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On the coupling of plastic slip and deformation-induced twinning in magnesium: A variationally consistent approach based on energy minimization

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Abstract

The present paper is concerned with the analysis of the deformation systems in single crystal magnesium at the micro-scale and with the resulting texture evolution in a polycrystal representing the macroscopic mechanical response. For that purpose, a variationally consistent approach based on energy minimization is proposed. It is suitable for the modeling of crystal plasticity at finite strains including the phase transition associated with deformation-induced twinning. The method relies strongly on the variational structure of crystal plasticity theory, i.e., an incremental minimization principle can be derived which allows to determine the unknown slip rates by computing the stationarity conditions of a (pseudo) potential. Phase transition associated with twinning is modeled in a similar fashion. More precisely, a solid-solid phase transition corresponding to twinning is assumed, if this is energetically favorable. Mathematically speaking, the aforementioned transition can be interpreted as a certain rank-one convexification. Since such a scheme is computationally very expensive and thus, it cannot be applied to the analysis of a polycrystal, a computationally more efficient approximation is elaborated. Within this approximation, the deformation induced by twinning is decomposed into the reorientation of the crystal lattice and simple shear. The latter is assumed to be governed by means of a standard Schmid-type plasticity law (pseudo-dislocation), while the reorientation of the crystal lattice is considered, when the respective plastic shear strain reaches a certain threshold value. The underlying idea is in line with experimental observations, where dislocation slip within the twinned domain is most frequently seen, if the twin laminate reaches a critical volume. The resulting model predicts a stress-strain response in good agreement

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with that of a rank-one convexification method, while showing the same numerical efficiency as a classical Taylor-type approximation. Consequently, it combines the advantages of both limiting cases. The model is calibrated for single crystal magnesium by means of the channel die test and finally applied to the analysis of texture evolution in a polycrystal. Comparisons of the predicted numerical results to their experimental counterparts show that the novel model is able to capture the characteristic mechanical response of magnesium very well.

1. Introduction

Light-weight materials are of great importance in transportation industries. Very promising candidates are magnesium and its alloys. Due to their high specific strength and their relatively low cost, they challenge aluminum alloys in some applications such as those in automotive industries, see Mordike and Ebert (2001). However, they exhibit a comparably poor formability under traditional metal forming processes. This originates from the hexagonal close-packed (HCP) structure of magnesium. In contrast to other metals such as aluminum with face-centered cubic (FCC) and iron with body-centered cubic (BCC) structure, the HCP structure of magnesium leads to a reduced number of energetically favorable dislocation systems. More precisely, with a reference lattice axial ratio of $c/a = 1.633$, magnesium with $c/a=1.624$ falls into the so-called *transition class*, see Christian and Mahajan (1995). The small difference to the reference lattice results in a complex mechanical interplay between dislocation slip and deformation-induced twinning. This has been observed in several experiments, see Hauser et al. (1955); Reed-Hill and Robertson (1957); Yoshinaga and Horiuchi (1963); Tegart (1964); Wonsiewicz and Backofen (1967); Roberts and Partridge (1966); Obara et al. (1973) and Ando and Tonda (2000). Though some of the characteristic deformation modes in single crystal magnesium are reasonably well understood such that the basal systems $\langle 11\bar{2}0 \rangle \{0001\}$ (Miller-Bravais indexing system for HCP lattices) and the prismatic systems $\langle 11\bar{2}0 \rangle \{\bar{1}100\}$ are mostly responsible for plastic deformation, many questions are still open and controversially discussed in the literature. For instance, although it is commonly accepted that twinning is activated in single crystal magnesium at the planes $\{\bar{1}012\}$ under tensile loading in $\langle 10\bar{1}1 \rangle$ direction, not much is known for the opposite loading direction. According to Wonsiewicz and Backofen (1967), twinning has been observed in this case as well. However, pyramidal slip on the system $\langle 11\bar{2}3 \rangle \{11\bar{2}2\}$ has also been frequently reported, see Obara et al. (1973); Lilleodden (2010).

While only little information are available about the qualitative mechanical response, even less is known about the quantitative behavior of single crystal magnesium. One effective way to get some further insight is provided by the so-called *channel die test*, see Wonsiewicz and Backofen (1967); Kelley and Hosford (1968) (cf. Sue and Havner (1984)). By using different crystal orientations within that test, classes of limited deformation systems can be enforced allowing to compute the respective hardening behavior (resolved shear stress vs. strain). However, except for rather simple deformation modes showing only a small number of active slip systems, significant further research is still required. For example, it is completely unknown for complex loading conditions, whether the twinned domain inherits the dislocations (i.e., plastic strains) corresponding to the initial phase, or if only a certain part of them is transferred. The present paper represents an additional step toward a better understanding of single crystal magnesium by combining experimental observations with physically sound material modeling.

An effective constitutive framework suitable for the modeling of dislocation slip was presented in the pioneering work Hill (1966); Rice (1971); Asaro and Rice (1977): *crystal plasticity theory*. In the late 90s, a variationally consistent reformulation of that theory was elaborated in Ortiz and Repetto (1999) (see also Carstensen et al. (2002); Miehe and Lambrecht (2003); Mosler and Bruhns (2009b)). This thermodynamically sound approach represents the fundament of the novel model discussed in the present paper. In contrast to conventional plasticity-like models, the approach advocated in Ortiz and Repetto (1999) allows to compute the unknown slip rates by minimizing a certain energy functional. Considering rate-independent problems, this potential turns out to be the stress power. In addition to its physical and mathematical elegance, the model proposed in Ortiz and Repetto (1999) shows also some numerical advantages. For instance, the determination of the set of active slip systems (see Peirce et al. (1982)) is naturally included within the aforementioned optimization problem and thus, a visco-plastic-type relaxation such as utilized in (Asaro, 1983; Asaro and Needleman, 1985) or other sophisticated regularization techniques similar to those in (Schmidt-Baldassari, 2003; McGinty and McDowell, 2006; Zamiri et al., 2007) can often be avoided.

Nowadays, a large number of (local) crystal plasticity theories suitable for the analysis of dislocation slip can be found in the literature. See Roters et al. (2010) for a recent overview. The opposite is true for the modeling of deformation-induced twinning and the coupling of the aforementioned deformation modes. Early attempts to combine twinning with dislocation slip were based on the concept of *pseudo-dislocation* (also referred to as PD-twinning), see e.g. Chin (1975) and references

cited therein. Conceptually, only the plastic shear strain caused by twinning has been accounted for within such approaches. First ideas related to the modeling of the reorientation of the crystal lattice due to deformation-induced twinning were addressed in Van Houtte (1978). Physically more sound descriptions of twinning as a phase transformation can be credited to the work Ericksen (1979). Therein, phase transformation is modeled by means of the theory of invariance groups of atomic lattices and the energy associated with their distortion, cf. Rajagopal and Srinivasa (1995). An elegant approximation of the kinematics associated with twinning goes back to James (1981), where Hadamard-like compatibility conditions were derived, see also Pitteri (1985); Ball and James (1987). According to James (1981), the deformation shows a weak discontinuity (discontinuous strain field) at the twin symmetry surface. More precisely, the deformation gradients on both sides of that surface differ from one another by a rank-one second-order tensor, cf. James (1981). As a consequence, twinning can be considered as a certain rank-one convexification (Ortiz and Repetto, 1999; Carstensen et al., 2002). This framework is nowadays well established for mechanical problems involving phase transformation. A typical example is the martensitic phase transformation occurring in shape memory alloys (Ball and James, 1987; Simha, 1997; Mueller, 1999; Idesman et al., 2000; James and Hane, 2000; Mielke et al., 2002). There, the aforementioned transition is modeled by means of a rank-one convexification. Physically speaking, a phase decomposition occurs within the cited models, if this is energetically favorable. Preliminary ideas to translate the underlying ideas into the modeling of deformation-induced twinning can be found in Kochmann and Le (2009). In that paper, first insight into the complex interplay between deformation-induced twinning and dislocation slip was obtained by analyzing a simple academic prototype problem showing only one active slip system.

Within the present paper, a thermodynamically consistent model suitable for the analysis of the fully coupled problem of dislocation slip and twinning is advocated. Though the discussed framework can be applied to a broad range of different materials, focus is on magnesium. In line with Ortiz and Repetto (1999) and Kochmann and Le (2009), the proposed approach is based on energy minimization, i.e., that particular combination between deformation-induced twinning and dislocation slip is chosen which minimizes the stress power. However, and in sharp contrast to Kochmann and Le (2009), a fully three-dimensional setting and a geometrically exact description (finite strains) is considered. Furthermore, all slip systems important for the mechanical response of single crystal magnesium are taken into account. For the modeling of the phase transition associated

with twinning, a novel approximation is discussed. Starting with a numerically very expensive rank-one convexification similar to those adopted in Ball and James (1987); Simha (1997); Mueller (1999); Idesman et al. (2000); James and Hane (2000); Mielke et al. (2002), the deformation induced by twinning is decomposed into the reorientation of the crystal lattice and simple shear. The latter is assumed to be governed by a standard Schmid-type plasticity law (pseudo-dislocation), while the reorientation of the crystal lattice is considered, when the respective plastic shear strain reaches a certain threshold value, cf. Staroselsky and Anand (2003). The underlying idea is in line with experimental observations, where dislocation slip within the twinned domain is most frequently seen, if the twin laminate reaches a critical volume. It will be shown that the resulting model predicts a stress-strain response in good agreement with that of a rank-one convexification method, while showing the same numerical efficiency as a classical Taylor-type approximation. Consequently, it combines the advantages of both limiting cases. The model is calibrated for single crystal magnesium by means of the channel die test. Since it is computationally very efficient, it can also be applied to the analysis of texture evolution in a polycrystal. Comparisons of the predicted numerical results to their experimental counterparts show that the advocated model is able to capture the characteristic macroscopic mechanical response of magnesium very well.

