$$

$$h_e^i(\bar{\gamma}) = h_0^i (1 - \tau_0^i / \tau_\infty^i) \exp(-h_0^i \bar{\gamma} / \tau_\infty^i) \quad (7b)$$

Slip systems are defined with respect to local material coordination for each Gauss point. Local material coordination can be assigned directly from the single crystal orientation, and in the case of polycrystals, from the discretised texture. Twinning as a bulk deformation alters the atomic structure and consequently in each grain locally changes ($s^i \otimes m^i$). It has been assumed that reorientation of a material point is controlled by a stepwise scalar function f_T , representing twinning:

$$f_T = f(\gamma_{\text{Twin}}, \alpha_k) \quad (8)$$

α_k is a statistical internal variable reflecting the net activation force and barriers and γ_{Twin} is a deterministic strain like threshold. Contraction and tensile twinning systems have definite orientation tensors $\mathbf{R}_{\text{Twin}}^k$ with predetermined Eulerian angles [3] and totally $k=12$ sets of possible rotation directions. Accordingly the definition of current material orientation after $k^{(\text{th})}$ twinning, follows this form:

$$(s^i \otimes m^i)_R = ((f_T * \mathbf{R}_{\text{Twin}}^k) + (1 - f_T) * \mathbf{I}) \cdot (s^i \otimes m^i)_0 \quad (9)$$

where $\mathbf{I}$ is unit tensor, $(*)$ and $(\cdot)$ operators represent scalar product and dot product. The portion of reoriented material points N_R is denoted as twinning volume fraction:

$$V_{\text{Twin}} = \frac{\sum N_R}{N_{\text{Total}}} \quad (10)$$

3 DEFINITION OF DEFORMATION SYSTEMS

Based on experimental observations in channel die tests [3, 8], four sets of deformation systems have been considered. Table 1 summarizes the deformation modes.

Table 1: Deformation modes considered in the present work.

Name	No.	Plane	Direction
Basal <a>	3	{0001}	<11-20>
Prismatic <a>	3	{-1100}	<11-20>
Tensile twin	6	{10-12}	<10-11>
Contraction twin	6	{10-11}	<10-1-2>

4 FINITE ELEMENT MODEL

The simulations of single crystal and polycrystalline aggregates have been done using 20-node 3D quadratic elements. Each discrete grain orientation was assigned to a finite element. Single crystal has been modelled by one finite element, Table 2. In order to map pure magnesium rolled plate texture, 512 discrete orientations which are based on experimental basal pole figure, have been assigned to an equal number of elements, Fig 1. R, T and Z represent rolling, transverse to rolling and thickness of rolled plate. Six possible configurations of cubic specimens have been coded by two letters: first letter defines compression direction, second represents extension direction. For instance sample RZ was exposed to compression in rolling direction and extension in thickness direction. The die and the loading punch are modelled by rigid surfaces. Friction between single and polycrystal samples with die and punch has been assumed to be Coulombian type with a constant coefficient of 0.05. Isotropic elasticity with Young's modulus $E = 45$ GPa and Poisson ratio $\nu = 0.3$ has been employed. To mimic rate-independent plasticity, the strain rate sensitivity exponent has been set identically for all deformation systems equal to 50. The set of constitutive equations have been implemented in a multipurpose finite element solver ABAQUSTM using a user material subroutine [11].

Table 2: Definition of the orientations used with the channel-die compression tests on single crystals [8].

Test	Loading	Constrained
A	<0001>	<10-10>
B	<0001>	<1-210>
C	<10-10>	<0001>
D	<1-210>	<0001>
E	<10-10>	<1-210>
F	<1-210>	<10-10>
G	<0001> at 45°	<10-10>

Figure 1: Right: Experimental [9], left: simulated {0001} pole figures of pure magnesium rolled plate material [10].

5 RESULTS

By using experimental stress-strain data of channel die test [8], the model parameters have been identified through a calibration procedure. Interaction (q_{ij}) and hardening parameters are listed in Table 3, 4. Figure 2 shows a comparison between simulation and experimental results. As in Fig. 3, microstructural reorientation due to twinning can be represented by the spatial motion of the basal poles. Symbols in Fig. 3 represent the basal poles during deformation for three single crystal orientations. The arrows show the angular difference caused by tensile and contraction twins. Figure 4 shows experimental and simulation results for six possible polycrystal sample orientations for channel die test. Figure 5 represents the evolution of both tensile twinning and contraction twinning volume fraction for polycrystal samples.

Table 3: Latent hardening parameters calibrated using experimental data in [8].

