Deformation Behavior of Magnesium Extrusions: Experiments and Modeling

Reverse tension-compression and compression-tension experiments are performed on an extruded AZ31B magnesium sheets using a newly-developed antibuckling device. In addition, combined tension and shear experiments are performed to investigate the material response to multiaxial loading. A constitutive model is proposed which makes use of a single crystal approach to describe the dominant twinning and detwinning response, while a quadratic anisotropic yield function is employed to model the slip-dominated material response. The model accounts for the characteristic tension-compression asymmetry in the hardening mechanisms. Both the convex-up shaped stress-strain response under twinning and concave-down shaped response for slip-dominated behavior are predicted accurately. Furthermore, the effect of latent hardening among slip and twinning systems is taken into account. Due to strong simplifications regarding the kinematics of twinning, the model is computationally efficient and suitable for large scale structural computations. [DOI: 10.1115/1.4023958]

Keywords: magnesium, twinning, plasticity, biaxial experiments, reverse loading

1 Introduction

Magnesium features the lowest mass density among common metallic engineering materials. It is about 35% lighter than aluminum and almost 80% lighter than steel, while its stiffness-to-density ratio is similar to that of aluminum and steel. The widespread use of magnesium in vehicle engineering is limited because of higher material and processing costs. Furthermore, virtual engineering with magnesium involves a lot of uncertainty because of the lack of reliable material models that can predict the complex mechanical behavior of magnesium.

At the crystal level, magnesium alloys feature a hexagonal closed packed (HCP) lattice structure. In addition to crystallographic slip, the large deformation behavior of magnesium is governed by the twinning and detwining of its crystal structure. The twinning mechanism is of polar nature which causes the characteristic asymmetry of its yield behavior under tension and compression (e.g., Kelley and Hosford [1]). The c/a ratio of the magnesium HCP crystal is $c/a = 1.624 > \sqrt{3}$ (Roberts [2]) and so-called tensile twinning is thus predominant on the {1012} planes. The c-axis of the HCP crystal is rotated by 86.6 deg within the portion of the grain that underwent twinning. This mechanism is responsible for the pronounced evolution of texture in polycrystalline magnesium. The tensile tests on extruded Mg alloys by Jiang et al. [3] show that contraction twinning on the {1011} planes is another active deformation mode. Jiang et al. [3] argue that contraction twins are more narrow than tensile twins because they produce a larger amount of shear per unit volume. Consequently, the effect of texture rotation is less pronounced for contraction twinning than for tensile twinning. The observations of Barnett [4,5] confirm that extension twins are typically thicker than the planar contraction twins. As pointed out by Lou et al. [6], no experimental data is available on the mechanical response of single AZ31B crystals. Since the single crystal data for pure magnesium is not representative, the Critical Resolved Shear Stresses (CRSS) for AZ31B have been determined from fitting polycrystal model simulations (e.g., Agnew [7], Agnew et al. [8], Staroselsky and Anand [9], and Styczynski et al. [10]). Even though there are strong variations among the estimated CRSS (see Table 1 in Lou et al. [6]), there is a common consensus that the CRSS for basal $<a>$ slip and tensile twinning are the lowest. The CRSS for prismatic and pyramidal $<-a>$ slip are probably at least twice as high, while pyramidal $<-c+a>$ slip features a much higher CRSS and is thus mostly inactive at room temperature. Chino et al. [11] performed tension and compression experiments on extruded Mg AZ31 alloys of three distinct grain sizes; in their samples, the material isotropy increases as the grain size decreases. They report a reduced twinning intensity for fine grained microstructures, speculating that nonbasal $<a-c>$ slip is more intense under the absence of twinning.

Twinning is not only responsible for the compression/tension yield asymmetry. It also has a strong effect on the strain hardening in magnesium: twinning is partially responsible for the sigmoidally-shaped stress-strain response for selected loading conditions and causes a strong loading path dependency. The hardening associated with twinning features a convex stress-strain response at the macroscopic level, whereas the concave stress-strain response is attributed to hardening on the slip systems. Proust et al. [12] performed compression experiments on small cubes with severe loading path changes (through-thickness compression followed by in-plane compression) showing that dislocation multiplication increases the twin nucleation stress. Lou et al. [6] reported the same effect after loading direction reversal during in-plane tension-compression experiments. It is speculated that dislocations act as barriers to twin nucleation and propagation. In a second series of experiments, Proust et al. [12] prestrain their specimens under twinning-dominant in-plane compression before applying through-thickness compression. The macroscopic results elucidate the importance of texture evolution throughout twinning: after preloading, the otherwise slip-dominated through-thickness compression response exhibits the convex hardening response that is characteristic for twinning. This effect is explained by the drastic change in texture during twinning which allows for detwinning upon reloading in the opposite direction.
The experiments by Lou et al. [6] confirm this observation and indicate that the yield stress for detwinning is lower than that for twinning. Jain and Agnew [13] show that the terminal flow stress after monotonic in-plane compression is higher than after through-thickness compression which is explained by the pronounced latent hardening effect of twinning on crystallographic slip. The uniaxial and shear experiments of Khan et al. [14] at different temperatures and strain rates on an AZ31 alloy show that tension along the rolling direction strengthens the basal texture, while the c-axes align with the loading direction under in-plane compression. They also report an increase of the deformation resistance for higher strain rates and temperatures. Experiments on the cyclic response of magnesium alloy AZ61A for fully reversed loading have been performed by Zhang et al. [15]. They observed asymmetric stress-strain hysteresis loops for tension-compression and combined axial-torsion because of twinning and detwinning.

Due to the complexity and importance of the underlying micro-structural deformation mechanisms, polycrystal plasticity models have been used to predict the macroscopic behavior of magnesium and its alloys. Staroselsky and Anand [9] proposed a set of constitutive equations for a single magnesium crystal that accounts for the lattice rotation associated with twinning; they added an isotropic model to account for grain boundary effects and estimated the macroscopic response using a collection of $7 \times 7 \times 7$ reduced integration solid elements; each element represents a different grain while the grain orientations are assigned such that the overall texture of the numerical model replicated the experimentally-measured initial texture. Graff et al. [16] performed polycrystal-line plasticity simulations on magnesium using a convex hardening function for the twinning systems. They consider a large number of slip systems including pyramidal $\langle a-1+c \rangle$ slip and a collection of $8 \times 8 \times 8$ full integration solid elements, but neglect the effect of twinning-induced lattice rotation. Jain and Agnew [13] used a Voce-type hardening rule at the slip system level along with the assumption that all slip systems feature equal self and latent hardening. Analogously to Staroselsky and Anand [9], twin systems are modeled as slip systems, while latent hardening of the slip modes is the highest for twinning. Furthermore, Jain and Agnew [13] adopt a self-consistent homogenization scheme that guarantees that the spatial averages of the local fields equal the macroscopic stress and strain rate (e.g., Lebensohn and Tomé [17]). Their model accounts for grain reorientation due to twinning, but neglects the effect of dislocation multiplication on twinning. The latter effect is taken into account by the viscoplastic self-consistent model of Proust et al. [12]. Their model includes the notion of a composite grain: each grain is considered as an evolving layered structure of twins that is characterized by the volume fraction of twins and the mean free path of dislocation motion. As a result, the deformation resistance to slip on planes parallel to the twin planes is lower than for nonparallel planes, thereby representing a directional Hall–Patch effect. Levesque et al. [18] made use of a rate-dependent crystal plasticity model to investigate the effects of crystallographic slip and twinning on the forming limits of alloy AM30. The forming limits of alloy AZ31B have also been investigated by Neil and Agnew [19]. Their crystal plasticity computations elucidate that the formability depends strongly on temperature and loading paths. A finite strain elastic-viscoplastic self-consistent model accounting for both rate dependent slip and twinning is presented by Wang et al. [20]. Unlike other viscoplastic self-consistent models, their model accounts for elastic anisotropy and predicts a smooth elastoplastic transition during loading path changes. This model is also used to investigate the forming limits of AZ31B through M-K analysis (Wang et al. [20]). The simulation results indicate a strong effect of the intensity of basal texture on the forming limits and confirm the strain path sensitivity reported by Neil and Agnew [19]. A comparative study on various self-consistent polycrystal plasticity models for magnesium AZ31B (Wang et al. [21]) reveals that models with a grain interaction stiffness halfway between the secant and tangent approximations provide the best estimates of the stress-strain response for uniaxial tension and compression.

