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Microscale Modelling of Deformation Twinning

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Abstract

A pseudoelastic micromodel that accounts for deformation twinning and crystallographic slip is used in conjunction with the representative volume element (RVE) technique. The material parameters are adopted to $\{10\bar{1}2\}\langle\bar{1}011\rangle$ twinning in a magnesium alloy. The simulation setup follows the commonly conducted compression tests on extruded Magnesium rods, where due to twinning a strong change of texture and a strength differential effect can be observed. The simulation setup allows to observe the twin propagation across grain boundaries. The predicted texture evolution is in good agreement with experimental findings, and the main feature of the macroscopic stress-strain-curve, namely the zero-hardening-plateau due to twinning in pure magnesium, could be reproduced as well. However, the hardening behaviour of magnesium-aluminium is, due to the complex twinning-particle-interaction in these materials, underestimated.

Keywords: $\{10\bar{1}2\}\langle\bar{1}011\rangle$, twinning, pseudoelasticity, nonconvex strain energy, magnesium, crystal plasticity.

1 Introduction

Many materials undergo solid to solid phase changes upon thermal or mechanical loading, which induces, e.g., the shape memory effect (SMA), the transformation induced plasticity effect (TRIP) or the twinning induced plasticity effect (TWIP). In this work, the focus lies on the isothermal and mechanically induced deformation twinning. Twinning can be considered as the homogeneous shearing of a crystal lattice, which leaves the atoms in positions such that a rotated copy of the parent lattice is generated. Although from a chemical point of view one might not want to speak about a phase change, some characteristic ingredients of phase changes are displayed.

Twinning produces sharp interfaces, at which the material properties that depend on the crystal orientation undergo a jump. The twins form as plates inside of grains, and can alter significantly the morphological and the crystallographic texture, both influencing significantly the yield surface and the elastic anisotropy. Due to its polarity, twinning can cause a pronounced differential effect on the strength of the material and the forming limit. For many materials, these effects are not negligible, and need to be incorporated in the material model. Especially the ductile TWIP steels and the lightweight hcp metals magnesium and titanium, which are interesting for engineering applications, display extensive twin formation at room temperature. For such materials, the proper prediction of forming processes requires a material model which includes mechanical twinning.

One approach, proposed by [1], is to treat phase changes by a non-convex elastostatic modelling. Summarising roughly, the overall modelling strategy is to construct an elastic strain energy w(E) which exhibits nonconvex regions. In this regions, no stable equilibrium state can be attained. Then, the convex branches are assigned to different phases, which are separated by the nonconvex regions. This leads to the pseudoelastic boundary value problem, which is ill-posed, since generally no unique energy-minimising configuration can be given. Different strategies to overcome the ill-posedness have been proposed, which can be roughly classified into "convexification" and "kinetisation".

A large amount of work has been contributed to the convexification strategies, beginning with introducing different forms of convexity [2]. Following the first approach, the ill-posedness may be overcome by confexifying w(E) in E, i.e. by replacing w(E) by a convexified strain energy $w_c(E)$. $w_c(E)$ should reproduce the main features of w(E). This procedure is also known as "relaxation". Unfortunately, the construction of $w_c(E)$ from w(E) is not a straightforward procedure. Mostly, several simplifying assumptions (small strains, elastic isotropy) are necessary. Moreover, the clear phase separation is lost, i.e. the relaxation is a special form of homogenisation. Another convexification strategy is to add a capillarity, i.e. $w_c(E, E \cdot \nabla) = w(E) + c(E \cdot \nabla)$, where $c(E \cdot \nabla)$ must be convex in $E \cdot \nabla$. This corresponds to a penalisation of interfaces at which the strains undergo a jump. The latter treatment is very challenging from the practical point of view.

The second line of work is to introduce a nucleation criterion and a kinetic relation for the phase growth, summarised in [3]. In doing so, the modelling approach is shifted from energy minimisation to evolution tracking. This may even be achieved by a kinetic relation which is not necessarily connected to the phase growth. E.g., by incorporating inertia forces, one has to track the propagation of waves in an elastic medium. Depending on the kinetic relation, the treatment can be complicated as well. It appears that this path has received less attention then the convexification methods, although it offers some advantages over the purely elastic modelling. Essentially, the strain path independence of a purely elastic modelling is resolved. Summaries on material modelling approaches which include phase mixtures are given by [4] and [5].

The material model relies on a nonconvex elastic stress-strain law plus a New-

tonian strain rate dependence, which serves as the kinetic relation. The nonconvex strain energy is constructed from the strain energies of the individual phases, which can be obtained through the isomorphy of the elastic laws from one elastic reference law [6]. In order to obtain results that are comparable to experiments conducted on the macroscale, the numerical homogenisation method of averaging over a representative volume element (RVE) has been used. Here, we compare the evolution of the twin volume fraction, of the crystallographic texture, and of the stress state to experimental results.