$i^{(th)}$ system	$j^{(th)}$	Basal	Prismatic	T- Twinning	C- Twinning
Basal		0.0	0.5	0.0	0.0
Prismatic		0.5	0.8	0.0	0.0
T-Twinning		5.0	2.0	0.2	8.0
C-Twinning		0.2	0.2	0.05	0.5

Table 4: Direct hardening parameters, calibrated using experimental data in [8].

	Basal	Prismatic	T- Twinning	C- Twinning
Hardening	Linear	Exponential	Linear	Exponential
τ_0 (MPa)	1	20	5	80
τ_∞ (MPa)	-	180	-	1160
h_0 (MPa)	10	7500	260	10500
γ_{Twin}	-	-	0.060	0.018

Figure 2: Comparison between experimental channel die test results [8] and simulation results on single crystals.

Figure 3: Simulated basal pole figure for channel die test of magnesium single crystal with orientations A, E and F. TT represents tensile twinning, CT contraction twinning and DT double twinning.

Figure 4: Comparison between experimental channel die test results [9] and simulation results for polycrystal samples.

Figure 5: Simulated twinning volume fraction for six polycrystal sample orientations in the channel die. TT represents tensile twinning and CT used for contraction twinning.

DISCUSSION

Crystal plasticity modelling incorporating material reorientation provides a way to study the effect of twinning reorientation on hardening behaviour of pure magnesium. As in Fig. 2, the different hardening modes are clearly visible for different crystalline orientations.

Cases A and B are handled by activation of contraction twinning. An exponential form of hardening continues until 0.02 of macroscopic strain. The same hardening form has been observed by Obara et. al [4] in uniaxial loading. However, these authors referred it to hardening of pyramidal slip systems. The strain type threshold γ_{Twin} fulfilled almost at the same time for all 27 Gauss points inside a finite element. But depending on activation internal variables α , reorientation happens in sequence. Figure 3 shows how contraction twinning rotates the basal pole of sample A, 56° degree toward the channel side wall. Consequently the Schmid's factors for basal systems become nonzero and because of their extreme activity ($\tau_0^{\text{Basal}} = 1$), the stress drops. Each oscillation in the stress-strain curves reflects local material softening. In the case of C and D orientation, no twinning is observed. In the cases of orientations E and F, extension in channel direction is favourable for activation of tensile twinning and compression compensated by mobility of prismatic systems. As can be seen in Fig. 2, the crystal reveals linear hardening (up to 0.056 for E and 0.072 for F) which can be associated with the initial stage of linear hardening for tensile twinning. At a certain point, twinning criteria are satisfied and reorientation of slip systems occurs. As it is clear in pole figure, basal plan follows 86° rotation to the centre. After first reorientation, the crystal orientation E look likes case A and the c-axis exposed to contraction, therefore contraction twinning is activated, which causes a rapid increase of macroscopic hardening. Afterwards the second reorientation happens and because of the increase in Schmid's factors of the basal slip systems, material becomes locally softer. The sum of reorientation angles corresponds to double twinning with 38° of rotation [3]. Crystal orientation F follows a different rotation path. Basal plane rotates toward the channel side wall and crystal orientation becomes similar to the D orientation, and hence prismatic slip systems become active. Therefore stress – strain curves for C, D and F are almost parallel in the range of macrostrains between 0.11 and 0.15. Orientation G with 45° initial rotation of the c-axis has maximum Schmid's factor for the basal slip systems, thus basal as dominant deformation system almost produce an ideally plastic deformation. As mentioned before, modelling of twinning by spatial reorientation, can change the set of active deformation systems.

The activity of both types of twinning defines the general form of macroscopic strain hardening in magnesium polycrystals. Depending on the plate texture and the sample configurations in the channel die, there are three categories of material responses that are caused by: activation of tensile twinning (RZ, TZ), activation of contraction twinning (ZR, ZT) and constrained c-axes (TR, RT). For all polycrystal cases, changes in the hardening slope happen near 0.03 of macrostrain. Simulated twinning evolutions that have been plotted in Fig. 5 show that microstructural rotations start at almost 0.03 of macrostrain. Figure 5 also clarifies the activities of twinning systems within the samples. ZR and ZT have

contraction twinning as dominant rotation system while RZ and TZ have tensile twinning. The constrained c-axes in TR and RT have a lower twinning volume fraction in comparison to the others. Because the discretised texture is not a perfect basal texture, some of the grains in RT and TR tilted toward the channel die, therefore twinning activity is expected.

CONCLUSIONS

A material reorientation technique has been introduced into classical crystal plasticity to model the twinning more physically. It has been shown that material reorientation can cover the special form of hardening for twinning systems. Also, double twinning as sequential reorientation has been simulated. Moreover, because of twinning evolutions in polycrystal samples, different hardening characteristics are observed.

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