Even though crystal plasticity models provide a good mathematical description of the current understanding of the micromechanics of magnesium alloys, these are seldom used for large scale computations because of limited computational power. Dorum et al. [22] made use of a pressure sensitive isotropic yield function along with a nonassociated flow rule (to ensure incompressibility) to model the inelastic response of nearly isotropic high pressure die castings. Dorum et al. [23] reported reasonable agreement between model predictions and monotonic experiments on high pressure die cast AM60 using the isotropic Hosford yield function along with an isotropic hardening model. The shape of the initial yield surface for anisotropic magnesium has been described by Cazacu and Barlat [24]. Starting with an isotropic yield function that depends on the second and third stress tensor invariants, they made use of a linear transformation formalism to obtain the corresponding anisotropic yield function. As far as the complex large deformation response of textured Mg alloys is concerned, Lee et al. [25] proposed an advanced phenomenological model that makes use of a two-surface concept (Dafalias and Popov [26]) to describe the hardening response. They introduce a reverse loading criterion to obtain good agreement between model and experiment for reverse loading. The model by Lee et al. [25] makes use of a modified Drucker–Prager yield surface. The same group of authors demonstrated the enhanced predictive capabilities of their model (as compared to standard plasticity models with kinematic hardening) in springback simulations (Lee et al. [27]). Li et al. [28] make use of a von Mises yield surface with nonzero back stress to describe the mechanical behavior of AZ31B under plane stress conditions. Their phenomenological model accounts for slip, twinning and untwining. The c-axis rotations are modeled through an explicit evolution rule. They report that the computational time for their phenomenological constitutive model is about two orders of magnitude shorter than that for a viscoplastic self-consistent polycrystal plasticity model.

In the present work, the mechanical behavior of extruded Mg AZ31B sheets is characterized experimentally for uniaxial tension, compression, tension followed by compression, and compression followed by tension. In-plane compressive strains as high as 9% are achieved through the use of a newly-developed anti-buckling device for sheet metal testing. In addition to uniaxial experiments, the multiaxial material behavior of the anisotropic sheet material is investigated for various combinations of tension and shear. A constitutive model is proposed which combines a single crystal description of the twinning and detwining behavior with a phenomenological plasticity model for crystallographic slip. The resulting anisotropic plasticity model accounts for texture evolution and is able to describe the characteristic macroscopic response of extruded magnesium: tension-compression asymmetry, the transition from concave up to concave down hardening, the activation and cessation of twinning and detwining, as well as the latent hardening among slip and twinning systems.

### Table 1 Description of twinning systems

<table>
<thead>
<tr>
<th>$c_i$</th>
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<td>6</td>
<td>$\varepsilon_s$</td>
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The experiments by Lou et al. [6] confirm this observation and indicate that the yield stress for detwinning is lower than that for twinning. Jain and Agnew [13] show that the terminal flow stress after monotonic in-plane compression is higher than after through-thickness compression which is explained by the pronounced latent hardening effect of twinning on crystallographic slip.
2 Material

All specimens are extracted from 4 mm thick and 200 mm wide Mg extrusions. According to the DIN 1729-1 standard, the composition of the AZ31 alloy is 2.5–3.5% aluminum, 0.5–1.5% zinc and 0.05–0.4% Si. Samples for microscopic analysis are prepared using a standard mechanical polishing procedure (abrasive paper and diamond paste) followed by OPS polishing. The grain size varies from about 10 to 100 μm with an average grain size of about 30 μm. The grain shapes appear to be random and unaffected by the direction of extrusion. Pole figures for the basal plane of the hexagonally closed packed magnesium lattice are obtained through Electron back scatter diffraction (EBSD) (Fig. 1). The results show that the extruded alloy exhibits a strong basal texture with the majority of basal planes being perpendicular to the normal direction. However, unlike cold-rolled AZ31 plates, the present extruded material features also a group of basal planes that are perpendicular to the transverse directions.

In the following, we will make use of the notation ED, TD and ND for extrusion direction, transverse direction and normal direction, respectively. The subscripts E, T and N are employed to denote quantities that are associated with one of the three material directions. For example, $\sigma_E$ denotes the Cauchy stress along the ED, while $c_N$ denotes a c-axis which is aligned with the ND.

3 Experiments

The experimental program includes monotonic uniaxial compression and tension experiments as well as reversed loading experiments with tension followed by compression and compression followed by tension. In addition, monotonic multiaxial experiments are performed for selected combinations of tension and shear. Both crystallographic slip and twinning are isochoric and hence the assumption of incompressibility is employed when calculating the true stresses. All results for uniaxial loading are presented in terms of true stresses and logarithmic strains. The results from biaxial experiments are depicted in terms of engineering stress-strain curves.

3.1 Loading Frame and Strain Measurement. A custom-made hydraulic dual actuator system is used for all experiments (Mohr and Oswald [29]). It is composed of a vertical actuator to apply tension or compression to the specimen and a horizontal actuator for possible shear loading. The position of the second actuator is locked whenever uniaxial experiments are performed. The loading frame is equipped with a special set of high pressure clamps that can transmit tension, compression and shear. The upper and lower clamps are aligned with great accuracy; their maximum eccentricity does not exceed 0.01 mm in both the horizontal and vertical planes. This feature is of particular importance when specimens are subject to compressive loading.

The vertical force is measured by a load cell that is located below a low friction sliding table. Further, a 50 kN load cell is positioned between the sliding table and the horizontal actuator. The strains are measured using 2D digital image correlation. For this, a black speckle pattern is applied to the specimen gauge section. A digital camera (Regita with Nikon Nikkor 105 mm lenses) is used to record pictures of the specimen gauge section at a frequency of 1 Hz. The optical extensometer function of the digital image correlation software VIC2D (Correlated Solutions) is employed to determine the average strains within the specimen gauge section.

3.2 Uniaxial Tension. Dogbone specimens with a 30 mm long and 8 mm wide gauge section are used to characterize the material response for uniaxial tension. The true stress-strain curves are depicted in Fig. 2 for uniaxial tension along the extrusion and transverse directions. An average elastic modulus of about 39 GPa is determined from all experiments. Based on the DIC measurements of the axial and width strain, we identified an average elastic Poisson’s ratio of 0.29. The r-ratio (ratio of thickness strain increment ratio) remains approximately constant for each experiment, but the r-ratios exhibit significant differences from specimen to specimen; r-ratios ranging from 0.7 to 0.9 are observed for tension along the ED and from 1.3 to 3.3 for the TD. The initial yield stress for the ED (154 MPa) is almost 50% higher than that for the TD (108 MPa). Conversely, the rate of strain hardening is much higher for uniaxial tension along the TD. As a result, the stress-strain curves intersect each other at an axial strain of about 0.09. However, the stress-strain curves seem to converge for large strains and the ultimate true stress at failure is only about 3% higher for the TD (302 MPa) than for the ED (293 MPa). The observed mechanical responses are tentatively explained through the texture and deformation mechanisms at the crystal level:

• For uniaxial tension along the ED, crystals with their c-axis in the TD and the ND are not expected to undergo twinning. Consequently, the inelastic material response is associated with crystallographic slip which requires a higher resolved shear stress than twinning.