1.1 Notation

Throughout the work a direct tensor notation is preferred. If an expression cannot be represented in the direct notation without introducing new conventions, its components are given with respect to orthonormal base vectors e_i , using the summation convention. Vectors are symbolised by lowercase bold letters $v = v_i e_i$, second order tensors by uppercase bold letters $T = T_{ij}e_i \otimes e_j$ or bold greek letters. The second order identity tensor is denoted by I. Fourth-order tensors are symbolised like \mathbb{C} . The dyadic product is defined as $(a \otimes b) \cdot c = (b \cdot c)a$. Matrices are denoted like [A]. A dot represents a scalar contraction. If more than one scalar contraction is carried out, the number of dots corresponds to the number of vectors that are contracted, thus $\boldsymbol{a} \otimes \boldsymbol{b} \otimes \boldsymbol{c} \cdots \boldsymbol{d} \otimes \boldsymbol{e} = (\boldsymbol{b} \cdot \boldsymbol{d})(\boldsymbol{c} \cdot \boldsymbol{e})\boldsymbol{a}, \alpha = \boldsymbol{A} \cdots \boldsymbol{B}$ and $\boldsymbol{\sigma} = \mathbb{C} \cdots \boldsymbol{\varepsilon}$. When only one scalar contraction is carried out, the scalar dot is frequently omitted, e.g., v = Fw, A = BC. The Rayleigh-product is defined by applying a second order tensor to all base vectors of a tensor. E.g., in case of a fourth order tensor, $P * \mathbb{C} = C_{ijkl} P e_i \otimes P e_j \otimes P e_k \otimes P e_l$, with $\mathbb{C} = C_{ijkl} e_i \otimes e_j \otimes e_k \otimes e_l$. Orthogonal tensors are denoted by $Q_{\beta v} = \tilde{e}_i \otimes e_i$, mapping one orthonormal basis e_i into another one \tilde{e}_i . If Q can be interpreted as a rotation, the optional indexing contains the amount of rotation β and the normalised axial vector v. Two-fold rotations are rotations of amount π . They are denoted as $\mathbf{R}_{\mathbf{v}} = -\mathbf{I} + 2\mathbf{v} \otimes \mathbf{v}$, with \mathbf{v} being the normalised axial vector. The derivative of a vector valued vector function with respect to its argument is denoted like $v'(w) = \partial v(w) / \partial w = \partial v_i / \partial w_i$ $e_i \otimes e_j$.

2 Uniaxial testing of extruded magnesium

Twinning in magnesium has been studied in detail firstly by [7, 8, 9, 10, 11, 12]. Since these pioneering works, a large amount of literature concerning twinning in magnesium and its alloys has been published. Usually, the twins are categorised as extension or compression twins, depending on whether they appear under elongation or compression along the *c*-axis. Magnesium has $c \approx 0.52103$ nm and $a \approx 0.32094$ nm, which gives $c/a \approx 1.62345$, i.e. it is quite close to the densest possible packing with $c/a = \sqrt{8/3}$. The unit cell is slightly less high than thick. This causes the $\{\bar{1}012\}\langle\bar{1}011\rangle$ twins to be extension twins (see Fig. 2), while twinning along the $\{10\bar{1}1\}$, $\{10\bar{1}3\}$, $\{30\bar{3}4\}$ and $\{10\bar{1}5\}$ planes [13] occurs under *c*-axis compression. Recently, [14] observed $\{11\overline{2}1\}$ -twinning in the magnesium alloy WE54.



Figure 1: Simple hexagonal lattice with Miller-Bravais basis (left), hexagonal close packed multilattice constructed from the simple lattice by introducing additional translations in $\boldsymbol{v} = \langle \frac{1}{3}0\frac{1}{3}\frac{1}{2} \rangle$ (right).



Figure 2: Visualisation of the effect of a variation of the c/a ratio on the magnitude of the shear deformation accompanying $\{10\overline{1}2\}$ twinning. Left: $c/a > \sqrt{3}$, twinning shear increases width of the structure, leading to *c*-axis compression. Centre: $c/a = \sqrt{3}$, width and height do not change (the mean deformation is zero, no $\{10\overline{1}2\}$ twinning). Right: $c/a < \sqrt{3}$, twinning shear increases the height of the structure, leading to *c*-axis elongation.

In a recent work [15], plane strain compression tests are carried out on cuboidshaped AZ31 samples with different processing histories. One of them is an extruded sample, that is compressed along the extrusion direction (Fig. 3). Extruded magnesium is textured such that the *c*-axes and one of the a_i directions are distributed approximately uniformly and perpendicular around the extrusion direction, i.e. a compression along the extrusion direction results in a *c*-axis elongation and vice versa. In a compression test, the strongly textured material undergoes a complete shift of texture, see Fig. 4.