The paper is organized as follows: Section 2 is concerned with a variational reformulation of crystal plasticity theory. Within the resulting approach all slip rates follow conveniently from minimizing the stress power. Twinning is described in Section 3 as a solid-solid phase transition. More precisely, it is modeled as a certain rank-one convexification. Based on the resulting scheme, the effect of different interface energies is analyzed (twinning symmetry surface). A computationally more efficient approximation is subsequently elaborated in Subsection 3.2. It relies on the aforementioned decomposition of twinning into the reorientation of the crystal lattice and a superposed shear deformation. By carefully analyzing an academic prototype problem, the differences and analogies between the original model and its approximation are shown. The implementation of the resulting model is finally summarized in Section 4. In addition to a variationally consistent algorithmic formulation, an approximation by means of crystal visco-plasticity is also discussed. In Section 5, the material parameters of the final model are calibrated. Comparisons of the numerically predicted results to their experimental counterparts (channel die test) show that the novel model is able to capture the macroscopic characteristic mechanical response of single crystal magnesium very well. The applicability of the presented model to the analysis of texture evolution in a polycrystal is

finally demonstrated in Section 6.

2. The variational structure of crystal plasticity theory

This section is concerned with a concise review of the variational formulation of classical crystal plasticity. Further details can be found, e.g., in Ortiz and Repetto (1999); Carstensen et al. (2002); Miehe and Lambrecht (2003); Mosler and Bruhns (2009b). While in Subsection 2.1 the fundamentals of crystal plasticity are briefly summarized, the aforementioned variational formulation is discussed in Subsection 2.2. This section is completed by a short remark on the numerical implementation.

2.1. Fundamentals of crystal plasticity theory

In what follows, the deformation of a solid $\Omega \subset \mathbb{R}^3$ is defined by the mapping $\varphi(\mathbf{X}) : \Omega \rightarrow \mathbb{R}^3$. For the modeling of inelastic processes such as those related to dislocation slip, a nowadays standard multiplicative decomposition of the deformation gradient is adopted, i.e., according to

$$\mathbf{F} = \mathbf{F}^e \cdot \mathbf{F}^p, \text{ with } \det(\mathbf{F}^e) > 0 \text{ and } \det(\mathbf{F}^p) > 0, \quad (1)$$

the deformation gradient $\mathbf{F} = \text{GRAD}\varphi(\mathbf{X})$ is decomposed into a plastic part $\mathbf{F}^p$, which transforms the reference body to an intermediate, incompatible, stress free configuration, and an elastic part $\mathbf{F}^e$ corresponding to the elastic distortion (Lee, 1969). Hardening effects are taken into account by means of a finite set of strain-like internal variables $\boldsymbol{\lambda} \subset \mathbb{R}^n$. Obviously, those variables are related to the accumulated shear strain caused by dislocations slip (Lubliner, 1972; Ortiz and Repetto, 1999). With the aforementioned definitions and by assuming isothermal conditions, an Helmholtz energy of the type

$$\Psi = \Psi(\mathbf{F}, \boldsymbol{\lambda}) \quad (2)$$

is postulated, cf. Lubliner (1972, 1997); Simo and Hughes (1998). Since the elastic stored energy depends only on the elastic distortion (the elastic response of a solid is not affected by plastic deformations), the Helmholtz energy can be additively decomposed into an elastic part Ψ^e and a plastic part Ψ^p corresponding to plastic work. Combining this with the principle of material frame indifference, the stored energy can thus be written as

$$\Psi = \Psi^e(\mathbf{C}^e) + \Psi^p(\boldsymbol{\lambda}). \quad (3)$$

Here and henceforth, $\mathbf{C}^e := \mathbf{F}^{eT} \cdot \mathbf{F}^e$ is the elastic right Cauchy-Green tensor. In what follows, Ψ^P is further decomposed into the part Ψ_{self}^P related to self hardening and Ψ_{lat}^P associated with latent hardening, i.e.,

$$\Psi^P = \Psi_{\text{self}}^P + \Psi_{\text{lat}}^P. \quad (4)$$

While the elastic response of a single crystal is completely defined by assuming a physically sound energy Ψ^e , plastic deformations require, in addition to the energy Ψ^P , suitable evolution equations fulfilling the second law of thermodynamics. For deriving those evolution equations, the Clausius-Planck dissipation inequality

$$\mathcal{D} = \mathbf{P} : \dot{\mathbf{F}} - \dot{\Psi} = \mathbf{S} : \frac{1}{2} \dot{\mathbf{C}} - \dot{\Psi} \geq 0 \quad (5)$$

is considered, cf. Coleman (1964). In Eq. (5), $\mathbf{P}$ and $\mathbf{S}$ are the first and second Piola-Kirchhoff stress tensors and the superimposed dot denotes the material time derivative. Applying the Coleman & Noll procedure to elastic unloading (Coleman, 1964), yields the elastic response

$$\mathbf{S} = 2 \frac{\partial \Psi}{\partial \mathbf{C}} = 2(\mathbf{F}^P)^{-1} \cdot \frac{\partial \Psi}{\partial \mathbf{C}^e} \cdot (\mathbf{F}^P)^{-T} \quad (6)$$

and finally, by inserting Eq. (6) into the Clausius-Planck inequality (5), the reduced dissipation inequality

$$\mathcal{D} = \boldsymbol{\Sigma} : \mathbf{L}^P + \mathbf{Q} \cdot \dot{\boldsymbol{\lambda}} \geq 0 \quad (7)$$

with $\boldsymbol{\Sigma} := 2\mathbf{C}^e \cdot \partial_{\mathbf{C}^e} \Psi^e$ being the Mandel stresses (Mandel, 1972), $\mathbf{L}^P := \dot{\mathbf{F}}^P \cdot (\mathbf{F}^P)^{-1}$ denoting the plastic velocity gradient (with respect to the intermediate configuration) and $\mathbf{Q}$ being a set of stress-like internal variables conjugate to the strain-like internal variable $\boldsymbol{\lambda}$, i.e.,

$$\mathbf{Q} = -\frac{\partial \Psi}{\partial \boldsymbol{\lambda}}. \quad (8)$$

For the modeling of isotropic hardening in single crystals, the vector $\mathbf{Q}$ contains n stress-like internal variables corresponding to the admissible slip systems, i.e., $\mathbf{Q} = [Q^{(1)}, \dots, Q^{(n)}]$. Each of those is defined according to

$$Q^{(a)} = -\partial_{\lambda^{(a)}} \Psi^P = -\frac{\Psi_{\text{self}}^P}{\partial \lambda^{(a)}} - \frac{\Psi_{\text{lat}}^P}{\partial \lambda^{(a)}} = Q_{\text{self}}^{(a)} + Q_{\text{lat}}^{(a)} \quad (9)$$

where $\lambda^{(a)}$ is the strain-like internal variables conjugate to $Q^{(a)}$.

For providing certain loading conditions, i.e., deciding whether elastic unloading or plastic loading occurs, the space of admissible stresses $\mathbb{E}_\sigma$

$$\mathbb{E}_\sigma = \{(\boldsymbol{\Sigma}, \boldsymbol{Q}) \in \mathbb{R}^{9+n} \mid \phi^{(a)}(\boldsymbol{\Sigma}, \boldsymbol{Q}^{(a)}) \leq 0, a = 1, \dots, n\} \quad (10)$$

is introduced. It is defined by n convex yield functions $\phi^{(a)}$. Each of those is associated with a certain slip system within the respective single crystal and assumed to be governed by Schmid's law. More explicitly,

$$\phi^{(a)}(\boldsymbol{\Sigma}, \boldsymbol{\lambda}) = |\boldsymbol{\Sigma} : \boldsymbol{N}^{(a)}| - (\Sigma_0^{(a)} - Q^{(a)}(\boldsymbol{\lambda})). \quad (11)$$

Accordingly, the applied resolved shear stress at slip system a (the slip activation force) computed by projecting the Mandel stresses $\boldsymbol{\Sigma}$ onto the slip plane using the Schmid tensor $\boldsymbol{N}^{(a)} := (\boldsymbol{s}^{(a)} \otimes \boldsymbol{m}^{(a)})$ is compared to the material's current strength which is decomposed into an initial yield stress $\Sigma_0^{(a)}$ and an additional hardening term $Q^{(a)}$. The time invariant orthogonal unit vectors $\boldsymbol{m}^{(a)}$ and $\boldsymbol{s}^{(a)}$ correspond to the normal of the slip plane and the direction of the plastic shear strain.

By combining dissipation inequality (7) with the space of admissible stresses (10), physically sound evolution equations can be derived. For that purpose, the postulate of maximum dissipation is considered here, cf. Hill (1972). A straightforward computation yields in this case

$$\boldsymbol{L}^P = \sum_{a=1}^n \varsigma^{(a)} \frac{\partial \phi^{(a)}}{\partial \boldsymbol{\Sigma}} = \sum_{a=1}^n \varsigma^{(a)} \text{sign}[\boldsymbol{\Sigma} : \boldsymbol{N}^{(a)}] \boldsymbol{N}^{(a)} \quad \text{and} \quad \dot{\lambda}^a = \varsigma^{(a)} \frac{\partial \phi^{(a)}}{\partial Q^{(a)}} = \varsigma^{(a)}, \quad (12)$$

together with the Karush-Kuhn-Tucker optimality conditions (Rice, 1971; Luenberger, 1984)

$$\varsigma^{(a)} \geq 0, \quad \varsigma^{(a)} \dot{\phi}^{(a)} = 0. \quad (13)$$

In these equations, $\varsigma^{(a)}$ is the plastic multiplier associated with slip system a . It can be computed from the consistency conditions $\dot{\phi}^{(a)} = 0$. By inserting Eq. (12) into the dissipation inequality (7), the dissipation is obtained as

$$\mathcal{D} = \sum_{a=1}^n \varsigma^{(a)} \left[\text{sign}[\boldsymbol{\Sigma} : \boldsymbol{N}^{(a)}] (\boldsymbol{\Sigma} : \boldsymbol{N}^{(a)}) + Q^{(a)} \right] \stackrel{\phi^a=0}{=} \sum_{a=1}^n \varsigma^{(a)} \Sigma_0^{(a)} \geq 0. \quad (14)$$

Since $\Sigma_0^{(a)} > 0$ and $\varsigma^{(a)} \geq 0$, the second law of thermodynamics is indeed fulfilled. The closed form expression for the dissipation is a direct consequence of the positively homogeneity of the equivalent stresses $|\boldsymbol{\Sigma} : (\boldsymbol{s}^{(a)} \otimes \boldsymbol{m}^{(a)})|$.