• For uniaxial tension along the TD, $c_T$-crystals are expected to form twins, while twinning of the $c_N$-crystals will remain inactive. As a result, the initial yield stress is lower than for tension along the ED. The apparent rapid strain hardening at the macroscopic level is then explained by the ceasing of twinning and the transition to crystallographic slip which requires much higher shear stresses. The intersection of the stress-strain curves for 0 deg and 90 deg is explained by the higher deformation resistance of the respective active slip systems. This is possibly due to the strong crystallographic
The above tentative explanations are supported by the observed r-values. For uniaxial tension along the TD, we observe exceptionally high r-values which indicates that the specimen thickness remains almost constant throughout the experiment. In other words, the shear driven crystal deformation takes place within the plane of the extruded sheet. This is clearly the case when ετ-crystals undergo twinning with c-axis rotations within the plane of the sheet.

3.3 Reverse Loading Experiments. Short dogbone shaped specimens with a 10 mm wide and 13 mm long gage section are used for reverse loading experiments. They feature a relatively short gauge section in order to reduce the effective buckling length. In addition, a special antibuckling device is used (Beese and Mohr [30]) to guarantee that the specimen remains straight from membrane to bending dominated loading in a compression experiment; all experiments are performed under displacement control at a cross-head speed of 1 mm/min.

3.3.1 Monotonic Compression. The short specimen for reverse loading and the antibuckling device are also used to obtain the stress-strain curve for monotonic uniaxial compression. The corresponding stress-strain curves are included in Fig. 2. The initial yield stress is about 75 MPa for both uniaxial compression along the extrusion and transverse direction. Subsequently, the stress-strain curves exhibit the characteristic sigmoidal shape. The initial slope is a convex curve which is usually associated with twinning. Beyond the deflection point, we observe a concave curve which is associated with crystallographic slip. Observe that the stress level increases faster for compressive loading along the TD. The stress-strain curves exhibit the characteristic sigmoidal shape. As the detwinning ceases, the stress level rises rapidly (convex up shape) until crystallographic slip becomes dominant which results in a concave down shaped stress-strain curve. It is interesting to observe that the initial threshold stress for detwinning increases as a function of the prestrain; for the TD, we have 63 MPa for −0.03, 87 MPa for −0.06 and 103 MPa for −0.09. The corresponding ultimate stress levels for large strains still seem to converge (when extrapolating the tensile stress-strain curves by eye). The present data clearly shows that the strain to fracture of the present magnesium alloy decreases with the amount of compressive prestrain.

3.3.2 Uniaxial Tension Followed by Uniaxial Compression. The specimen for the ED is loaded under tension up to a true strain of 0.13 before it is unloaded and reloaded under compression (solid black curve in Fig. 3). The maximum tensile stress prior to unloading is 293 MPa whereas the apparent yield stress for reloading under compression is 154 MPa. The stress-strain curve for reloading features the characteristic sigmoidal shape for compression. The yield stress for reloading (154 MPa) is much higher than that for monotonic uniaxial compression (78 MPa) which indicates some latent hardening of the twinning systems during slip. Furthermore, the stress level at compressive failure is much higher (396 MPa versus 326 MPa) when the specimen is subject to tension prior to compression.

Simultaneous observations are made for the specimen that is subject to a tensile strain of 0.10 prior to compressive loading along the TD (blue curves in Fig. 3). For reference, we show the monotonic stress-strain curves from Fig. 2 as dashed lines in Fig. 3. These curves are close to the initial loading branches of the specimens subject to reverse loading. This is seen as a partial validation of the short dogbone specimen geometry. The observed differences are attributed to scatter in the material properties.

3.4 Combined Tension and Shear. The specimen for biaxial experiments comprises a 5 mm high and 50 mm wide rectangular gauge section. The specimen thickness is reduced from 3 mm to 1 mm within the gauge section to avoid plastic deformation in the 10 × 80 mm large gripping areas. The vertical actuator of the hydraulic dual actuator systems is used to apply tensile loads while the horizontal actuator is used to apply shear loading to the gauge section boundaries. The reader is referred to Mohr and Oswald [29] for more details on the experimental procedure. The experimental results are reported in terms of engineering stresses and strains. The engineering normal and shear stresses correspond to the normalized vertical and horizontal forces,

$$\sigma = \frac{F_N}{A_0} \quad \text{and} \quad \tau = \frac{F_H}{A_0}$$

The corresponding engineering normal and shear strains are determined from optical displacement measurements on the gauge.
section surface. We introduce the so-called biaxial loading angle $\beta$ to characterize the loading path in the stress space,

$$\tan \beta = \frac{\sigma}{\tau}$$

(2)

According to this definition, $\beta = 0$ deg corresponds to pure shear loading. $\beta = 90$ deg defines pure tensile loading. Note that the strain along the specimen width direction is zero. Thus, “pure tensile loading” corresponds to transverse plane strain tension.

The specimens are prepared with either the ED or the TD aligned with the tensile axis. The ED specimens are tested for $\beta = 0$ deg, 49 deg, 68 deg, 75 deg and 90 deg while the TD specimens are subject to combined loading for $\beta = 0$ deg, 38 deg, 62 deg, 77 deg and 90 deg. The experiments for $\beta = 90$ deg are performed under displacement control, while all other experiments are performed under force control. From each experiment, we obtain a normal stress-strain curve and a shear stress-strain curve.

The two upper graphs in Fig. 4 depict the stress-strain curves for the ED specimens ($\alpha = 0$ deg). The lower two graphs (Figs. 4(c) and 4(d)) show the corresponding experimental results for the TD specimens. Most curves feature three distinct dots which indicate the points where the total plastic work is 2mJ (solid circular dot), 5mJ (star symbol) and 8mJ (open circular dot). All curves are in hierarchical order except for the shear stress-strain curves for the ED specimens. Note that the curves for $\beta = 49$ deg lies initially above that for 0 deg.

4 Constitutive Model

The constitutive model consists of three major parts. A first set of equations describes the deformation behavior associated with crystallographic slip while the second part is associated with twinning. A third part is introduced to model the interaction of crystallographic slip and twinning.

4.1 Model For Crystallographic Slip. The material response for crystallographic slip dominated deformation modes is described through a phenomenological plasticity model at the macroscopic level. The key ingredients of this model are an anisotropic quadratic yield surface with initial back stress and a combined isotropic/nonlinear kinematic hardening model.