Figure 3: Schematic diagram of the extrusion process and the resulting texture.



Figure 4: (0002) (left) and $(10\overline{1}0)$ (right) pole figures before (above) and after (below) the compression test at $\varepsilon = 0.28$ (courtesy of [15]). The projection direction is parallel to the extrusion direction. As $\{10\overline{1}2\}$ twinning reorients the *c*-axis about approximately 86°, the outer ring (upper left figure) transforms into the centre peek (lower left figure). The slight deviation from the approximately rotational symmetric starting texture comes from the asymmetry of the loading (plane strain compression, two opposing faces are kept fixed).



Figure 5: Strength differential effect in the AZ31 magnesium alloy (left, courtesy of [16]), sketch of $\langle \bar{1}101 \rangle \{ 1\bar{1}02 \}$ extension and $\langle \bar{1}102 \rangle \{ 1\bar{1}01 \}$ compression twinning (right). Note that the extension twins show in the compression test along the extrusion direction and vice versa.

However, the impressive change of texture does not occur when the loading direction is reversed. Moreover, one observes a pronounced strength differential effect. The cause for this is the uni-directionality of twinning. The *c*-axis elongation is accommodated by $\{\bar{1}012\}$ twins, while compression twins (mostly $\{\bar{1}011\}$) accommodate *c*-axis compression, i.e. elongation along the extrusion direction. These twinning modes exhibit strong morphological differences. The $\{\bar{1}012\}$ tension twins are activated very easily, (namely at a shear stress of approximately 2.7MPa in pure magnesium, [17]), and their boundaries are mobile. The $\{\bar{1}011\}$ compression twins are thin, pinned lamellas. Instead of growing in thickness like the elongation twins, double twinning (first $\{10\bar{1}1\}$ compression followed by $\{10\bar{1}2\}$ extension twins) is observed as loading continues [18].

Therefore, in a compression test, the major deformation mechanism are the $\{\overline{1}012\}$ elongation twins. After virtually occupying the entire volume, elongation twinning is no more disposable. Due to the reorientation of the *c*-axis of approximately 86°, the deformation is then accommodated by $\{\overline{1}011\}$ compression twinning [11, 12], as it occurs from the beginning if the contrary loading direction is chosen. As depicted in Fig. 5, the stress level is then approximately the same as in the tension test. Due to the immobile interfaces of the compression twins, the deformation accommodated before fracture is much lesser than in case of elongation twinning. The double twins have been identified to be crack initiation sites [19, 20].

3 Characteristics of $\{\overline{1}012\}$ and $\{\overline{1}011\}$ twinning

Summarising roughly, $\{\overline{1}012\}$ tension twins allow for large deformation accommodation, while $\{\overline{1}011\}$ compression twins precede fracture. A similar behaviour is observed in titanium [21, 22] and zinc [23], which suggests that the morphological difference between the twinning modes is intrinsic to the hexagonal lattice structure. It is explained by the characteristics of the distinct interfaces and partial dislocations belonging to each twinning mode. In a series of articles, Serra and Bacon [24, 25, 26, 21] analysed twinning with the molecular dynamics technique. Firstly, they examined which of the different many-body potentials given in the literature suite best to each hcp metal [24]. [27] even adopted parameters of the many-body potentials such that they reproduce the elastic properties and c/a ratio for eight hcp metals. With the potentials at hand, the stacking fault and interface energies have been calculated, and found to be in agreement with experiments [25]. In [26], the mobility of partial dislocations belonging to different twin interfaces has been studied by means of molecular dynamics. It is found that dislocations in $\{10\overline{1}2\}$ and $\{11\overline{2}1\}$ boundaries are very glissile, but sessile in $\{1011\}$ and $\{1122\}$ interfaces. In [21], the interaction between basal slip dislocations and different twin interfaces has been studied. It is found that if a basal slip dislocation hits a $\{1012\}$ interface, a source for $\{1012\}$ partial dislocations is created, which forms pairs of partial dislocations if a shear strain of approximately ± 0.005 is applied. The source therefore provides a mechanism to move the interface gradually by generating a pair of partial dislocations, as long as the load is not removed and no obstacle is met. The converse is reported for a basal slip dislocation that hits a $\{10\overline{1}1\}$ interface. It creates there a pair of partial dislocations, but not an independent source for twinning dislocations. Together with the findings from [26], a convincing explanation for $\{10\overline{1}2\}$ -twinning being the most prominent twinning mode in hcp metals is obtained.