2.2. A variational reformulation of crystal plasticity theory

A variational reformulation of the crystal plasticity model summarized in the previous section is discussed here. Although such a framework is not frequently applied, it is already relatively well developed. Further details concerning the variational structure of plasticity theory can be found, e.g., in Ortiz and Stainier (1999); Mosler and Bruhns (2009b). Without going too much into detail, the underlying idea is to minimize the stress power. This idea is directly related to the postulate of maximum dissipation, cf. Hackl and Fischer (2008).

Considering the crystal plasticity model presented in the previous subsection, the stress power is given by

$$\tilde{\mathcal{E}}(\dot{\varphi}, \dot{\mathbf{F}}^p, \dot{\boldsymbol{\lambda}}, \boldsymbol{\Sigma}, \mathbf{Q}) = \dot{\Psi}(\dot{\varphi}, \dot{\mathbf{F}}^p, \dot{\boldsymbol{\lambda}}) + \mathcal{D}(\dot{\boldsymbol{\lambda}}) + J(\boldsymbol{\Sigma}, \mathbf{Q}) \quad (15)$$

Here, the characteristic function of the admissible stress space

$$J := \begin{cases} 0 & \forall (\boldsymbol{\Sigma}, \mathbf{Q}) \in \mathbb{E}_\sigma \\ \infty & \text{otherwise} \end{cases} \quad (16)$$

has been introduced. Accordingly, J penalizes the functional (15) for inadmissible stress states. It can be shown that the stationarity conditions of functional (15) are equivalent to the crystal plasticity model discussed in the previous section, cf. (Carstensen et al., 2002), i.e.,

$$\begin{aligned} \partial_{\boldsymbol{\Sigma}} \tilde{\mathcal{E}} = 0 & \Rightarrow \mathbf{L}^p = \sum_{a=1}^n \varsigma^{(a)} \frac{\partial \phi^{(a)}}{\partial \boldsymbol{\Sigma}} \\ \partial_{\mathbf{Q}} \tilde{\mathcal{E}} = 0 & \Rightarrow \dot{\boldsymbol{\lambda}}^a = \varsigma^{(a)} \frac{\partial \phi^{(a)}}{\partial \mathbf{Q}^{(a)}} \\ \partial_{\dot{\boldsymbol{\lambda}}^{(a)}} \tilde{\mathcal{E}} = 0 & \Rightarrow Q^{(a)} = -\partial_{\dot{\boldsymbol{\lambda}}^{(a)}} \Psi^p \\ \partial_{\dot{\mathbf{F}}^p} \tilde{\mathcal{E}} = 0 & \Rightarrow \boldsymbol{\Sigma} = 2 \mathbf{C}^e \cdot \partial_{\mathbf{C}^e} \Psi^e. \end{aligned} \quad (17)$$

Hence, this stationarity problem represents a variational reformulation of crystal plasticity theory. By enforcing the postulate of maximum dissipation (maximization with respect to the stress-like variables) the reduced stress power, now a function in terms of strain-like variables only, reads

$$\mathcal{E}(\dot{\varphi}, \dot{\mathbf{F}}^p, \dot{\boldsymbol{\lambda}}) = \dot{\Psi}(\dot{\varphi}, \dot{\mathbf{F}}^p, \dot{\boldsymbol{\lambda}}) + J^*(\dot{\mathbf{F}}^p, \dot{\boldsymbol{\lambda}}). \quad (18)$$

Here, J^* is the Legendre transformation of the characteristic function J . Physically speaking and considering associative evolution equations, it is the dissipation. Hence, in case of admissible states, J^* can be computed in closed form and is given by Eq. (14). Interestingly and in contrast to the

stationarity problem $\text{stat}\tilde{\mathcal{E}}$, the crystal plasticity model described in the previous subsection can now be formulated as a minimization problem of the type $\inf \mathcal{E}$. More precisely, the evolution equations (12) are equivalent to

$$(\dot{\mathbf{F}}^{\text{p}}, \dot{\boldsymbol{\lambda}}) = \arg \inf_{\dot{\mathbf{F}}^{\text{p}}, \dot{\boldsymbol{\lambda}}} \mathcal{E}(\dot{\boldsymbol{\varphi}}, \dot{\mathbf{F}}^{\text{p}}, \dot{\boldsymbol{\lambda}}). \quad (19)$$

Minimization principle (19) gives rise to the introduction of the reduced functional

$$\hat{\mathcal{E}}(\dot{\boldsymbol{\varphi}}) := \inf \mathcal{E} = \mathbf{P} : \dot{\mathbf{F}}. \quad (20)$$

Accordingly and in line with hyperelastic materials, this pseudo potential defines the stress response, i.e.,

$$\mathbf{P} = \partial_{\dot{\mathbf{F}}} \hat{\mathcal{E}}. \quad (21)$$

2.3. Numerical implementation - Variational constitutive updates

Based on minimization principle (19), effective numerical implementations can be developed. For that purpose, a time discretization of the continuously defined functional (18) of the type

$$I_{\text{inc}} = \int_{t_n}^{t_{n+1}} \tilde{\mathcal{E}} \, dt = \Psi_{n+1} - \Psi_n + \sum_{a=1}^n \Delta \varsigma^{(a)} \Sigma_0^{(a)}, \quad \Delta \varsigma^{(a)} := \int_{t_n}^{t_{n+1}} \varsigma^{(a)} \, dt \quad (22)$$

is considered. Here, t_n and t_{n+1} are two pseudo times. For computing the Helmholtz energy Ψ at time t_{n+1} , the plastic part of the deformation gradient is approximated by means of an exponential integration scheme, while a classical backward Euler discretization is applied to the strain-like internal variables, i.e.,

$$\mathbf{F}_{n+1}^{\text{p}} = \exp(\Delta t \mathbf{L}^{\text{p}}) \cdot \mathbf{F}_n^{\text{p}}, \quad \lambda_{n+1}^a = \lambda_n^a + \Delta \varsigma^{(a)}. \quad (23)$$

Inserting these approximations into Eq. (22), together with the flow rule (12)₁, the incrementally defined functional I_{inc} depends on the unknown slip rates (discrete increments) as well as on the current deformation gradient (the old state is known in numerical schemes such as the finite element method). As a consequence,

$$I_{\text{inc}} = I_{\text{inc}}(\mathbf{F}_{n+1}, \Delta \varsigma^{(1)}, \dots, \Delta \varsigma^{(n)}). \quad (24)$$

Based on this functional the slip rates can be computed according to

$$(\Delta \varsigma^{(1)}, \dots, \Delta \varsigma^{(n)}) = \arg \inf_{\Delta \varsigma^{(1)}, \dots, \Delta \varsigma^{(n)}} I_{\text{inc}}|_{\mathbf{F}_{n+1}} \quad (25)$$

and finally, the stresses are defined by

$$\mathbf{P} = \partial_{\mathbf{F}_{n+1}} \inf_{\Delta_{\zeta(1)}, \dots, \Delta_{\zeta(n)}} I_{\text{inc}}. \quad (26)$$

Further details on variational constitutive updates are omitted. They can be found, for instance, in Mosler and Bruhns (2009a,b).

In addition to its physical and mathematical elegance, the variational constitutive update presented here shows further advantages. For instance, the determination of the set of the active slip systems is naturally included within the optimization problem and thus, sophisticated regularization techniques such as those in (Schmidt-Baldassari, 2003; McGinty and McDowell, 2006; Zamiri et al., 2007) are not required. Even more importantly, energy principles provide a physically sound basis for coupling different models, cf. Mosler and Cirak (2009), i.e., the energetically most favorable combination between the respective models is considered. Such a canonical coupling is also proposed in the present paper for combining plastic slip and deformation-induced twinning.

3. Modeling of deformation-induced twinning as a solid-solid phase transition

In the previous section, constitutive models suitable for the analysis of dislocation slip were briefly discussed and reformulated within a variationally consistent framework. In the present section, focus is on the solid-solid phase transitions associated with deformation-induced twinning. In line with the previous subsection and for the sake of consistency, the aforementioned phase transition is assumed to be governed by energy minimization, i.e., a twin forms, if this is energetically favorable. While twinning is considered as a certain rank-one convexification in Subsection 3.1, a computationally more efficient approach is elaborated in Subsection 3.2. It is based on decomposing the deformation induced by twinning into a shear strain and the re-orientation of the crystal lattice.

3.1. Modeling twinning by rank-one convexification

Twinning is characterized by a laminate structure, cf. James (1981). A powerful mathematical tool for analyzing such problems is provided by the concept of rank-one convexification, cf. Carstensen et al. (2002). Within this concept, the energy of a solid is further minimized by allowing for certain phase-decompositions (micro-structures). Continuity of the sub-deformations is guaranteed by enforcing a Hadamard-type (Ball and James, 1987) compatibility condition between the deformation gradients within the different phases.