4.1.1 Hill’48 Yield Function With Back Stress. The yield surface is defined through the equation

$$f = \sigma - k = 0$$

(3)

where $\sigma$ defines an equivalent stress measure and the scalar $k$ is the deformation resistance. The Hill’48 equivalent stress reads

$$\sigma = \left[ F(\sigma_{22} - \sigma_{33})^2 + G(\sigma_{33} - \sigma_{11})^2 + H(\sigma_{11} - \sigma_{22})^2 
+ L(\sigma_{12}^2 + \sigma_{21}^2) + M(\sigma_{13}^2 + \sigma_{31}^2) + N(\sigma_{32}^2 + \sigma_{23}^2) \right]^{1/2}$$

(4)

where $\sigma_{ij}$ are the components of the symmetric Cauchy stress tensor as written in a Cartesian coordinate system that is aligned with the principal axes of orthotropy. Here, we introduce the deviatoric back stress tensor $\mathbf{x}$ and substitutive the components $\sigma_{ij}$ in Eq. (4) by $\sigma_{ij} - x_{ij}$. Thus, for plane stress conditions, we obtain

$$\sigma = \left[ F(\sigma_{22} - x_{22} + x_{33})^2 + G(-\sigma_{11} + x_{11} - x_{33})^2 
+ H(\sigma_{11} - \sigma_{22} - x_{11} + x_{22})^2 + 2L(\sigma_{12} - x_{12})^2 \right]^{1/2}$$

(5)
Introducing the stress vector \( \sigma = \{\sigma_{11}, \sigma_{22}, \sigma_{12}\} = \{\sigma_e, \sigma_T, \tau\} \) and the back stress vector \( \beta \) with the components \( \beta_1 = \sigma_{11} - \sigma_{33}, \beta_2 = \sigma_{22} - \sigma_{33} \) and \( \beta_3 = \sigma_{12} \), Eq. (5) may be rewritten as

\[
\tilde{\sigma} = \sqrt{\mathbf{P}(\sigma - \beta) \cdot (\sigma - \beta)}
\]

with the anisotropy coefficient matrix

\[
\mathbf{P} = \begin{bmatrix} G + H & -H & 0 \\ -H & F + H & 0 \\ 0 & 0 & 2L \\ \end{bmatrix}
\]

4.1.2 Associated Flow Rule and Hardening Laws. An associated flow rule is assumed to describe the evolution of the plastic strain vector \( \mathbf{d}^p = \{\epsilon_{e}, \epsilon_T, \gamma\} \)

\[
d^p = \frac{d\lambda}{\alpha} \mathbf{P}(\sigma - \beta)
\]

where \( d\lambda \geq 0 \) is the plastic multiplier and \( \lambda = \int d\lambda \) is referred to as the equivalent plastic strain. We assume a modified Swift law to describe isotropic hardening,

\[
dk = H(\lambda) \cdot d\lambda \quad \text{with} \quad H(\lambda) = nA(\lambda_0 + \lambda)^{n-1}
\]

where \( A, \epsilon_0 \) and \( n \) are model parameters. The kinematic hardening is described using a Frederick–Armstrong approach (e.g., Chaboche [31]). In 3D, the Frederick–Armstrong rule is typically written as

\[
d\alpha = \frac{2}{3} \epsilon a(d^p - \epsilon) \mathbf{d}^p
\]

with the kinematic hardening parameters \( c \) and \( a \). For plane stress, the corresponding expression in vector notation reads

\[
d\beta = \epsilon a \mathbf{G} \mathbf{d}^p - \epsilon \mathbf{b} \mathbf{d}^p
\]

with the coefficient matrix

\[
\mathbf{G} = \frac{2}{3} \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 0.5 \\ \end{bmatrix}
\]

Recall that the normal components of \( \beta \) correspond to the differences in back stresses \( \dot{\beta}_i = \beta_{ij} - \beta_{ik} \) which requires the introduction of a coefficient matrix in the plane stress version of the Frederick–Armstrong rule.

4.2 Model for Twinning and Detwinning. The twinning and detwinning model is developed based on the assumption that the c-axis of the hexagonal crystals in extruded magnesium are either aligned along the extrusion direction, the transverse direction, or the thickness direction. This assumption is not only made for the initial configuration, but also for subsequent deformed configurations. It is justified by the strong initial texture (see pole figures in Fig. 1) and the fact that the c-axis rotates by 86.3 deg \( \pm 90 \) deg as a crystal undergoes twinning (Fig. 5). The key simplification is the kinematic restriction of forcing the rotated crystal orientations to remain aligned with one of the initial material axes. For example, if a crystal is initially aligned with the ND, it can only rotate to the ED or TD direction, while all other orientations in the (E,T)-plane are eliminated by this kinematic restriction. Detwinning is considered as another twinning event. For instance, if a crystal axis rotates from \( \epsilon_1 \) to \( \epsilon_2 \) throughout twinning, detwinning is modeled as another twinning event that rotates the c-axis from \( \epsilon_2 \) to \( \epsilon_1 \).

Figure 5 shows a schematic of the twinning of a single hexagonal crystal. A twinning system is described by the normal \( \mathbf{n} \) of the twinning plane and the twinning direction \( \mathbf{m} \). In pure magnesium, we have \( c/a = 1.624 \) which corresponds to an angle of 43.2 deg between the c-axis before twinning and the normal of the twinning plane. Denoting the Cauchy stress tensor as \( \sigma \), the resolved shear stress for this twinning system reads

\[
\tau_i = \sigma \cdot (\mathbf{m} \otimes \mathbf{n})
\]

According to our model assumptions, the c-axis rotates by 90 deg in the (\( \mathbf{n}, \mathbf{m} \))-plane as the resolved shear stress exceeds the twinning resistance \( s_i \). According to the above modeling assumptions, we consider all transformations \( \epsilon_i \rightarrow \epsilon_j \), with \( i \neq J \): (1) \( \epsilon_1 \rightarrow \epsilon_2 \), (2) \( \epsilon_2 \rightarrow \epsilon_3 \), (3) \( \epsilon_2 \rightarrow \epsilon_3 \), (4) \( \epsilon_T \rightarrow \epsilon_2 \), (5) \( \epsilon_3 \rightarrow \epsilon_E \) and (6) \( \epsilon_T \rightarrow \epsilon_F \). Note that there are two possible twinning systems for each transformation from \( \epsilon_i \) to \( \epsilon_j \) when considering the exact rotation of 86.3 deg (the second twinning system corresponds to the horizontal mirror image of Fig. 5). However, when approximating the rotation by 90 deg, the corresponding resolved shear stresses and associated shear deformations are identical. Thus, in the approximate model, we have only six possible twinning systems (instead of twelve). Moreover, for twinning from \( \epsilon_i \) to \( \epsilon_j \), we have

\[
\mathbf{n} = \frac{1}{\sqrt{2}} (\mathbf{c}_i + \mathbf{c}_j) \quad \text{and} \quad \mathbf{m} = \frac{1}{\sqrt{2}} (\mathbf{c}_i - \mathbf{c}_j)
\]

The components of the \( \mathbf{n} \) and \( \mathbf{m} \) vectors for all six twinning systems considered in the present model are summarized in Table 1.

4.2.1 Polar Twinning Conditions. Twinning occurs on a twinning system \( i \) if the twinning condition

\[
f_i = \tau_i - s_i = 0
\]

is satisfied with \( s_i > 0 \) denoting the corresponding twinning resistance. Note that typical slip conditions in crystal plasticity compare the absolute value of the resolved shear stress on a slip system with the deformation resistance. However, Eq. (15) includes the sign of \( \tau_i \) and therefore accounts for the polar nature of twinning. Each function

\[
f_i = \tau_i - s_i = 0
\]

defines a plane in the stress space. The orientations of these planes do not change when twinning takes place, but their distances to the origin, \( s_i \), can increase. For plane stress conditions, it is convenient to rewrite the resolved shear stresses in the form

\[
\frac{1}{\sqrt{2}} (\mathbf{c}_i \cdot \mathbf{m})
\]
with the normal vectors

\[
\begin{align*}
\mathbf{q}_1 &= \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}, \\
\mathbf{q}_2 &= \begin{bmatrix} 1 & \sqrt{2} & 0 \end{bmatrix}, \\
\mathbf{q}_4 &= \begin{bmatrix} 1 & 0 & \sqrt{2} \end{bmatrix}, \\
\mathbf{q}_5 &= \begin{bmatrix} 0 & 1 & 0 \end{bmatrix}, \\
\mathbf{q}_6 &= \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}, \\
\mathbf{q}_7 &= \begin{bmatrix} 0 & \sqrt{2} & 0 \end{bmatrix}, \\
\mathbf{q}_8 &= \begin{bmatrix} -1 & 1 & 0 \end{bmatrix}, \\
\mathbf{q}_9 &= \begin{bmatrix} 0 & 0 & -1 \end{bmatrix}
\end{align*}
\]

(18)

Note that the third component of all vectors \(\mathbf{q}_i\) is zero which implies that the in-plane shear stress does not affect the twinning according to the model assumptions. The twinning conditions therefore correspond to boundary lines of the elastic domain in the \((\sigma_E, \sigma_T)\)-plane (Fig. 6).