Another explanation for the needle-like $\{10\overline{1}1\}$ twinning and the extensive $\{10\overline{1}2\}$ twinning is that the $\{10\overline{1}1\}$ twins produce a larger shear strain. Therefore, to accommodate a certain deformation, compared to $\{10\overline{1}2\}$ twinning, less volume fraction of $\{10\overline{1}1\}$ twins is necessary [28, 29]. At least for magnesium this explanation is rather improbable, as the corresponding shear numbers $\gamma_{\{10\overline{1}2\}} \approx 0.13$ and $\gamma_{\{10\overline{1}1\}} \approx 0.137$ differ only slightly.

Li [30] recently modelled the development of a $\{10\overline{1}1\}$ twin and its interface movement in magnesium by molecular dynamics. In their simulations, a magnesium single crystal is subjected to a strain driven tensile test. The crystal orientation is such that 2 of the 6 possible twin variants are not triggered, while 4 of them are equally preferable. It is found that in the process of twin nucleation, initially two twin variants develop, one of which is assimilated by the other one as the simulation continues. As the model is symmetric, it is to conclude that a small perturbation, like a dislocation, can cause the unfortunate twin to be the other one. This underlines the affinity of twinning to bifurcation. In order to obtain reproducible results, both the simulation and experimental setups should avoid ambiguities like equally preferred twin systems. Another interesting result is that 3 kinds of interface steps are observed, namely 1,2 and 4-layer steps. While the 1-layer step is sessile, the 2-layer step is glissile. The 4-layer step is unstable and dissociates into two 2-layer steps, between which a repulsive force is acting. The movement of the interface is connected to the generation of prismatic dislocation. In another work, [31] focused on the atomic modelling of a $\{10\overline{1}2\}$ twin interface in magnesium, employing the embedded atom model by [32]. It has been found that the morphological difference between $\{1011\}$ and $\{1012\}$ twinning in magnesium can be explained by the mechanism underlying to the interface movement. In case of the $\{10\overline{1}1\}$ twinning, the interface movement rests upon the movement of partial dislocations, while in case of the $\{10\overline{1}2\}$ twinning, atomic shuffling appears to play the leading role, and no pronounced partial dislocation is observed. Therefore, unlike $\{10\overline{1}2\}$ twinning, the $\{10\overline{1}1\}$ twin propagation is restricted by the partial dislocation density, which renders the $\{10\overline{1}2\}$ interfaces more glissile compared to the $\{10\overline{1}1\}$ interfaces.

4 The material model

The material model is based on a nonconvex elastic energy. The elastic energy is obtained by combining the elastic energies of the possible configurations in a regularised version of the Ball and James-approach $\tilde{w}(\mathbf{C}) = \min(w_1(\mathbf{C}), w_2(\mathbf{C})...w_n(\mathbf{C}))$ [33]. The individual strain energies are obtained by exploiting the isomorphy of the parent and the twin lattices [6]. To avoid an overestimation of the critical twinning stress, a modification of the strain energy in the transition zones is necessary. Inside the parent configuration, basal slip is possible, which is approximated by the card glide mechanism. As kinetic relation, a viscous regularisation is introduced.

The index 0 indicates the parent configuration, while the indices 1...n run over the possible twin variants, and sums are explicitly written.

The plastic transformations map the elastic reference law of each phase to the reference placement. P_0 is given by the parent crystal orientation, and P_i , i = 1..n are given by

$$\boldsymbol{P}_i = \boldsymbol{P}_0 \boldsymbol{P}_{0i} \qquad i = 1...n, \tag{1}$$

with the plastic transformations P_{0i}

$$\boldsymbol{P}_{0i} = \boldsymbol{S}_i^{-1} \boldsymbol{R}_{\boldsymbol{n}_i} \tag{2}$$

$$= (\boldsymbol{I} - \gamma_0 \boldsymbol{d}_i \otimes \boldsymbol{n}_i)(-\boldsymbol{I} + 2\boldsymbol{n}_i \otimes \boldsymbol{n}_i)$$
(3)

$$= -\boldsymbol{I} - \gamma_0 \boldsymbol{d}_i \otimes \boldsymbol{n}_i + 2\boldsymbol{n}_i \otimes \boldsymbol{n}_i \qquad i = 1...n.$$
(4)

 S_i denotes the shear deformation with respect to the parent crystal, while R_{n_i} accounts for the reorientation of the crystal lattice. d_i and n_i are the normalised shear directions and the shear plane normals of the $\{10\overline{1}2\}\langle\overline{1}011\rangle$ twin systems in the parent lattice, γ_0 represents the twinning shear. With the P_i , Green's strains E_i are obtained by

$$\boldsymbol{E}_{i}(\boldsymbol{C}) = \frac{1}{2} (\boldsymbol{P}_{i}^{T} \boldsymbol{C} \boldsymbol{P}_{i} - \boldsymbol{I}).$$
(5)