Figure 1: Lattice rotation associated with deformation-induced twinning

3.1.1. Kinematics

A twin $\partial\Omega_{\text{Tw}}$ partitions the initial domain $\Omega \subset \mathbb{R}^3$ into the sub-bodies Ω_{ini} and Ω_{Tw} , i.e., $\Omega = \Omega_{\text{ini}} \cup \Omega_{\text{Tw}} \cup \partial\Omega_{\text{Tw}}$. While the crystal lattice in Ω_{ini} is equivalent to that in Ω , the simple shear parallel to the twin plane $\partial\Omega_{\text{Tw}}$ changes the crystal lattice in Ω_{Tw} . Such a transformation can be described by a proper orthogonal tensor $\mathbf{R}$. More precisely, denoting the lattice vectors of the initial phase as $\mathbf{e} := \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ and those corresponding to the twinned configuration as $\tilde{\mathbf{e}}$, the transformation

$$\tilde{\mathbf{e}} = \mathbf{R} \cdot \mathbf{e}. \quad (27)$$

holds, see Fig. 1. With $\mathbf{n}$ being the normal vector of the twin interface, $\mathbf{R}$ is defined by (Pitteri, 1985)

$$\mathbf{R} = -\mathbf{I} + 2(\mathbf{n} \otimes \mathbf{n}) \text{ with } \det \mathbf{R} = 1. \quad (28)$$

Commonly observed micro-structures suggest that twinning occurs with laminate topology. Here, a first-order approximation is considered. More precisely and following James (1981); Ortiz and Repetto (1999); Carstensen et al. (2002), the deformation gradient $\mathbf{F}_{\text{ini}}$ associated with the initial phase Ω_{ini} and $\mathbf{F}_{\text{Tw}}$ belonging to Ω_{Tw} are decomposed according to

$$\mathbf{F}_{\text{Tw}} = \mathbf{F}_{\text{ini}} - \lambda_{\text{Twin}}(\mathbf{a} \otimes \mathbf{n}). \quad (29)$$

For guaranteeing a resulting physically reasonable macroscopic strain, the additional compatibility conditions

$$\mathbf{F} = \xi_{\text{ini}}\mathbf{F}_{\text{ini}} + \xi_{\text{Tw}}\mathbf{F}_{\text{Tw}} \quad (30)$$

and

$$\xi_{\text{ini}} + \xi_{\text{Tw}} = 1 \quad (31)$$

are enforced, see Silhavy (1997). Henceforth, the subscript (Tw) is omitted from ξ_{Tw} , i.e., ξ denotes the volume fraction of the twinning phase. As evident from Eq. (29), the rank-one deformation tensor $\lambda_{\text{Tw}}(\mathbf{a} \otimes \mathbf{n})$ defines the deformation jump across the twinning interface. In this connection, the normal vector $\mathbf{n}$ corresponds to the twinning plane (interface), while $\mathbf{a}$ and λ_{Tw} define the jump direction and the amplitude of the shear deformation. In contrast to conventional rank-one convexification (Carstensen et al., 2002), the direction and the amplitude of the twinning shear are a priori prescribed by the respective lattice structure. For instance, in case of magnesium tensile twinning ($\mathbf{a} := \langle 10\bar{1}1 \rangle$, $\mathbf{n} := \{\bar{1}012\}$), it is obtained as $\lambda_{\text{Tw}} = f(c/a)$, see Christian and Mahajan (1995).

Remark 1. *Generally, deformation-induced twinning can occur successively by several twinning variants. In this case, the aforementioned phase decomposition has to be considered several times. However, within the present paper, only first-order laminates will be modeled. Since the resulting approach predicts the mechanical response of magnesium single crystal very well, computationally more expensive higher-order approximations will not be analyzed here.*

3.1.2. Energy

According to the previous subsection, the presence of twin laminates induces deformation fluctuations in the initial phase. More precisely, the deformation gradient decomposes as stated in Eq. (29). Consequently, the Helmholtz energy of the whole solid can be described by a volume averaging of the energies associated with each phase, i.e.

$$\Psi_{\text{C}}(\mathbf{C}, \mathbf{F}_{\text{ini}}^{\text{p}}, \boldsymbol{\lambda}_{\text{ini}}, \mathbf{F}_{\text{Tw}}^{\text{p}}, \boldsymbol{\lambda}_{\text{Tw}}, \xi) = (1 - \xi)\Psi_{\text{ini}}(\mathbf{C}_{\text{ini}}^{\text{e}}, \boldsymbol{\lambda}_{\text{ini}}) + \xi \Psi_{\text{Tw}}(\mathbf{C}_{\text{Tw}}^{\text{e}}, \boldsymbol{\lambda}_{\text{Tw}}) + \Psi^{\text{mix}}(\xi). \quad (32)$$

In Eq. (32), an additional mixture energy Ψ^{mix} has been introduced. It primarily depends on the coherency of the neighboring phases in the vicinity of the interface. It vanishes in case of unconstrained twinning, e.g., Fig. 1. The purpose of this mixture energy is twofold. First, as mentioned before, it allows to include interface effects, i.e., it leads to a physically more sound model. Second, by choosing different energies, different approximations of phase transition can be analyzed within a unique framework. For instance, by choosing

$$\Psi^{\text{mix}} = \begin{cases} 0 & \forall \xi \in \{0; 1\} \\ \infty & \forall \xi \in (0, 1) \end{cases} \quad (33)$$

a classical Taylor-type approximation is obtained, i.e., either phase Ω_{ini} or Ω_{Tw} will be active. Mixture cannot occur, if energy minimization is the overriding principle. Clearly, by neglecting the

mixture energy, the rank-one convexification method is obtained. It represents a lower bound of the energy, i.e.,

$$\inf_{\xi} \Psi_C \leq \Psi. \quad (34)$$

Remark 2. *In the present subsection, the concept of rank-one convexification was briefly discussed. Although only the Helmholtz energy has been considered, the same concept can also be applied to the dissipation or to the incrementally defined potential associated with variational constitutive updates, cf. Subsection 2.2. For the sake of understandability, dissipative effects have been excluded here. However, the final model combining deformation-induced twinning and dislocation slip will show such features.*

Remark 3. *The notation Taylor-type approximation has been chosen, since the introduction of pseudo-dislocations allows to consider only one phase ($\xi \in \{0; 1\}$) with a constant strain field for each grain.*

3.1.3. Effect of mixture energy on phase transition

The mixture energy Ψ^{mix} in Eq. (32) governs implicitly the phase transition induced by deformation-induced twinning. By using a simple prototype model, this effect is analyzed here. For the sake of simplicity, it is assumed that the initial and the twinning phase are dislocation free (i.e., no plastic strains) and further dissipative processes are also excluded (fully reversible model). The more general case, including dissipation will be discussed later.

With these assumptions and adopting a St. Venant material model, the Helmholtz energy of the initial phase is given by

$$\Psi_{\text{ini}}(\mathbf{E}_{\text{ini}}) = \frac{1}{2} \mathbf{E}_{\text{ini}} : \mathbb{K}_{\text{ini}} : \mathbf{E}_{\text{ini}} \quad (35)$$

where $\mathbf{E}_{\text{ini}} = \frac{1}{2}(\mathbf{F}_{\text{ini}}^T \cdot \mathbf{F}_{\text{ini}} - \mathbf{I})$ is the Green-Lagrange strain tensor and $\mathbb{K}_{\text{ini}}$ denotes the fourth-order elastic stiffness tensor. It is supposed that the material shows twinning at the system ($\mathbf{a} := \{01\bar{1}1\}, \mathbf{n} := \{0\bar{1}12\}$). Accordingly, the twinning shear strain $\mathbf{E}_{\text{Twin}}$ which defines the stress free state of the twinning phase is obtained by

$$\mathbf{E}_{\text{Twin}} = \frac{1}{2}(\mathbf{F}_{\text{Twin}}^T \cdot \mathbf{F}_{\text{Twin}} - \mathbf{I}) \quad (36)$$

with

$$\mathbf{F}_{\text{Twin}} = \mathbf{I} + \lambda_{\text{Twin}}(\mathbf{a} \otimes \mathbf{n}). \quad (37)$$

Since the material properties of both phases are similar, the elastic strain energy of the twinning phase can be derived from that of the initial phase simply by translating the stress free state. More

explicitly, the energy of the new phase reads

$$\Psi_{\text{Tw}}(\mathbf{E}_{\text{Tw}}) = \frac{1}{2}(\mathbf{E}_{\text{Tw}} - \mathbf{E}_{\text{TwIn}}) : \mathbb{K}_{\text{Tw}} : (\mathbf{E}_{\text{Tw}} - \mathbf{E}_{\text{TwIn}}) + \alpha. \quad (38)$$

Here, the scalar-valued parameter α corresponds to the thermal activation energy of twinning which is taken as a constant. Following the previous subsection, the total energy obtained by volume averaging is thus given by

$$\Psi = (1 - \xi)\Psi_{\text{ini}}(\mathbf{E}_{\text{ini}}) + \xi \Psi_{\text{Tw}}(\mathbf{E}_{\text{Tw}}) + \Psi_{\text{mix}}(\xi). \quad (39)$$

Consequently, by considering the Hadamard-type compatibility condition Eq. (29) and taking into account that the vectors $\mathbf{a}$, $\mathbf{n}$ as well as the shear strain λ_{TwIn} are a priori known from crystallographic information, the energy Ψ depends only on the macroscopic deformation gradient as well as on the unknown volume fraction ξ , i.e.,

$$\Psi = \Psi(\mathbf{F}, \xi). \quad (40)$$

Despite the fact that several parameters such as the laminate morphology, chemical composition, temperature and dislocation structures have deterministic effects on the mixture energy Ψ^{mix} , a simplified model of the type

$$\Psi^{\text{mix}}(\xi) = \frac{f\mu}{(1 + \exp[c(\xi - a)])(1 + \exp[-c(\xi - b)])}, \quad (41)$$

solely depending on the current twinning volume fraction ξ is adopted, cf. Mueller and Bruhns (2006). In Eq. (41), μ is the elastic shear modulus and $\{a, b, c, f\}$ is a set of adjustable scalar shape function parameters defining the mixture energy Ψ^{mix} , see Fig. 2. In case of a fully coherent interface not showing any residual stresses, the mixture energy "Coh" is set to zero. The other limiting case is the Boxcar-type function. It describes a highly incoherent interface. Depending on the shear modulus, this function is a good approximation of the classical Taylor-type homogenization. More precisely, if energy minimization is the overriding principle and μ is large enough, phase mixture cannot occur.