4.2.2 Evolution of Twinning Deformation. In close analogy with the flow rule for plastic flow, we introduce the twinning rule to determine the evolution of the twinning strain vector \(\dot{\gamma}^w\) at the macroscale. In tensor notation, the macroscopic rate of twinning deformation is expressed as

\[
\mathbf{D}^w = \sum_{i=1}^{6} \dot{\gamma}^w_{\text{sym}} (\mathbf{m}_i \otimes \mathbf{n}_i)
\]

(19)

while the corresponding spin is set to zero. In vector notation, Eq. (19) is rewritten as

\[
\dot{\gamma}^w = \sum_{i=1}^{6} \dot{\gamma}^w_i \mathbf{q}_i
\]

(20)

while the through-thickness strain increment is computed from the incompressibility constraint,

\[
\dot{\varepsilon}_{N}^w = -(\dot{\varepsilon}_E^w + \dot{\varepsilon}_T^w)
\]

(21)

4.2.3 Twinning Resistance. Formally, the resistance \(s_i\) of the twinning system \(i\) is written as

\[
s_i = s_{\text{tw}}(\dot{\gamma}_i, \dot{\gamma}_t) + s_{\text{detw}}(\gamma_{tw})
\]

(22)

The first term accounts for the direct hardening of the twinning system, while the second term describes the latent hardening among twinning systems. It is expressed as a function of the accumulated twinning strain,

\[
\dot{\gamma}_{tw} = \sum_{i=1}^{6} \dot{\gamma}_i
\]

(23)

Note that the twinning on a system \(\mathbf{c}_i \rightarrow \mathbf{c}_j\) ceases as the volume fraction \(\gamma_i\) of the crystals of orientation \(\mathbf{c}_i\) approaches zero. Thus, the direct hardening term is decomposed further into

\[
s_{\text{tw}} = s_{\text{d}}(\dot{\gamma}_i) + s_{\text{p}}(\gamma_i)
\]

(24)

where \(s_{\text{p}}\) is a penalty function; it is a monotonically decreasing function of \(\gamma_i\), which increases the twinning resistance as \(\gamma_i \rightarrow 0\). According to the above numbering of the twinning systems, we have \(\dot{\gamma}_1 = \dot{\gamma}_2 = \dot{\gamma}_3, \dot{\gamma}_4 = \dot{\gamma}_5 = \dot{\gamma}_6\) and \(\dot{\gamma}_7 = \dot{\gamma}_8 = \dot{\gamma}_9\).

4.2.4 Texture Evolution. As mentioned above, one of the strong model assumptions is the restriction to three crystal orientations: \(\mathbf{c}_E, \mathbf{c}_T, \mathbf{c}_N\). The texture is thus defined through the three corresponding volume fractions: \(\gamma_E, \gamma_T, \gamma_N\). The evolution of the volume fractions is bound by the lower limit

\[
\gamma_i \geq 0
\]

(25)

and the constraint

\[
\gamma_E + \gamma_T + \gamma_N = 1
\]

(26)

When a crystal undergoes twinning on the system \(\mathbf{c}_i \rightarrow \mathbf{c}_j\) from the initial configuration \((\gamma_i = 0, \dot{\gamma}_i = 1)\) to the fully-twinned configuration \((\gamma_i = 0, \dot{\gamma}_i = 1)\), the corresponding theoretical twinning shear strain is \(\gamma_{\text{max}} = 0.13\). For twinning on a single system, it follows from [26] that

\[
\dot{\gamma}_i = -\hat{\gamma}_i \geq 0
\]

(27)

Furthermore, it is assumed that the rate of volume fraction evolution is proportional to the shear strain rate \(\dot{\gamma}_i\) of the corresponding active twinning system. For the six twinning systems considered in this model, we obtain the texture evolution equations

\[
\dot{\gamma}_E = \frac{1}{\gamma_{\text{max}}} (\dot{\gamma}_3 + \dot{\gamma}_5 - \dot{\gamma}_1 - \dot{\gamma}_2)
\]

(28)

\[
\dot{\gamma}_T = \frac{1}{\gamma_{\text{max}}} (\dot{\gamma}_1 + \dot{\gamma}_6 - \dot{\gamma}_3 - \dot{\gamma}_4)
\]

(29)

\[
\dot{\gamma}_N = \frac{1}{\gamma_{\text{max}}} (\dot{\gamma}_2 + \dot{\gamma}_4 - \dot{\gamma}_5 - \dot{\gamma}_6)
\]

(30)

The constraint, Eq. (26), is automatically satisfied by the Eqs. (28)-(30), while Eq. (21) is enforced indirectly through the penalty function, Eq. (24). Unlike the shear increments which are always positive, \(\dot{\gamma}_i \geq 0\), the evolution of the volume fractions is reversible and \(\dot{\gamma}_i\) can also be negative.

4.3 Coupling of Crystallographic Slip and Twinning/ Detwinning. The models for crystallographic slip and twinning/detwinning are coupled through the flow rule. Furthermore, additional latent hardening terms are introduced as twinning may increase the deformation resistance for crystallographic slip and vice versa. The resulting model corresponds to an anisotropic rate-independent multisurface plasticity model with cross-hardening.

4.3.1 Coupled Flow Rule. The separate flow rules for slip and twinning are replaced by a single flow rule which corresponds to the addition of Eqs. (8) and (19),

\[
\sum_{i=1}^{6} \dot{\gamma}^w_i \mathbf{q}_i = \sum_{i=1}^{6} \dot{\gamma}^s_i \mathbf{q}_i + \sum_{i=1}^{6} \dot{\gamma}^{st}_{\text{tw}}(\gamma_{tw}) \mathbf{q}_i
\]
\[ \dot{\varepsilon}^P = \dot{\varepsilon}^p + \dot{\varepsilon}^{tw} = \frac{P(\sigma - \beta)}{\sigma} \dot{\lambda} + \sum_{i=1}^{6} \dot{\gamma}_i \mathbf{q}_i \]  

(31)

In sum, the model comprises seven plastic multipliers, \( \dot{\lambda}, \dot{\gamma}_1, \ldots, \dot{\gamma}_6 \), while each plastic multiplier is associated with a different yield or twinning surface. Under the absence of slip, a maximum of two twinning systems may become active simultaneously (corresponds to a loading path that crosses the intersection point of two twinning envelopes). Due to the coupling of slip and twinning, up to three surfaces may intersect at a single point in stress space. The corresponding plastic multipliers are then determined from the three corresponding consistency conditions \( \dot{d}_i = 0 \) for the active deformation systems.

4.3.2 Latent Hardening. The twinning model accounts already for the latent hardening among twinning systems. Here, we add a third term to Eq. (22) to include the effect of latent hardening of a twinning system due to crystallographic slip,

\[ s_t = s_{tw}(\gamma_t, \lambda) + s_{sc}(\gamma_{sc}) + s_{sc}(\lambda) \]

(32)

\( s_{sc}(\lambda) \geq 0 \) is a function of the equivalent plastic strain \( \dot{\varepsilon}^p \) of the slip model and needs to be determined from experiments where crystallographic slip is followed by twinning.