For clarity, the chain like dependence $w_i(E_i(C))$ is omitted in the following. The strain energies, based on the St. Venant-Kirchhoff strain energy, are given in terms of

Greens strain by

$$w_i = \frac{1}{2} \boldsymbol{E}_i \cdots \boldsymbol{\mathbb{C}} \cdots \boldsymbol{E}_i \qquad \text{if } \phi_i(\boldsymbol{E}_i) \le 0 \qquad (6)$$

$$w_{i} = \boldsymbol{E}_{i} \cdot \cdot \mathbb{C} \cdot \cdot \boldsymbol{E}_{i,\text{crit}} - \frac{1}{2} \boldsymbol{E}_{i,\text{crit}} \cdot \cdot \mathbb{C}_{0} \cdot \cdot \boldsymbol{E}_{i,\text{crit}} \qquad \text{if } \phi_{i}(\boldsymbol{E}_{i}) > 0, \qquad (7)$$

with the elasticity tetrad \mathbb{C} . The functions ϕ_i indicate whether a critical strain state has been reached. As mentioned before, the w_i have to be modified in order to not over-predict the twinning stresses. This is achieved by a linear continuation of the quadratic strain energy when a critical strain state is reached. The functions $\phi(\mathbf{E}_i)$ are given by

$$\phi_0(\boldsymbol{E}_0) = \sum_{i=1}^n \langle \gamma_j / \gamma_{\text{twin}} \rangle^m - 1 \qquad \qquad \gamma_j = 2\boldsymbol{E}_0 \cdots \boldsymbol{M}_j \quad (8)$$

$$\phi_i(\boldsymbol{E}_i) = \frac{\gamma_i}{\gamma_{\text{twin}}} - 1 \qquad \gamma_i = 2\boldsymbol{E}_i \cdot \boldsymbol{M}_i \qquad i = 1...n, \quad (9)$$

where $M_i = d_i \otimes n_i$. In the parent configuration (index 0), there are *n* possible twin configurations to be reached, while the twins (index 1...*n*) are allowed to transform only back to the parent, i.e. the model does not include higher order twins. The w_i can now be inserted into a regularised version of the Ball and James-approach,

$$\tilde{w} = \sum_{i=0}^{n} a_i w_i$$
 $a_i = \frac{g_i}{\sum_{j=0}^{n} g_j}$ $g_i = \frac{h(w_i)}{1 - h(w_i)}$ $h_i = \exp(-kw_i)$, (10)

with k being a preferably large regularisation parameter. With \tilde{w} on hand by the latter system of equations, the second Piola Kirchhoff stresses are

$$\boldsymbol{T} = \frac{\partial \tilde{w}}{\partial \boldsymbol{E}} \approx \sum_{i=0}^{n} a_i \boldsymbol{T}_i \tag{11}$$

$$\boldsymbol{T}_{i} = \frac{\partial w_{i}}{\partial \boldsymbol{E}} = \boldsymbol{P}_{i} \frac{\partial w_{i}}{\partial \boldsymbol{E}_{i}} \boldsymbol{P}_{i}^{T}.$$
(12)

This is, so far, the elastic law. Incorporating the viscous regularisation corresponds to adding the deviatoric part of $\frac{J\eta}{2}C^{-1}\dot{C}C^{-1}$ to the second Piola Kirchhoff stresses, with η being the viscosity. In order to account for basal slip, the collective of basal slip systems is approximated by the card glide mechanism. n_b corresponds to the base plane normal, while the slip direction d_b is obtained by projecting the stress vector into the base plane. The plastic transformation of the parent evolves corresponding to

$$-\boldsymbol{P}_{0}^{-1}\dot{\boldsymbol{P}}_{0}=\dot{\gamma}\boldsymbol{d}_{b}^{*}\otimes\boldsymbol{n}_{b},\qquad \boldsymbol{d}_{b}^{*}=\frac{\boldsymbol{d}_{b}}{\|\boldsymbol{d}_{b}\|},$$
(13)

with

$$\boldsymbol{d} = ((\boldsymbol{I} - \boldsymbol{n}_b \otimes \boldsymbol{n}_b) \tilde{\boldsymbol{F}}^{-1} \boldsymbol{\sigma} \tilde{\boldsymbol{F}}^{-T}) \cdot \boldsymbol{n}_b, \qquad \tilde{\boldsymbol{F}} = \boldsymbol{F} \boldsymbol{P}_0.$$
(14)

 $\dot{\gamma}$ is determined consistently with the elastic law. I.e., during the plastic flow, the resolved shear stress in the card glide system is equal to the flow stress.