The prototype model discussed before is subjected to a shear strain

$$\mathbf{F} = \mathbf{I} + \varepsilon(\mathbf{a} \otimes \mathbf{n}) \quad (42)$$

parallel to the twinning plane. Here, ε denotes the strain amplitude. Subsequently, the stable state of the system is obtained by minimizing the total energy, i.e.,

$$\inf_{\xi} \Psi(\varepsilon, \xi). \quad (43)$$

Function label	a	b	c	f
Boxcar	0.99	0.01	1000	1
Bell _A	0.70	0.30	15	1
Bell _B	0.60	0.40	10	1
Coh	0.45	0.55	1000	1

Figure 2: Mixture energies (41) as a function of the twinning volume fraction ξ

The resulting energies are summarized in Fig. 3 (left). There, the thin lines correspond to the energies of the single phases. The evolution of the computed volume ratio ξ is shown in Fig. 3 (right). As expected, the interface energy strongly governs the phase transition. In the case of a coherent interface, the total energy is identical to the rank-one convex hull which results in a linear evolution of the twinning volume fraction. By way of contrast, the Boxcar mixture energy leads to a Taylor-type phase transition. The Gaussian mixture energies range between the aforementioned limiting cases.

Certainly, although the energy governs phase transition within the presented model, this physical quantity can not be measured in experiments. For that reason, the stress response is analyzed as well. Fig. 4 summarizes the respective diagrams. Since the considered deformations are comparably small, the stress-strain diagrams are piecewise linear. In case of coherent phases (Fig. 4f), a classical stress plateau can be seen, i.e., the stress increases linearly except for within the transition range $\xi \in (0, 1)$. By way of contrast, for the other limiting case, being the Boxcar-type mixture energy, a Taylor transition is observed. More precisely, the stress-strain diagram is discontinuous and shows a jump at the transition point. Experimental evidence of such a behavior can be found, e.g., in Salje et al. (2009); Harrison et al. (2004). However, considering sufficiently large samples of single crystal magnesium, a continuous stress-strain response is expected, cf. Kelley and Hosford (1968); Lilleodden (2010). Hence, the Taylor-type model, although computationally very efficient cannot be utilized. The opposite is true for the coherent case being identical to a rank-one convexification:

Figure 3: Left: elastic strain energy of the initial and twinning phase and the resulting homogenized energy using the mixture energies illustrated in Fig.(3); Right: evolution of the twinning volume fraction ξ depending on the considered mixture energy

It leads to physically sound results, but it is numerically very expensive. For this reason, an approximation combining the advantages of these limiting cases will be elaborated in the next subsection.

3.2. An approximation of the solid-solid phase transition induced by twinning

Although the modeling of a solid-solid phase transition by means of the concept of rank-one convexification is physically sound, its application to complex systems showing dislocation slip and deformation-induced twinning is numerically very expensive (in case of magnesium, the interplay between twelve dislocation systems and six different twinning modes has to be considered). More precisely, the respective computational costs corresponding to the numerical analysis of a polycrystal would be prohibitive. Therefore, an approximation of the rank-one convexification method which is significantly more efficient will be elaborated here.

3.2.1. Fundamentals

The underlying idea of the proposed novel model suitable for the analysis of solid-solid phase transition originates from experimental observations (Barber and Wenk, 1979; Terlinde and Luetjering, 1982; Chia et al., 2005; Li and Ma, 2009). According to the cited works, experiments show that the width of a twin laminate has to be large enough to allow for dislocation slip inside this laminate. Consequently, observable plastic deformations within the twin require a sufficient twin

volume. This phenomenon is strongly pronounced particularly in the case of magnesium with a very low twinning activation energy.

The aforementioned experimental observations suggest to decompose twinning into two stages. Within the first of those, the twin laminate is comparably small and hence, plastic deformations within the reoriented phase can be neglected. If the twin volume reaches a critical threshold, the slip systems corresponding to the reoriented crystal lattice may become active. For modeling the first stage, the concept of *pseudo-dislocation* is utilized, cf. Chin (1975). Hence, instead of computing the twin volume explicitly, the shear strain caused by twinning is considered. If this shear strain equals the twinning strain (unconstrained twinning), the crystal lattice is reoriented. For the sake of computational efficiency, the reorientation is applied to the whole underlying representative volume. Consequently, the deformation systems associated with the original crystal lattice may be active in the first stage, while only the systems related to the reoriented crystal are considered in the second stage.

Accounting for standard dislocation slip ($\varsigma^{(a)}$) as well as for the aforementioned pseudo-dislocation-related slip ($\varsigma_{\text{pd}}^{(j)}$) caused by twinning within the first transformation stage yields a plastic velocity gradient of the type

$$\mathbf{L}^p = \sum_{a=1}^n \varsigma^{(a)} \text{sign}[\boldsymbol{\Sigma} : \mathbf{N}^{(a)}] \mathbf{N}^{(a)} + \sum_{j=1}^m \varsigma_{\text{pd}}^{(j)} \text{sign}[\boldsymbol{\Sigma} : \mathbf{N}^{(j)}] \mathbf{N}^{(j)} \quad (44)$$

with

$$\mathbf{N}_{\text{pd}}^{(j)} = \mathbf{a}^{(j)} \otimes \mathbf{n}^{(j)}. \quad (45)$$

Accordingly, the slip caused by pseudo-dislocations is assumed to be governed by a standard Schmid-type law. Further extending this analogy, the Helmholtz energy describing the initial (not twinned) phase is chosen as

$$\Psi_{\text{ini}}(\mathbf{C}^e, \boldsymbol{\lambda}, \boldsymbol{\lambda}_{\text{pd}}) = \Psi^e(\mathbf{C}^e) + \Psi^p(\boldsymbol{\lambda}) + \Psi_{\text{pd}}^p(\boldsymbol{\lambda}_{\text{pd}}). \quad (46)$$

Here, $\lambda_{\text{pd}}^{(i)}$ are internal variables associated with the pseudo-dislocation ($\dot{\lambda}_{\text{pd}}^{(i)} = \varsigma_{\text{pd}}^{(i)}$). Once the critical twinning strain is reached, the energy of the reoriented phase is active. Since, the original and the twinned domain show the same mechanical properties (except for the orientation of the crystal lattice), the Helmholtz energy of the reoriented phase reads

$$\Psi_{\text{Tw}}(\mathbf{C}^e, \boldsymbol{\lambda}) = \Psi^e(\mathbf{C}^e) + \Psi^p(\boldsymbol{\lambda}). \quad (47)$$

Having defined the Helmholtz energies of the different phases, the total energy can be computed in standard manner. In line with the previous subsections, it is given by

$$\Psi(\mathbf{C}^e, \boldsymbol{\lambda}, \boldsymbol{\lambda}_{\text{pd}}, \boldsymbol{\lambda}_{\text{Tw}}, \xi) = (1 - \xi)\Psi_{\text{ini}}(\mathbf{C}^e, \boldsymbol{\lambda}, \boldsymbol{\lambda}_{\text{pd}}) + \xi \Psi_{\text{Tw}}(\mathbf{C}_{\text{Tw}}^e, \boldsymbol{\lambda}_{\text{Tw}}) + \Psi_{\text{mix}}(\xi), \quad \forall \xi \in \{0; 1\}. \quad (48)$$

Although Eq. (48) looks formally identical to Eq. (32), both models are significantly different. While a continuous evolution for ξ is considered within the framework provided by the rank-one convexification, the novel approximation is based on a discontinuous transition, i.e., $\xi \in \{0; 1\}$. Clearly, the mixture energy can thus be neglected and consequently, a minimization of Eq. (48) w.r.t. ξ simplifies to

$$\inf_{\xi \in \{0; 1\}} \Psi(\mathbf{C}^e, \boldsymbol{\lambda}, \boldsymbol{\lambda}_{\text{pd}}, \boldsymbol{\lambda}_{\text{Tw}}, \xi) = \min[\Psi_{\text{ini}}(\mathbf{C}^e, \boldsymbol{\lambda}, \boldsymbol{\lambda}_{\text{pd}}), \Psi_{\text{Tw}}(\mathbf{C}_{\text{Tw}}^e, \boldsymbol{\lambda}_{\text{Tw}})]. \quad (49)$$

Remark 4. *During the first stage in which twinning is described by the concept of pseudo-dislocation, the elastic energy of the reoriented phase has been neglected. Such an approximation is admissible, since the elastic deformations are comparably small in magnesium. However, the more general case is also included in the framework as discussed here.*

Remark 5. *As mentioned before, it is completely unknown for complex loading conditions, whether the twinned domain inherits the dislocations corresponding to the initial phase, or if only a certain part of them is transferred. Therefore and focusing on the model presented here, it is not clear which initial conditions are to be chosen for $\boldsymbol{\lambda}_{\text{Tw}}$. Within the present paper, the final values of $\boldsymbol{\lambda}$ serve as initializers of $\boldsymbol{\lambda}_{\text{Tw}}$. Hence, it is assumed that the whole dislocation history is kept.*

Remark 6. *Within the presented model, phase transition occurs, if the slip caused by pseudo-dislocations reaches a certain threshold. In this respect, the transformation is strain-based. However, by choosing $\Psi_{\text{pd}}^p(\boldsymbol{\lambda}_{\text{pd}})$ properly, an equivalent energy depending criterion can be derived. Such a criterion will be elaborated for the final model.*

Remark 7. *Although only the Helmholtz energy has been considered within the present subsection, the discussed ideas can also be applied to the dissipation and the stress power. Accordingly, the final model will capture dissipative effects as well.*

3.2.2. Illustrative examples

In this subsection, the characteristics of the novel phase transition model as discussed in the previous subsection are illustrated. It will be shown that this model combines the advantages of a classical Taylor-type approximation and the computationally more expensive concept of rank-one convexification. More precisely, the continuous stress-strain response as predicted by the model is in line with that of the rank-one convexification, while it is as efficient as the Taylor-type model. First, a fully reversible prototype is considered. Subsequently, dissipative effects are considered as well.