Experimental results also indicate latent hardening of the twinning systems due to twinning. Therefore, we also rewrite Eq. (9) as

\[ dk = H_d \dot{\lambda} + H_{sc} d_{sc} \]

(33)

where the modulus \( H_{sc} \) describes the latent hardening due to twinning. Recall that \( \dot{\gamma}_{sc} \) is the accumulated twinning strain which increases \( d\dot{\gamma}_{sc} \geq 0 \) as twinning takes place on at least one of the six twinning systems.

4.4 Dissipation. For plane stress conditions, the rate of intrinsic dissipation (difference of applied work and stored energy) per unit volume reads

\[ (\sigma - \beta) : \dot{\varepsilon}^p + \sigma : \dot{\varepsilon}^{tw} \geq 0 \]

(34)

Due to the use of the normality flow rule, the rate of intrinsic dissipation associated with crystallographic slip is always positive,

\[ (\sigma - \beta) : \dot{\varepsilon}^p = \sigma : \dot{\varepsilon}^p \geq 0 \]

(35)

Twinning is considered as dissipative at a rate of

\[ \sigma : \dot{\varepsilon}^{tw} = \sigma : \sum_{i=1}^{6} \dot{\gamma}_i \mathbf{q}_i = \sum_{i=1}^{6} \dot{\gamma}_i (\sigma : \mathbf{q}_i) = \sum_{i=1}^{6} \dot{\gamma}_i \mathbf{t}_i \geq 0 \]

(36)

Due to the polar nature of the twinning condition, Eq. (15), twinning can only occur for \( \tau > 0 \). According to our definition \( \dot{\gamma}_i > 0 \), the rate of dissipation associated with twinning is always positive.

5 Model Parameter Identification

The elastic response of the material is assumed to be linear and isotropic. We thus make use of the average Young’s modulus \( E = 39 \text{ GPa} \) and elastic Poisson’s ratio \( v = 0.29 \) as determined from the uniaxial tension experiments along different material directions. In the following, we discuss the model parameters and functions that need to be determined to describe the inelastic behavior. A first set of material model parameters is identified in a deterministic way. These parameters are subsequently used as seed values for a model parameter optimization through Monte Carlo simulations.

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5.1 Crystallographic Slip. The first part of the constitutive model requires the identification of

- the anisotropy coefficients \( P_{22}, P_{12}, P_{13} \) (which are directly related to the Hill coefficients \( H, F \) and \( L \) as given by Eq. (7))
- the initial back stresses \( \beta_{01}, \beta_{02}, \beta_{03} \)
- the kinematic hardening coefficients \( c \) and \( a \), and
- the isotropic hardening function \( H = H(\lambda) \) along with the initial deformation resistance \( k_0 \)

5.1.1 Anisotropy Coefficients. First estimates for the anisotropy coefficients \( P_{22} \) and \( P_{12} \) are obtained from the Lankford ratios for tension along the extrusion and transverse directions. Assuming the approximations

\[ r_0 = \frac{-P_{12}(\sigma_0 - \beta_{01}^1) + P_{22}\beta_{02}^1}{(1 + P_{12})(\sigma_0 - \beta_{02}^1) - (P_{22} + P_{12})\beta_{02}^1} \geq -\frac{P_{12}}{1 + P_{12}} \]

(37)

and

\[ r_0 = \frac{-P_{12}(\sigma_{20} - \beta_{01}^2) + P_{22}\beta_{02}^2}{(P_{22} + P_{12})(\sigma_{20} - \beta_{02}^2) - (1 + P_{12})\beta_{02}^2} \geq -\frac{P_{12}}{P_{22} + P_{12}} \]

(38)

We find \( P_{12} \approx -0.47 \) and \( P_{22} \approx 0.84 \) for \( r_0 = 0.9 \) and \( r_0 = 1.3 \).

5.1.2 Initial Back Stresses. Seed values for the back stresses \( \beta_{01}^1 \) and \( \beta_{02}^1 \) are identified from the combined tension and shear experiments. Based on the current experimental data, we cannot determine \( \beta_{01}^2 \) and we assume \( \beta_{02}^2 = 0 \). Recall that plane stress conditions prevail along the horizontal direction of the biaxial plasticity specimen. In the case of tension along the ED (\( \phi = 0 \) deg), evaluation of the plane stress condition for the plasticity model for crystallographic slip yields

\[ d\dot{\varepsilon}_E = 0 \Leftrightarrow \sigma_E - \beta_1 = -\frac{P_{12}}{P_{22}}(\sigma_E - \beta_1) \]

(39)

which corresponds to a yield envelope of

\[ (1 - \frac{P_{12}}{P_{22}}) (\sigma_E - \beta_1)^2 + P_{33} \tau^2 = k^2 \]

(40)

In the case of tension along the transverse direction (\( \phi = 90 \) deg), the plane strain condition yields

\[ d\dot{\varepsilon}_E = 0 \Leftrightarrow \sigma_E - \beta_2 = -\frac{P_{12}}{P_{22}}(\sigma_T - \beta_2) \]

(41)

and hence

\[ (P_{22} - P_{12}^2)(\sigma_T - \beta_2)^2 + P_{33} \tau^2 = k^2 \]

(42)

The discrete yield envelopes in the \( (\sigma_E, \tau) \)-plane for \( \phi = 0 \) deg and in the \( (\sigma_T, \tau) \)-plane for \( \phi = 90 \) deg are determined from the combined tension and shear experiments using a plastic work definition of the yield point. For each biaxial experiment, we calculate the plastic work and extract the stress point for a plastic work density of \( 2 \text{MJ/mm}^3 \). The corresponding experimental data points are shown by solid dots and stars in Fig. 7. Observe that the initial back stress becomes apparent from the position of the maximum shear stress in the case of \( \phi = 0 \) deg. A fit of the quadratic yield envelopes (solid lines) leads to the seed values \( \beta_{01}^1 = 80 \text{ MPa} \) and \( \beta_{02}^1 = 0 \).

5.1.3 Isotropic and Kinematic Hardening Parameters. The isotropic and kinematics hardening parameters are identified based on the uniaxial tension experiments. A simple finite difference scheme is used to solve the constitutive equations for crystallographic slip for monotonic uniaxial loading. The isotropic hardening parameters \( A = 330 \text{ MPa}, \quad c_0 = 0.002 \) and \( n = 0.167 \)
with the parameters 

\( a = 40 \text{ MPa} \) are then identified from a fit to the experimental data for uniaxial tension along the ED and TD.

5.2 Twinning and Detwinning. The second part of the constitutive model requires the identification of

- the initial volume fractions \( \gamma_E^0, \gamma_t^0 \) and \( \gamma_N^0 \)
- the penalty function \( s_p(\gamma_t) \)
- the latent hardening function \( s_{I\rightarrow T}(\gamma_{tw}) \)

The initial volume fractions characterize the initial texture of the material. Based on the pole figures shown in Fig. 1, we assume \( \gamma_E^0 = 0.05, \gamma_t^0 = 0.2 \) and \( \gamma_N^0 = 0.75 \) as starting values in our numerical identification study.

Parametric models are assumed for the three functions describing the twinning resistance (Fig. 8). We assume

\[ s_d(\gamma_t) = p_0 + p_1\gamma_t + p_2\gamma_t^3 \]  

(43)

with the parameters \( p_0, p_1 \) and \( p_2 \). Seed values for these parameters may be determined from a monotonic uniaxial compression experiment along the TD. In this experiment, it is expected that twinning occurs only on system \#6 (\( \gamma_N \rightarrow \gamma_T \)) as the initial condition \( \gamma_E^0 = 0.05 \) prevents the possible activation of system \#1 (\( \gamma_E \rightarrow \gamma_t \)). According to Eqs. (16), (17), and (20), we have \( d\epsilon^p = -d\epsilon_t \) and \( \sigma = -s_6 \). From a fit to the compressive stress versus strain curve, we obtain \( p_0 = 77 \text{ MPa}, p_1 = 2 \text{ GPa} \) and \( p_2 = 291 \text{ GPa} \).