The material parameters are given with respect to the elastic reference law. e_1 is parallel to a_1 while e_3 is parallel to the *c*-axis. The elastic stiffness tetrad of magnesium [34], with respect to the basis $B_1 = e_1 \otimes e_1$, $B_2 = e_2 \otimes e_2$, $B_3 = e_3 \otimes e_3$, $B_4 = \sqrt{2}/2(e_1 \otimes e_2 + e_2 \otimes e_1)$, $B_5 = \sqrt{2}/2(e_1 \otimes e_3 + e_3 \otimes e_1)$, $B_6 = \sqrt{2}/2(e_2 \otimes e_3 + e_3 \otimes e_2)$ is

$$\mathbb{C} = \begin{bmatrix} 56.49 & 23.16 & 18.10 & 0 & 0 & 0 \\ 56.49 & 18.10 & 0 & 0 & 0 \\ & 58.73 & 0 & 0 & 0 \\ & & 2 \times 16.81 & 0 & 0 \\ & & & & 2 \times 16.81 & 0 \\ & & & & 56.49 - 23.16 \end{bmatrix} \boldsymbol{B}_i \otimes \boldsymbol{B}_j,$$
(15)

in GPa. B_i is an orthonormal vector basis for symmetric 2nd order tensors, i.e. a fourth order tensor with both subsymmetries can be denoted as a second order tensor with respect to B_i . The six structural tensors belonging to the $\{10\overline{1}2\}\langle\overline{1}011\rangle$ twin systems are given by

$$\boldsymbol{M}_1 = \boldsymbol{d}_1 \otimes \boldsymbol{n}_1 \tag{16}$$

$$\boldsymbol{d}_1 = \cos(\alpha)\boldsymbol{e}_2 + \sin(\alpha)\boldsymbol{e}_3 \tag{17}$$

$$\boldsymbol{n}_1 = -\sin(\alpha)\boldsymbol{e}_2 + \cos(\alpha)\boldsymbol{e}_3 \tag{18}$$

$$M_i = Q_{\pi/3}^{i-1} e_3 * M_1, \qquad i = 2...6$$
 (19)

i.e. by rotating the twin system M_1 in the sixfold symmetric hexagonal cell, with

$$\alpha = \operatorname{atan}(c/(a\sqrt{3})). \tag{20}$$

For magnesium and its alloys, $c/a \approx 1.623$. The twinning shear for the $\{10\overline{1}2\}\langle\overline{1}011\rangle$ twin systems is given by

$$\gamma_0 = \frac{\sqrt{3}}{c/a} - \frac{c/a}{\sqrt{3}},\tag{21}$$

i.e. $\gamma_0 \approx 0.13$. The regularisation parameter k and the viscosity are taken as k = 0.25 and $\eta = 10000$ MPa s.

The regularisation parameter of the phenomenological model adaption of the strain energy is taken to be m = 10. The used critical shear strain is $\gamma_{\text{twin}} = 0.006\gamma_0$. The critical shear stress for twinning is therefore approximately $\tau_{\text{crit}} = G\gamma_{\text{twin}} \approx 0.006 \times 0.13 \times 17000 \text{ MPa} \approx 13 \text{ MPa}.$

For the basal glide, only the critical shear stress τ_{basal} enters the card glide. It is observed that the critical $\{10\overline{1}2\}\langle\overline{1}011\rangle$ twinning stress and the basal slip shear stress are related by $\tau_{\text{crit}}/\tau_{\text{basal0}} \approx 4$. Therefore, τ_{basal} is set to 4 MPa, and strain hardening is neglected.



Figure 6: FE Model of the RVE, with schematic pole figure of the c-axes. The greyscale exemplifies the periodic Voronoi structure of the grains.

5 Simple compression of an RVE

In order to obtain results that are comparable to experimental data, the RVE method is used to simulate the simple compression of an extruded magnesium alloy along the extrusion direction. The crystallographic texture of the latter is such that the *c*-axes are aligned approximately perpendicular to the extrusion direction, i.e., the compression along the extrusion direction results in *c*-axis elongation, which is accommodated by $\{10\overline{1}2\}\langle\overline{1}011\rangle$ twinning (see [29, 15]).

5.1 Model setup

The FE model of the RVE consist of a regularly meshed cube with $30 \times 30 \times 30$ linear hexahedron elements. The initial microstructure has been approximated by a periodic Voronoi tessellation, consisting of 20 grains, Fig. 6. The limited number of grains is necessary to provide a reasonable discretization of each grain, though the grains are partitioned by twinning. The crystal orientations are restricted such that the *c*-axes do not deviate more than α from the plane of compression, and are uniformly distributed. No preferred orientation of the remaining degree of freedom (rotating the a_i around the *c*-axis) has been established. The displacement boundary conditions are periodic on the entire surface of the cube. The 11-component of the mean displacement gradient with respect to the orthonormal base system used for the model description have been constrained,

$$\boldsymbol{H} = \begin{bmatrix} f(t) & 0 & 0\\ 0 & \cdot & 0\\ 0 & 0 & \cdot \end{bmatrix} \boldsymbol{e}_i \otimes \boldsymbol{e}_j, \tag{22}$$

while H_{22} and H_{33} have not been constrained. Instead, the mean reaction forces along the e_2 and e_3 directions have been constrained at the corresponding faces to be equal to zero, in order to obtain the average uniaxial stress state along the e_1 direction.