Prototype model. The mechanical prototype model analyzed here is in line with that previously discussed in Subsection 3.1.3. The sole difference is that pseudo-dislocation slip caused by twinning is already considered within the initial phase. Accordingly, the plastic deformations in the initial phase are described by

$$\mathbf{F}_{\text{ini}}^{\text{p}} = \mathbf{I} + \lambda_{\text{pd}}(\mathbf{a} \otimes \mathbf{n}) \quad (50)$$

with λ_{pd} being the magnitude of the PD's plastic shear. With Eq. (50) and assuming a St. Venant model, the stored energy of the initial phase is given by

$$\Psi_{\text{ini}}(\mathbf{E}_{\text{ini}}, \lambda_{\text{pd}}) = \frac{1}{2}(\mathbf{E}_{\text{ini}} - \mathbf{E}_{\text{ini}}^{\text{p}}) : \mathbb{K}_{\text{ini}} : (\mathbf{E}_{\text{ini}} - \mathbf{E}_{\text{ini}}^{\text{p}}) + \Psi_{\text{pd}}^{\text{p}}(\lambda_{\text{pd}}) \quad (51)$$

with $\mathbf{E}_{\text{ini}} = 1/2(\mathbf{F}_{\text{ini}}^T \cdot \mathbf{F}_{\text{ini}} - \mathbf{1})$ and $\mathbf{E}_{\text{ini}}^{\text{p}} = 1/2(\mathbf{F}_{\text{ini}}^{\text{p}T} \cdot \mathbf{F}_{\text{ini}}^{\text{p}} - \mathbf{1})$ being the total Green-Lagrange strain tensor and its plastic part. The model is completed by assuming a suitable energy $\Psi_{\text{pd}}^{\text{p}}(\lambda_{\text{pd}})$. Here, the choice

$$\Psi_{\text{pd}}^{\text{p}}(\lambda_{\text{pd}}) = \beta \lambda_{\text{pd}} + \Pi(\lambda_{\text{pd}}) \quad (52)$$

is made. In Eq. (52), $\Pi(\lambda_{\text{pd}})$ can be understood as a penalty function guaranteeing that the plastic shear of PD-twinning is properly bounded, i.e., $\lambda_{\text{pd}} \in [0, \lambda_{\text{Twin}}]$. This can be realized by defining

$$\Pi(\lambda_{\text{pd}}) := \begin{cases} 0 & \text{if } \lambda_{\text{pd}} \in [0, \lambda_{\text{Twin}}) \\ \infty & \text{if } \lambda_{\text{pd}} \geq \lambda_{\text{Twin}} \end{cases} \quad (53)$$

Consequently, if energy minimization is the overriding principle, the second phase is energetically more favorable, if the PD-twinning strain λ_{pd} approaches the threshold λ_{Twin} . In this respect, $\Pi(\lambda_{\text{pd}})$ defines an energy-based transformation condition. However, other penalty functions are also admissible. More precisely, they have only to be monotonically increasing and converge to infinity for $\lambda_{\text{pd}} \rightarrow \lambda_{\text{Twin}}$. In line with self and latent hardening, the best choice for $\Pi(\lambda_{\text{pd}})$ depends on experimental measurements.

Having discussed the second term in Eq. (52), the linear summand $\beta \lambda_{\text{pd}}$ remains to be explained. Although the Helmholtz energy is addressed here, this term looks formally identical to the dissipation (product of plastic multiplier and the yield strength). According to Eq. (53), $\Psi_{\text{pd}}^{\text{p}}(\lambda_{\text{pd}}) = \beta \lambda_{\text{pd}}$ for $\lambda_{\text{pd}} \in [0, \lambda_{\text{Twin}})$. Consequently, no additional hardening is active within the first stage. As a result, the Helmholtz energy can be decomposed in this case into a standard elastic part and a dissipation-like term. Hence, the predicted mechanical response is expected to be similar to that of perfect plasticity, i.e., the model will show a stress plateau within the interval $\lambda_{\text{pd}} \in [0, \lambda_{\text{Twin}})$.

Non-dissipative process. In this paragraph, a fully reversible process is analyzed. More precisely, the model introduced within the previous paragraph is utilized. The only difference compared to the model employed in Subsection 3.1.3 is that the PD-twinning system is included within the initial phase and a Boxcar mixture energy is considered for enforcing a Taylor-type approximation, see Fig. 2. Hence and in line with Eq. (43), the minimization problem to be solved reads

$$\inf_{\lambda_{\text{pd}}, \xi} \Psi(\varepsilon, \lambda_{\text{pd}}, \xi). \quad (54)$$

As evident, the slip caused by PD-twinning represents an additional unknown variable within optimization problem (54). Fig. 4j shows the minimizer of the total energy in terms of the prescribed strain amplitude. Accordingly, although the transition of the volume fraction ξ is approximated in a discontinuous fashion (see Fig. 4k), the resulting energy evolution is sufficiently smooth and thus, the stress-strain-relation is continuous (see Fig. 4l). More precisely, the stress-strain diagram is piecewise linear (comparably small deformations) and shows a plateau. This is a direct consequence of the term $\beta \lambda_{\text{pd}}$ included within Ψ^{p} . A more careful comparison reveals that the energy response as well as that of the stresses predicted by the advocated model are in excellent agreement with those corresponding to the computationally more expensive rank-one convexification method (cf. Fig. 4d and Fig. 4f). However, the evolution of the volume fraction ξ is discontinuous as seen for the Taylor-type approximation (see Fig. 4h). As a result, the presented model combines indeed the advantages of the aforementioned limiting cases.

Dissipative process. Although the example discussed in the previous paragraph illustrated the characteristics of the proposed phase transition model, deformation-induced twinning cannot be considered as fully reversible. Hence, dissipative mechanisms are added here. Consequently, the Helmholtz energy in Eq. (54) is replaced by the incrementally defined integrated stress power, cf. Section 2.3. More explicitly, the integrated stress power of the initial phase and that of the twinned phase are given by

$$\begin{aligned} I_{\text{ini}}(\varepsilon, \Delta\lambda_{\text{pd}}) &= \Psi_{\text{ini}}|_{n+1}(\varepsilon, \Delta\lambda_{\text{pd}}) - \Psi_{\text{ini}}|_n + A \Delta\lambda_{\text{pd}} \\ I_{\text{Tw}}(\varepsilon) &= \Psi_{\text{Tw}}|_{n+1}(\varepsilon) - \Psi_{\text{Tw}}|_n. \end{aligned} \quad (55)$$

Here, $A \Delta\lambda_{\text{pd}} = \Delta\mathcal{D}$ is the dissipation integrated over the time interval $[t_n; t_{n+1}]$ and A is an additional material parameter governing the dissipation amplitude. With Eqs. (55), the resulting energy is computed from the (discrete) minimization problem

$$I_{\text{inc}}(\varepsilon) = \min\left\{ \inf_{\Delta\lambda_{\text{pd}}} I_{\text{ini}}; I_{\text{Tw}} \right\}. \quad (56)$$

Figure 4: Fully reversible prototype model: Illustration of different phase transition models: energy evolution (left row); evolution of the twinning volume fraction (middle row); resulting stress-strain response (right row). Thick lines show the resulting minimum energy, while thin lines are associated with the single phases.

Figure 5: Prototype model including dissipation: a) incremental minimizers of I_{inc} (see Eq. (56)), b) stored energy corresponding to each phase, c) stress-strain diagram

Fig. 5a shows the evolution of I_{inc} as a function of the applied strain ε . During the first stage, PD-twinning is active resulting in a vanishing energy I_{inc} . When the threshold value λ_{Twin} is reached, the phase showing the new orientation becomes energetically more favorable yielding an increasing energy. The same holds for the Helmholtz energy. The computed stress-strain response is depicted in Fig. 5c. Accordingly, the stress diagram shows a plateau until the threshold value λ_{Twin} is reached and the crystal is reoriented. Subsequently, the stresses increase linearly (small deformations). In summary, the mechanical response predicted by the novel model is again in excellent agreement with that of the computationally more expensive rank-one convexification method.

4. Numerical implementation

In this section, the numerical implementation of the proposed model suitable for the analysis of deformation-induced twinning coupled to plastic slip is summarized. While in Subsection 4.1 the advocated energy-driven variational constitutive update is presented, an approximation of the novel model by means of visco-plastic crystal plasticity theory is briefly discussed in Subsection 4.2.

4.1. Variational constitutive update

In this subsection, the resulting variational model is briefly summarized. Its calibration, together with the choice of admissible hardening evolution laws, will be described in Section 5. First, the Helmholtz energies $\Psi = \Psi^e + \Psi^p$ describing the initial phase and the reoriented phase are explained. Subsequently, the dissipation functionals are introduced. This subsection is completed by the numerical implementation.