As penalty function (Fig. 8(b)), we propose,

\[ s_p(\gamma_t) = \begin{cases} p_3 \left(1 - \frac{\gamma_t}{\tilde{\gamma}} \right)^3 & \text{for } 0 \leq \gamma_t \leq \tilde{\gamma} \\ 0 & \text{for } \tilde{\gamma} \leq \gamma_t \leq 1 \end{cases} \]  

(44)

where the parameter \( p_3 = 300 \text{ MPa} \) determines the magnitude of the penalty; this numerical parameter it is chosen such that system \#1 remains inactive during compression along the TD. The parameter \( \tilde{\gamma} \) determines the volume fraction at which the penalty term becomes active. Here, a value of \( \tilde{\gamma} = 0.39 \) provided a good agreement of the simulations and the experiments.

The effect latent hardening among twinning systems is described by the linear function

\[ S_{I\rightarrow T} = H_{I\rightarrow T}\gamma_{tw} \]  

(45)

Note that due to the definition of \( \gamma_{tw} \), Eq. (41) also includes a direct contribution of the active twinning system. The latent hardening modulus \( H_{I\rightarrow T} = 230 \text{ MPa} \) is determined from reversed loading experiments along the TD with compression (twinning from \( c_N \rightarrow c_T \)) followed by tension (twinning from \( c_T \rightarrow c_N \)).

The point of the onset of twinning after reversal of the loading direction is clearly visible on the stress-strain curve (Fig. 3). An increase of about \( \Delta \sigma = 6 \text{ MPa} \) is observed when increasing the plastic strain to the point of load reversal by \( \Delta \epsilon_p = 0.026 \); we have \( d\gamma_{tw} = d\gamma_t = -d\epsilon_p \) during compressive loading along the TD; hence a modulus of \( H_{I\rightarrow T} = 6/0.026 \approx 230 \text{ MPa} \) is chosen.

5.3 Coupling of Crystallographic Slip and Twinning. There are two more latent hardening functions that need to be identified to describe the coupling between slip and twinning:

- the function \( s_{s\rightarrow t}(\lambda) \) for the latent hardening of a twinning system due to slip
- the modulus \( H_{s\rightarrow t}(\gamma_{tw}) \) for the latent hardening of a slip system due to twinning

Due to the limited experimental data, a linear function is assumed for \( s_{s\rightarrow t}(\lambda) \),

\[ s_{s\rightarrow t} = H_{s\rightarrow t}\lambda \]  

(46)

while a modulus of \( H_s = 441 \text{ MPa} \) has been identified from the reversed tension-compression loading experiment along the TD.

The latent hardening of a slip system due to twinning becomes apparent in all experiments that show a transition from twinning to slip-dominated behavior (Fig. 3). As illustrated in Fig. 8(c), an
exponential function is adopted for \( H_{t \rightarrow a}(\gamma_{tm}) \) to ensure that the effect of twinning induced slip system hardening ceases for large accumulated twinning shear strains,

\[
H_{t \rightarrow a}(\gamma_{tm}) = \begin{cases} 
0 & \text{for } \gamma_{tm} \leq \gamma_0 \\
 h_0 \exp \left( \frac{\gamma_{tm} - \gamma_0}{h_1} \right) & \text{for } \gamma_{tm} > \gamma_0 
\end{cases} \tag{47}
\]

The seed parameters \( \gamma_0 = 0.04, h_0 = 3.5 \, \text{GPa}, \) and \( h_1 = 0.02 \) are determined from the simulation of monotonic uniaxial compression experiment along the TD.

5.4 Numerical Parameter Identification. The introduction of the parametric models for the direct and latent hardening functions results in a large number of model parameters. In sum, we have 23 model parameters:

- Description of the initial state of the material
  - 3 anisotropy coefficients \( (P_{12}, P_{22}, P_{33}) \)
  - 3 initial back stresses \( (p_0^0, \tilde{p}_0^0, \tilde{p}_0^0) \)
  - 2 initial volume fractions \( (\lambda_T^0, \lambda_N^0) \)
- Crystallographic slip
  - 3 parameters \( (A, \varepsilon_B, n) \) associated with \( H(i) \)
  - 2 parameters \( (c, a) \) associated with kinematic hardening
- Twinning
  - 3 parameters \( (p_0, p_1, p_2) \) associated with \( s_k(\gamma_i) \)
  - 2 parameters \( (p_0, \tilde{p}) \) associated with \( s_k(\lambda_i) \)
  - 1 hardening modulus \( H_{t \rightarrow a} \) associated with \( s_k(\gamma_{tm}) \)
- Interaction of slip and twinning
  - 3 parameters \( (\gamma_0, h_0, h_1) \) associated with \( H_{t \rightarrow a}(\gamma_{tm}) \)
  - 1 hardening modulus \( H_{t \rightarrow a} \) associated with \( s_k(\lambda) \)

This large number of parameters is needed since distinct features of rather complex deformation mechanisms at the microscale (slip, twinning, and detwining) become visible at the macrosopic level when a polycrystalline magnesium alloy with strong basal texture is subject to mechanical loading.

The interaction of various mechanisms even for rather simple loading conditions such as uniaxial tension or compression makes it impossible to determine an analytical solution of the constitutive equations. Instead, a user material subroutine as implemented into the finite element software Abaqus/explicit is used for inverse parameter identification. Recall that the model features seven surfaces that describe the boundary of the elastic domain. However, due to the position of these surfaces with respect to each other, a maximum of three slip/twinning systems may become active simultaneously. Different from conventional single surface algorithms, the plastic multiplier becomes a vector. There exists a consistency condition for each component of this vector which poses a well-defined algebraic problem for determining the plastic multipliers. Based on the trial stress state, the potentially active systems are identified. Subsequently, a return-mapping is performed. In case of a negative plastic multiplier, the corresponding deformation system is deactivated and the return mapping repeated for the remaining potentially active systems only. Using this time integration scheme, simulations are performed to predict the model response for all uniaxial experiments, for pure shear and transverse plane strain tension.

The parameters \( P_{12}, P_{22}, P_{33}, \tilde{p}_0^0, \tilde{p}_f, A, a, c, p_0, h_0 \) and \( \tilde{\lambda} \) are then determined through Monte Carlo simulations. After defining a finite interval around the seed value of each parameter, more than 1000 independent random parameter combinations are generated assuming a uniform distribution for each parameter. For each set of parameters, the stress-strain curves are computed for tension followed by compression, compression followed by tension, transverse plane strain tension and simple shear. Based on the comparison with the corresponding experimental results, the “optimal” parameter set is chosen among the 1000 combinations. Table 2 summarizes the final model parameters. The left columns in Figs. 9 and 10 show a comparison of the corresponding model predictions (solid lines) with the experimental results (dashed lines). In addition, the evolution of the crystal volume fractions are shown in the left columns of these figures; \( \lambda_T \) is shown in blue, \( \tilde{\lambda} \) is shown in red, and \( \lambda_N \) is shown in green. The volume fractions are

![Fig. 9](image-url) Comparison of model predictions (solid black curves) with experiments (dashed blue lines) for uniaxial loading along the extrusion direction
Fig. 10 Comparison of model predictions (solid black curves) with experiments (dashed blue lines) for uniaxial loading along the transverse direction.

Fig. 11 Comparison of model predictions (solid black curves) with experiments (dashed blue lines) for combined tension and shear loading for $\alpha = 0$ deg (a)-(b) and for $\alpha = 90$ deg (c)-(d).
plotted as a function of a time like parameter. The corresponding axial strain is plotted as a gray dotted curve; its value is shown on the secondary axis. A comparison of the simulations and experiments for combined tension and shear is shown in Fig. 11.