Figure 7: Propagation of a twin (black) over a grain boundary. The grey-scaling represents the grain structure.



Figure 8: Twin spreading on the RVE, at a nominal compression strain of 2.5%, 2.9% and 4.6%, from left to right.

5.2 General observations

In the simulations, twins nucleate and spread rapidly over the FE model. In Fig. 7, the propagation of a twin over a grain boundary is illustrated. In Fig. 8, a sequence of states illustrating the twin spreading in the RVE is given. Both Figures are obtained from the simulation with a maximum deviation of $\alpha = 30^{\circ}$ of c from the plane of compression. The incorporation of basal glide does not significantly alter the results, which is due to the approximately perpendicular alignment of the basal planes to the principal stress direction.

5.3 Comparison to experimental findings

As a reference, the works of [35] and [29] have been used, where compression tests for two magnesium alloys and pure magnesium are documented. In Fig. 9, graphs for the twin volume fraction evolution in the experiments and the simulations are depicted.

One notes that the evolution of the twin volume fraction is in good agreement with the experimental findings. The rapidly increasing twinning rate at 3 to 5% of logarithmic strain, as well as the saturation to 100% twin volume fraction are captured by the model. In Figs. 9 and 10, the twin volume fraction and the nominal compression stress are plotted. Therefore, it is to be expected that the crystallographic texture evolution are in good accordance, as twinning dominates the texture evolution for this particular experiment.

However, comparing to the stress strain response given by [29], one finds that the experimental results display a pronounced hardening behaviour, which is not found in the simulations. This is due to the fact that the hardening behaviour of the magnesium alloy under consideration is very complex due to precipitates, which is not captured by the model. This explanation is furnished by the fact that the stress strain response is in considerable agreement with the compression experiments with pure magnesium [35], which displays a less complicated hardening behaviour due to the lack of particles and precipitates, see Fig. 10. It is found that the zero-hardening-plateau at approximately $60 \text{ MPa} (\approx 8.7 \text{ ksi})$ corresponds to the twin nucleation phase. At approximately 3% of logarithmic strain, the nominal stress increases constantly, which coincides with the point where volume-filling twinning starts seriously. Similar findings are given in [36]. The hardening is explained by the fact that the twins form firstly at stress concentration points, or expressed differently, at the most favourable twinning sites. For further twinning, the loading must be increased in order to activate the less favoured twinning sites. One notes that the hardening rate is overpredicted in the simulations. This is due to the fact that the material model does not capture secondary twinning and slipping inside the twins, which renders them stiffer as in reality.

5.3.1 Texture evolution

The RVE-simulations allow to compare the texture evolution with experimental results. At a material point, the significant orientation is assumed to be given by the phase with the smallest strain energy. Due to the phenomenological model adaption, the strain energy invariance is not exactly met by the model, i.e. a definite orientation can be extracted at each of the 8×30^3 integration points of the FE model. The *c*-axes of 20 initial orientations deviate at most by 15° from the compression plane, see Fig. 11 for pole figures of the initial orientation distribution. The sequence of *c* and *a* pole figures for the compression test is given in Fig. 12. One notes that the texture evolution corresponds qualitatively well to experimental results of [29], although the rate at which the texture shifts is overestimated.

6 Conclusions

The presented micro-model is able to predict, in conjunction with the representative volume element method as the numerical homogenisation scheme, twinning-induced effects on the macroscale. Simulations of characteristic compression tests on textured



Figure 9: Comparison of the experimental [29] and the RVE-simulated twin volume fraction evolution. The simulated curves are obtained with different texture sharpnesses, the maximum deviation of the c axis from the compression plane is given.



Figure 10: Comparison of the experimental and the RVE-simulated stress evolution (Cauchy stress over logarithmic strain). Courtesy of S.N. Monteiro, experimental data firstly published in [35].



Figure 11: c and a pole figures of the initial orientation distribution, with $I_{c_{\text{max}}} = 9.403$ and $I_{a_{\text{max}}} = 5.173$. The projection plane is parallel to the compression direction. The pole figures are calculated using a Mises-Fisher [37] distribution with a half-width of 20° around the individual orientations.