The elastic response of magnesium within the initial and the reoriented phase is approximated means of a neo-Hooke model of the type

$$\Psi^e(\mathbf{C}^e) = \frac{\lambda_E}{2}(\ln(J^e))^2 - \mu \ln(J^e) + \frac{\mu}{2}(\text{tr}(\mathbf{C}^e) - 3), \quad (57)$$

where J^e is the determinant of the elastic deformation gradient and $\{\lambda_E, \mu\}$ are the Lamé constants. The elastic deformations in magnesium are comparatively small and consequently, the elastic material model does not influence the results significantly. Accordingly, by neglecting the macroscopic anisotropy in magnesium, Eq. (57) represents a suitable choice.

The opposite is true for the plastic deformations. Taking 12 slip systems and 6 PD-twinning systems into account, the part of the Helmholtz energy associated with plastic work is assumed as

$$\Psi^P = \Psi_{\text{self}}^P + \Psi_{\text{lat}}^P + \Psi_{\text{pd}}^P. \quad (58)$$

Here, Ψ_{self}^P and Ψ_{lat}^P describe latent and self hardening of the slip systems, while Ψ_{pd}^P is related to PD-twinning. This decomposition, together with the classical Schmid-type yield functions (11), results in the dissipation

$$\mathcal{D} = \sum_{i=1}^{12} \Sigma_0^{(a)} \zeta^{(a)} + \sum_{i=1}^6 \Sigma_{\text{pd}0}^{(a)} \zeta_{\text{pd}}^{(a)} \geq 0. \quad (59)$$

Again, the first part governs the standard slip systems, while the second part is associated with PD-twinning. Integration of the stress power $\mathcal{P} = \dot{\Psi} + \mathcal{D}$ yields finally the incrementally defined functional

$$I_{\text{inc}}^{(\alpha)} = \Psi|_{n+1} - \Psi|_n + \sum_{i=1}^{12} \Sigma_0^{(a)} \Delta \zeta^{(a)} + \sum_{i=1}^6 \Sigma_{\text{pd}0}^{(a)} \Delta \zeta_{\text{pd}}^{(a)}. \quad (60)$$

Here, $\alpha \in \{\text{ini}; \text{Tw}\}$. Hence, the same incremental energy is used for the initial as well as for the reoriented phase. However, the crystal lattice orientation of both phases and the internal variables are, of course, not necessarily identical. For computing energy (60), the underlying evolution equations are again integrated by the implicit scheme (23). Finally, the stress power of the crystal can be determined from the discrete minimization

$$I_{\text{inc}} = \min\{\inf I_{\text{inc}}^{\text{ini}}; \inf I_{\text{inc}}^{\text{Tw}}\}. \quad (61)$$

In this connection, the optimization problems $\inf I_{\text{inc}}^{(\alpha)}$ depending on $\Delta \zeta^{(a)}$ and $\Delta \zeta_{\text{pd}}^{(a)}$ have to be solved for a given strain. Based on Eq. (61), the first Piola-Kirchhoff stress tensor $\mathbf{P}$ can be computed in standard manner, i.e., $\mathbf{P} = \partial_{\mathbf{F}} I_{\text{inc}}$.

4.2. Viscous approximation

The algorithm summarized in the previous subsection describes twinning and crystal slip by means of a fully variational method. Although it is physically sound and numerically efficient, so-called *variational constitutive updates* can nowadays still not be considered as standard. By ways of contrast, implementations for standard crystal plasticity theory are available for a broad range of different finite element programs. For this reason, an approximation of the novel variational model is discussed here which allows to use standard visco-plastic crystal plasticity models. A similar strategy has already been reported earlier, e.g., in Staroselsky and Anand (2003); Forest and Parisot (2000). It bears emphasis that the additional viscosity is not related to the material, but it is introduced for relaxing the ill-posed problem of rate-independent crystal plasticity theory, cf. Schmidt-Baldassari (2003).

Instead of computing the plastic multipliers $\zeta^{(a)}$ from the consistency condition $\dot{\phi}^{(a)} = 0$, the viscous-type over-stress model

$$\dot{\zeta}^{(a)} = \zeta_0^{(a)} \left\langle \frac{\phi^{(a)}(\boldsymbol{\Sigma}, \boldsymbol{Q})}{\Upsilon} \right\rangle^n \quad (62)$$

is introduced. Here, Υ and $\zeta_0^{(a)}$ are additional material parameters, $\langle \bullet \rangle$ are the Macaulay brackets and n determines the rate sensitivity, see Rice (1971); Peirce et al. (1982). Since this viscous law is utilized here only for regularizing the rate-independent limiting case, the admissible choice $\Upsilon = 1$ and $\lambda_0 = 1$ is made. Clearly, by choosing n sufficiently large, Eq. (62) is a good approximation of the rate-independent case. This is precisely, the underlying idea of the viscous-type approximation. For dislocation slip and PD-twinning, a yield function $\phi^{(a)}$ of the type (11) is adopted. The remaining variables such as those defining the hardening response (Ψ^p) are chosen in line with those utilized for the variational model discussed in the previous subsection. With this, the model describing the initial phase and that corresponding to the twinned phase are completed.

The final point to be addressed is a criterion for the phase transition. In principal, the energy based strategy as employed within the variational method could also be applied here. However, this would require an additional computation of the energies. Instead an equivalent strain-based criterion is employed. As explained in Section 3.2.2, twinning occurs, when the PD-twinning slip λ_{pd} reaches a critical threshold. Hence, for the advancing time step Δt , the final algorithm reads

$$\boldsymbol{e}_{t+\Delta t} = \begin{cases} \boldsymbol{e}_t & \text{if } (\lambda_{pd} < \lambda_{\text{Twin}}) \\ (-\mathbf{1} + 2(\boldsymbol{n} \otimes \boldsymbol{n})) \cdot \boldsymbol{e}_t & \text{if } (\lambda_{pd} \geq \lambda_{\text{Twin}}) \end{cases} \quad (63)$$

Test label	Loading direction	Constrained direction
A	[0001]	[1010]
C	[1010]	[0001]
E	[1010]	[1210]
G	[0001] at 45°	[1010]

Figure 6: Schematic representation of the channel die setup and the crystal orientations

where the vector $\mathbf{e}$ determines the local material orientation, and the threshold λ_{Twin} corresponds to the twinning-induced shear.

5. Calibration of the model - identification of the material parameters

The application of the numerical models summarized in the previous section requires the calibration of their material parameters. In principal, they can be determined by a standard optimization problem in which the error between the experimentally observed response and the predictions by the model is minimized. However, since the number of material parameters is large (12 slip systems, 6 PD-twinning systems, latent hardening, etc.), it seems to be more promising to separate the different deformation modes.

5.1. Experimental setup

One possible experimental setup for achieving this is provided by the channel die test, cf. Kelley and Hosford (1968). Within this test, four different sample configurations of the crystal are analyzed, see Fig. 6. Assuming rigid walls, the resulting strain state can be approximated by a deformation gradient of the type

$$\mathbf{F} = \mathbf{I} - \varepsilon(\mathbf{e}_3 \otimes \mathbf{e}_3) + \tilde{\varepsilon}(\mathbf{e}_1 \otimes \mathbf{e}_1), \quad (64)$$

where ε and $\tilde{\varepsilon}$ characterize the compression and extension strains in the punching direction ($\mathbf{e}_3$) and the channel direction ($\mathbf{e}_1$). Clearly, Eq. (64) represents an approximation of the more complex, inhomogeneous strain state, see Sue and Havner (1984). The crystal symmetry and the constrained

loading conditions, reduce the number of potentially active slip systems in each sample. More precisely, the following deformation modes are active:

- Sample A: pyramidal slip systems $\{[2\bar{1}\bar{1}\bar{3}](2\bar{1}\bar{1}2), [\bar{2}11\bar{3}](\bar{2}112)\}$
- Sample C: prismatic slip systems $\{[1\bar{2}10](10\bar{1}0), [11\bar{2}0](1\bar{1}00)\}$
- Sample E:
 - Initial phase: PD-twinning $\{[01\bar{1}1](0\bar{1}12), [0\bar{1}11](01\bar{1}2)\}$
 - Twinning phase: pyramidal slip systems $\{[11\bar{2}\bar{3}](11\bar{2}2), [\bar{1}\bar{2}1\bar{3}](\bar{1}\bar{2}12), [\bar{1}\bar{1}2\bar{3}](\bar{1}\bar{1}22), [1\bar{2}1\bar{3}](1\bar{2}12)\}$
- Sample G: basal slip systems $[01\bar{1}0](0001)$

Pairs of energetically equivalent slip systems result in a symmetric plastic deformation for samples A, C and E. By way of contrast, only one deformation system is potentially active in sample G resulting in a lattice rotation.

5.2. Hardening models

The results of the channel die experiments (see Kelley and Hosford (1968)) suggest that the mechanical response of prismatic and pyramidal slip systems can be approximated by an exponential hardening law, while only slight hardening effects have been observed for the basal and the PD-twinning systems. Hence, their hardening response is assumed as linear with comparably small moduli. Unlike dislocation slip, the strain related to PD-twinning is bounded by λ_{Twin} . For guaranteeing a physically sound phase transition, the hardening law corresponding to PD-twinning is thus, superposed by the additional function Π converging to infinity, if the critical transformation strain λ_{Twin} is reached. Consequently and analogous to the interface energy, Π governs the type of phase transition. In line with self and latent hardening, the best choice of the shape for $\Pi(\lambda_{\text{pd}})$ depends on experimental measurements. In summary, self-hardening is approximated by

$$Q_{\text{self}}^{(a)} = \frac{\partial \Psi_{\text{self}}^{\text{p}}}{\partial \lambda^{(a)}} = \begin{cases} h_0 \lambda^{(a)} & \text{Basal} \\ \Sigma_{\infty}(1 - \exp(-h_0 \lambda^{(a)} / \Sigma_{\infty})) & \text{Prismatic and Pyramidal} \\ h_0(\lambda^{(a)} + (\frac{\lambda^{(a)}}{\lambda_{\text{Twin}}})^m) & \text{PD - twinning} \end{cases} \quad (65)$$

where h_0 , n , Σ_0 and Σ_{∞} are material parameters, while $m \gg 1$ is a numerical parameter smoothing the discrete phase transition. The resulting hardening functions are depicted in Fig. 7. A similar set

Figure 7: Self hardening of the different deformation systems in magnesium

of self hardening functions has been proposed by Graff et al. (2007). However, in sharp contrast to the new model, Graff et al. (2007) used piecewise linear hardening functions specifically designed to agree with the stress-strain-response observed in experiments. In the novel approach, the piecewise linear stress-strain-response is a result of new slip systems activated in the twinning phase.