6 Discussion

6.1 Comparison of Experiment and Simulation. The comparison of the simulation results with the experiments for uniaxial loading (Figs. 9 and 10) demonstrates the model’s ability to capture the characteristic features of the deformation behavior of extruded magnesium:

- Strong anisotropy for uniaxial tension: The model follows closely the experimental stress-strain curve for uniaxial tension along the ED (first branch of curve shown in Fig. 9(a)) and the TD (corresponding branch in Fig. 10(a)). The significant differences in stress level between the ED and TD are described accurately. Observe from Figs. 9(b) and 10(b) that the model predicts twinning from CT to CN (decreasing red curve, increasing blue curve) for tension along the TD, while the volume fractions remain unchanged (crystallographic slip only) for tension along the ED.

- Tension-compression asymmetry: The model predicts twinning from CN to CE and CT to CE for compression along ED (Fig. 9(d)), while twinning remained inactive for tension along the ED (Fig. 9(b)). Consequently, the apparent initial yield stress for compression is much lower than that for tension. The same observation is made for loading along the TD, where the model predicts intensive twinning from CN to CT for compression (Fig. 10(f)), while the tensile response is slip-dominated with only a small amount of twinning from CT to CN (Fig. 10(b)). Note that initial yield asymmetry can also be predicted through single macroscopic yield surface which is either pressure or Lode angle dependent. However, the strength of the present multisurface plasticity model lies its ability to associate different hardening responses to each yield surface. As a result, the concave and convex shaped hardening curves are predicted correctly including the transition from twinning-dominated to slip-dominated behavior.

- Detwinnng after load reversal: Figs. 9(e) and 9(f) show an example of the predicted change from twinning to detwinnng. The evoluction of the c-axis volume fractions show an increase of tE under compression (twinning) followed by a decrease of tE during subsequent tensile loading.

- Latent hardening: For example, the predicted increase in slip resistance due to twinning agrees well with that measured experimentally. Note that the yield stress may reach values as high as 400 MPa when twinning precedes slip, while the maximum stress level under monotonic tension is less than 250 MPa.

The model is also able to provide a reasonable prediction of the stress-strain response for combined tension and shear loading (Fig. 11). In particular, the pronounced difference between transverse plane strain tension along the ED and TD is captured by the model. The model performs less well for shear-dominated loading where the predicted curves typically lie above those measured experimentally. Moreover, the shapes of the predicted and experimental curves are different which indicates some more fundamental shortcomings within the model formulation.

6.2 Evolution of the Elastic Domain Boundary. The elastic domain in stress space is bound by the yield surface for crystallographic slip and by six planes associated with twinning. The solid black envelope in Fig. 12(a) shows the boundary surface in the (σE, σT)-plane after calibration. For uniaxial tension along the ED, the elastic loading path is limited by the curved envelope for slip. For uniaxial tension along the TD, the boundary envelope features a corner. It corresponds to the intersection of the yield envelope and the plane for twinning system #4 (CT → CN). As a result, both slip and twinning occurs for tension along the TD. The loading paths for uniaxial compression along the ED and TD are bound by the twinning surfaces #5 (CN → CE) and #6 (CN → CT), respectively. The twinning surfaces #1 (CE → CT) and #2 (CE → CN) do not intersect with the initial elastic domain because of the low initial volume fraction tE.

In addition to the initial elastic domain boundary (EDB), Fig. 12(a) shows the EDB evolution along the reverse loading path (compression followed by tension) described in Fig. 9(e). The blue envelope corresponds to the EDB at the point of load reversal. Except for the point of uniaxial compression along the ED, the elastic domain is bound by twinning planes only. Throughout uniaxial compression, the volume fraction tE has increased; consequently, twinning of CE-crystals becomes more likely which is reflected by a decrease of the twinning resistance for systems #1 and #2. As the material is reloaded under uniaxial tension, the elastic domain initially remains bound by the twinning systems only. However, the loading path for tension along the ED also hits the yield envelope for slip. The EDB at the end of the experiments (red envelope) therefore features a corner at which the twinning planes #1 and #2 intersect with the yield envelope for slip.

For illustration, we also show the evolution of the EDB for tension followed by compression along the TD in Fig. 12(b). The initial black envelope is the same as the one shown in Fig. 12(a). Upon compressive loading, twinning occurs on system #6 (CN → CT). Due to the increasing volume fraction tE, the resistance to twinning on system #4 (CT → CN) decreases. Thus, at the point of load reversal (blue envelope), the loading path for uniaxial tension along the TD is now limited by twinning plane #4. After load reversal, the EDB remains bound by the same twinning systems (see final red envelope). In other words, the evolution is mostly driven by self and latent hardening. Observe that the systems #3 (CT → CE) does not become active as the twinning on system #4 continuously decreases the volume fraction tE.
6.3 Future Work. Throughout the development of the present material model, we focused on the description of first order effects in an attempt to come up with a simple model formulation. The constitutive equations can still be solved numerically using a standard return mapping scheme. The resulting computational material model is suitable for large scale computations as far as its computational efficiency is concerned. However, as the simulations for combined tension and shear loading demonstrate, there is a need to improve the model further, in particular for multiaxial loading conditions. It is expected that a higher number of twinning systems needs to be considered for improved model predictions. Recall that the present model is limited to only three possible c-axis orientations. It is speculated that this model simplification is responsible for poor predictions when the loading is not aligned with the ED or TD. This aspect needs to be investigated experimentally in more detail in order to identify the dominant twinning systems for multiaxial loading. Moreover, it is highly desirable to calibrate (or at least validate) the proposed constitutive model based on experimental measurements of the texture evolutions. The assumed yield surface for crystallographic slip needs to be revisited as well. Here, we made use of Hill’s quadratic yield function with a back stress because of its simplicity and the lack of discriminating experimental data. It is relatively straightforward to determine a single initial yield surface for both twinning and slip. However, the key challenge lies in the separation of slip and twinning which is needed to come up with models that can predict the complex evolution of the elastic domain boundary under nonproportional and nonmonotonic loading conditions.

7 Conclusions

Using a newly designed anti-buckling device, the deformation response of extruded Mg AZ31 sheets is investigated experimentally for monotonic uniaxial tension and compression as well as tension followed by compression, and tension followed by compression. In addition, combined tension and shear experiments are performed for monotonic loading conditions. Due to the pronounced anisotropy of the material, specimens have been extracted along two different material directions. The measured stress-strain curves show the known characteristic features associated with the underlying microstructural deformation mechanisms: twinning, detwinning, crystallographic slip and their interaction.

A multifield plasticity model is presented with different surfaces for twinning and crystallographic slip. The material is considered as a single crystal (as far as twinning is concerned) because of the strong basal texture of the polycrystalline microstructure. The slip-driven deformation behavior is described through an anisotropic quadratic yield function. Latent hardening functions are introduced and calibrated such that they describe the observed stress-strain responses. The combination of a single crystal approach for twinning with a macroscopic plasticity model for slip results in a simple multisurface plasticity model which can describe the strong material anisotropy and tension-compression asymmetry in both initial yield and strain hardening. Furthermore, the transition from twinning-dominated to slip-dominated behavior as well as the evolution of texture is taken into account. As compared to polycrystal plasticity models, the model is highly efficient from a computational point of view and is suitable for use in large scale structural analyses.

Acknowledgment

The partial financial support by Volkswagen R&D is gratefully acknowledged. Dr. Eva Heripré from Ecole Polytechnique is thanked for characterizing the material microstructure.

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