Figure 12: c and a pole figures for the compression test. The projection plane is parallel to the compression direction. The pole figures are calculated using a Mises-Fisher distribution with a half-width of 20° around the individual orientations.

magnesium polycrystals have been carried out. The following has been found:

• The twin volume fraction evolution shows a qualitatively good agreement to the experimental findings of [29]. Quantitatively, it is slightly overestimated.

• The impact on twinning on the texture evolution is linked directly to the twin volume fraction, which allows to obtain a reasonable estimation of the texture evolution.

• The twinning-induced zero-hardening plateau observable in pure magnesium samples could be reproduced.

• The overall setup (material model and FE model) allows for grain to grain interaction, which manifests in twin propagation across grain boundaries.

However, the model fails to predict the stress-strain curves for magnesium-aluminium alloys, which has several reasons.

• Firstly, multiple twinning is not included. The reason herefore is that the elastic modelling would allow for, due to its inherent strain-path independence, arbitrary configuration changes. To exclude this unrealistic behaviour, only first-order twins are considered.

• Secondly, inside the twins, no further deformation mechanism, like slip or fracture, is accounted for.

• Thirdly, no twin-particle interaction and no grain-particle has been considered, which is known to have a considerable influence on the hardening behaviour. This is a special feature of MgAl-alloys, which owe there relative strength compared to Mg to precipitate-hardening. At least, this shortcoming is not an artifact of the model, but of the finite element setup, which allows in principle the inclusion of particles in the RVE calculation.

Appendix A

For a hexagonal lattice, it is convenient to use the Miller-Bravais basis

$$\boldsymbol{a}_1 = a\boldsymbol{e}_1, \qquad \boldsymbol{a}_2 = a\left(-\frac{1}{2}\boldsymbol{e}_1 + \frac{\sqrt{3}}{2}\boldsymbol{e}_2\right),$$
 (23)

$$\boldsymbol{a}_3 = a \left(-\frac{1}{2} \boldsymbol{e}_1 - \frac{\sqrt{3}}{2} \boldsymbol{e}_2 \right), \qquad \boldsymbol{c} = c \boldsymbol{e}_3$$
 (24)

see Fig. 1, [38, 39]. The lattice parameters c and a represent the height of the cell and the edge length of the base hexagon, respectively, and correspond to the norms of c and a, $c = \sqrt{c \cdot c}$ and $a = \sqrt{a \cdot a}$. Although one usually does not appreciate the use of linearly dependent base vectors, this basis has the advantage that it reflects the hexagonal symmetry. Permutations of the components belonging to $a_{1...3}$, a change of sign of the c-component or a simultaneous change of sign of all $a_{1...3}$ yield crystallographically equivalent directions, which are denoted as $\langle a_1 a_2 a_3 c \rangle$. Usually, negative components are denoted by \bar{x} instead of -x. Further, due to the linear dependence of $a_{1...3}$, the condition $a_1 + a_2 + a_3 = 0$ is imposed, and therefore sometimes the third component a_3 is omitted.

To indicate planes, it is advantageous to introduce another basis. This is done by taking the dual basis $(\tilde{a}_1, \tilde{a}_2, \tilde{c})$ of (a_1, a_2, c) and defining the base vectors

$$a_1^* = \frac{2}{3}\tilde{a}_1 - \frac{1}{3}\tilde{a}_2 = \frac{2}{3a^2}a_1, \qquad a_2^* = -\frac{1}{3}\tilde{a}_1 + \frac{2}{3}\tilde{a}_2 = \frac{2}{3a^2}a_2,$$
 (25)

$$a_3^* = -\frac{1}{3}\tilde{a}_1 - \frac{1}{3}\tilde{a}_2 = \frac{2}{3a^2}a_3,$$
 $c^* = \tilde{c} = \frac{1}{c^2}c.$ (26)

This basis again satisfies $a_1^* + a_2^* + a_3^* = 0$, but it is not the dual basis of (a_1, a_2, a_3, c) . It also has the advantage that crystallographically equivalent planes are connected by permutations of the components and changes of sign as stated above. Again, the components should be restricted to $a_1^* + a_2^* + a_3^* = 0$. If this is done, several practical simplifications are obtained: If a normal vector is given with respect to the basis $(a_1^*, a_2^*, a_3^*, c^*)$, the reciprocals of its components correspond to the piercing point distances of the plane with the base vectors (a_1, a_2, a_3, c) . Therefore, the plane $\{10\overline{1}2\}$ can be visualised by considering the points $a_1, -a_3$ and 1/2c (see Fig. 1). Moreover, one can easily see whether direction and normal vectors are perpendicular to each other by calculating the scalar product as if (a_1, a_2, a_3, c) and $(a_1^*, a_2^*, a_3^*, c^*)$ were dual bases.

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