The hardening response is completed by assuming a linear latent hardening model of the type

$$\Psi_{\text{lat}}^{\text{p}} = \frac{1}{2} \boldsymbol{\lambda} \cdot \mathbf{L} \cdot \boldsymbol{\lambda}. \quad (66)$$

Its resulting moduli are constant and given by

$$l^{ab} := \frac{\partial^2 \Psi_{\text{lat}}^{\text{p}}}{\partial \lambda^{(a)} \partial \lambda^{(b)}}. \quad (67)$$

Alternatively, Voce-type latent hardening models are frequently applied to the analysis of magnesium deformation systems, cf. Agnew et al. (2001); Staroselsky and Anand (2003); Agnew and Duygulu (2005); Agnew et al. (2005); Bohlen et al. (2007); Graff et al. (2007). Conceptually, this class of models depends on a multiplicative decomposition of hardening into an scalar-valued amplitude and a matrix. The diagonal components correspond to self hardening, while the off-diagonal components are related to latent hardening. Accordingly, Eq. (67) falls also into this framework. In Staroselsky and Anand (2003) and Bohlen et al. (2007) latent hardening was completely neglected, while in (Agnew et al., 2001; Agnew and Duygulu, 2005; Agnew et al., 2005; Graff et al., 2007) a unit matrix or relatively small off-diagonal elements were chosen. In the proposed model, latent hardening is considered only for slip systems of the same type such as basal-basal. This is a direct consequence of the channel die experiment in which only one family of slip systems is active.

By comparing the experimentally observed mechanical response to the respective predictions by the model, the set of material parameters as summarized in Tab. 1 was found.

Table 1: Material parameters used in the numerical analysis of magnesium at room temperature

Elastic Properties	$\lambda = 34(\text{GPa})$			$\mu = 17 (\text{GPa})$		
Hardening parameters						
	Σ_0 (Mpa)	h_0 (Mpa)	Σ_∞ (Mpa)	m	λ_{Twin}	l^{ab}
Basal	0.48	10	-	-	-	0
Prismatic	20	9000	75	-	-	20
Pyramidal	25	7100	105	-	-	25
Pseudo-dislocation twinning	1	20	-	150	0.17	10

5.3. Comparison between experimental observations and predictions by the model

The results as computed by applying the variationally consistent method described in Subsection 4.1, together with the respective experimental observations, are shown in Fig. 8. For improving the numerical efficiency of the model, the symmetry conditions associated with the different crystal orientations were taken into account. According to the right row in Fig. 8, the computed stress-strain response is in good agreement with the experimentally observed results. The left row illustrates the evolution of the integrated stress power. For the PD-twinning system, two energy wells are plotted: one for the initial phase and one for the reoriented phase. From this figure it can be seen that the energy of the reoriented system becomes energetically more favorable, when the critical twinning transformation strain is reached. The effect of this transition on the stresses is evident in the respective stress-strain. While hardening is comparably small during the first loading stage, new slip systems are active within the reoriented phase resulting in more pronounced hardening.

5.4. Comparison between the variationally consistent model (Subsection 4.1) and its visco-plastic approximation (Subsection 4.2)

The numerical results reported in the previous subsection were obtained by applying the variationally consistent model (see Subsection 4.1). Here, the quality of its visco-plastic approximation (see Subsection 4.2) is analyzed. Particularly, the influence of the rate sensitivity power n is studied. Clearly, from a physical point of view, n has to be chosen sufficiently large. However, if n is too large, numerical problems can occur. The results for different rate sensitivity powers are summarized in Fig. 9. According to Fig. 9, $n = 100$ approximates the rate-independent case sufficiently

Figure 8: Channel die test: Comparison between the experimentally observed results by Kelley and Hosford (1968), denoted by "Exp", and the model predictions, denoted by "Sim": evolution of the incrementally defined energy (left row); true stresses vs. true strains (right row).

Figure 9: Channel die test: Comparison between the numerical results of the rate-independent variational method (Subsection 4.1) and the over-stress visco-plastic model (Subsection 4.2). n denotes the rate sensitivity power and RI denotes the rate-independent case (Subsection 4.1)

Figure 10: Simulation of a rolling process: Pole figure (normalized densities) showing the evolution of the basal texture

accurately by not causing any numerical problems. Therefore, $n = 100$ seems to be a promising choice.

6. Texture evolution in a polycrystal

Having discussed the presented crystal plasticity model in detail, its application to the analysis of a polycrystal is investigated here. More precisely, texture evolution of a polycrystal during a rolling process is considered. For that purpose, a representative volume element (RVE) consisting of $8 \times 8 \times 8 = 512$ eight-noded linear 3D hexahedron elements with 8 integration points is considered. In line with computational homogenization theory (see Miehe (2002)), periodic boundary conditions are enforced. The prescribed macroscopic strain inducing certain constraints at the boundary of the RVE (see (Miehe, 2002; Graff et al., 2007; Levesque et al., 2010)) is assumed to be plain strain compression $\text{diag} \mathbf{F} = \{\varepsilon; \bar{\varepsilon}; 1\}$. The pole figure in Fig. 10a depicts the initial texture with 4096=512x8 randomly distributed grain orientations which represents the texture of an as-cast ingot, cf. (Agnew et al., 2001; Lee et al., 2010). These individual material orientations are assigned to the respective material points (integration points). The texture evolution is governed by plastic deformations as well as by twinning. For the basal planes it is presented in Fig. 10a-c. The saturation of the basal poles toward the compression axis implies that basal slip is very pronounced. However, after 0.68 compression strain, the basal poles are inclined about 20 degrees out of the compression axis toward the extension direction. This is in good agreement with the results reported in Agnew et al. (2001) using a visco-plastic self consistent approach and also cf. (Agnew and Duygulu, 2005; Levesque et al., 2010; Proust et al., 2009; Beausir et al., 2007). The incremental activities of the different deformation systems versus the true compression strain are depicted in Fig. 11. Fig. 11

Figure 11: Simulation of a rolling process: Activities of the magnesium deformation systems versus the true compression strain. V_R denotes the volume fraction of the rotated grains.

also includes the total volume $V_R = \frac{n_R}{512 \times 8}$ of the reoriented grains, where n_R denotes the number of those grains. According to Fig. 11, the contribution of basal and pyramidal slip to the total plastic deformation is about 60%. Although PD-twinning is active during the early stages of loading, further slip is bounded by the penalty function ($\Pi(\lambda_{pd})$). Consequently, the reoriented volume is bounded and reaches only 25% (at 0.6 compression strain). The deformation activities of the basal slip systems are fully consistent with the texture evolution shown in Fig. 10, i.e., basal slip is very pronounced.

Remark 8. From an applicational point view, the analysis of the stress-strain-response characterizing the polycrystal is, in addition to the texture evolution, also very important. Evidently, this response depends strongly on the grain topology, e.g., the shape of the grains, cf. Lenhart (1955); Mathis et al. (2004); Gan et al. (2009). For the simulation of the polycrystal presented here, the material parameters as calibrated according to the channel die test have been used. However, the topology of the grains in the channel dies test (cubic single crystal) and that of the grains in the polycrystal are significantly different. Therefore, the results obtained from the numerical analysis of the polycrystal can only be interpreted in a qualitative manner. Consequently, for a quantitative description of a polycrystal, the material parameters have to be calibrated again for the considered grain topology.

Remark 9. If twinning is decomposed into continuous pseudo-dislocation slip and instantaneous lattice reorientation, the activity of twinning can be measured by two different methods. The first of those is the shear strain of the pseudo-dislocation compared to the final (maximum) twinning strain, i.e., $\lambda_{pd}/\lambda_{Twin}$. The second choice which was adopted in the present paper is the volume of the secondary phase (reoriented grains) compared to the total volume.

7. Conclusion

A novel model suitable for the numerical analysis of the mechanical response of magnesium has been proposed. It captures both relevant deformation modes being slip caused by dislocations as well as the reorientation of the crystal lattice induced by twinning. In contrast to previous works, the advocated approach is fully variational, i.e., every single aspect is driven by energy minimization. More precisely, the stable configurations of the considered solid are characterized by a combination between plastic slip and twinning that minimizes the respective energy. Furthermore, the presented model accounts for finite strains as well as for all 12 slip systems and 6 twinning modes. Having started by describing the phase transformation caused by twinning as a numerically expensive rank-one convexification, a more efficient model has been elaborated. It is based on decomposing the deformation of twinning into a simple shear mode and the reorientation of the crystal lattice. The underlying idea of that method is in line with experimental observations, where dislocation slip within the twinned domain is most frequently seen, if the twin laminate reaches a critical volume. It has been shown that the resulting model predicts a stress-strain response in good agreement with the numerically expensive rank-one convexification method, while showing the same numerical efficiency as a classical Taylor-type approximation. In addition to the analysis of a single crystal, the efficiency of novel model allows to investigate numerically more complex problems such as those related to texture evolution in a polycrystal. Comparisons of the predicted numerical results to their experimental counterparts showed that the novel model is also able to capture the characteristic mechanical response at the macroscale (polycrystal).

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