Dependence of twinned volume fraction on loading mode and schmid factor in randomly textured magnesium.

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Abstract

The twinning activity in random textured cast magnesium during room temperature tension and compression tests was monitored by neutron diffraction (ND). Variation of integrated intensities of selected diffraction peaks, characterizing the twinned volume in particularly oriented grains was compared with calculated Schmid factors for extension twinning of these grains. It is shown that *in tension* there is a direct proportion between the twinned volume and the maximum value of the Schmid factor for a given grain orientation. In contrast, *in compression* this relation is not valid. The twinned volume in this case is influenced by both deviation of the grain from the ideal orientation and its rotation around the c-axis. The experimental results are in good agreement with those obtained from elasto-plastic self-consistent (EPSC) modeling.

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1. Introduction

$\{10\bar{1}2\}\{10\bar{1}1\}$ extension twinning is an important deformation mechanism in magnesium alloys [1-3]. It exhibits polar behavior and differently oriented grains undergo twinning during tensile and compressive deformation. Thus, the plastic behavior and texture evolution depends strongly on the loading direction. There is discussion in the literature [4-8] as to the extent that activation of a given twin variant depends on its Schmid factor (SF). The SF-volume correlation is not necessarily straightforward, since the stresses that drive twinning vary locally and the accommodation of the twinning strain also has to be taken into account [9, 10]. The common approach for answering this question usually includes statistical analysis of EBSD data. However, this technique is limited in terms of the volume of material that can be examined.

In-situ neutron diffraction has been proved to be useful for investigation of deformation twinning [11-13]. The large penetration depth of the thermal neutrons facilitates the investigation of relatively large sample volumes and provides good statistics also in the case of coarse-grained ($>50\text{ }\mu\text{m}$) materials. The information about twinning can be obtained by following the intensity changes of particular diffraction peaks [11, 14, 15].

In this work we employ the neutron diffraction method to study the Schmid factor dependence of twinning. Correspondence between the experimentally established twinned volume fraction and the calculated Schmid factors for extension twinning in

particular orientation families is analyzed¹. The experimental data, measured on randomly textured Mg-Al alloy are compared with predictions of an EPSC model.

2. Material and experimental methods

Binary Mg- 2 wt. % Al (Mg2%Al) alloy having a grain size of approximately $100\mu\text{m}$ was used for the experiment[16]. The testing was carried out using cylindrical specimens with a diameter of 9mm and gauge length of 20mm. Inverse pole figures show that the initial samples have a random grain orientation distribution (Fig. 1). Monotonic compression and tensile tests were performed at room temperature at a strain rate of 10^{-3}s^{-1} . The test was stopped for approx. 70 min at particular true strain values (0.1%, 0.5%, 1%, 2%, 3%, 4%, 5%, and 6%) in order to collect the neutron diffraction data. The SMARTS engineering instrument at LANSCE was used for collecting the diffraction pattern [17]. The diffraction patterns were measured using two detector banks at $\pm 90^\circ$ to the incident beam. The angle between the incident beam and the loading direction was 45° . This setup provides diffraction measurement of crystallographic planes both perpendicular (axial detector) and parallel (transversal detector) to the loading direction. We evaluated data from the axial detector which shows the grain orientation with respect to the loading direction. The measured data were fitted by EPSC model in order to better understand the changes in peak intensity.

Direct observations of the microstructure of the specimen deformed to 1% strain were performed by scanning electron microscope FEI Quanta 200F. The electron back-scatter diffraction (EBSD) was used to study of the activated twin variants. The specimens for EBSD investigations were polished by standard methods down to OPS

¹ Contraction $\{10\bar{1}1\}$ twins were not considered due to the low strain levels achieved

colloidal silica suspension. The final electropolishing was done by means of Struers AC-2-II electrolyte.

3. Results

Examples of the microstructure after 1% deformation in a) tension; b) compression are shown in Fig 2. The loading direction in both cases is perpendicular to the figure plane. It is obvious that the number of twin variants and size of twins depends significantly on the loading mode. Grains, designated as T1 and C1, are almost ideally oriented for extension twinning in tension and compression, respectively. Several twin variants, having moderate thickness can be observed in grain T1. In contrast, grain C1 includes only one twin variant, which has reoriented almost half of the parent grain. In the grains less favorably oriented for twinning (T2, C2), the number of twin variants is larger for the compression case than for tension.

3.1 Neutron diffraction experiments

The overall twin volume fraction (TVF) during the deformation has been determined from the diffraction data by performing a 2-bank Rietveld refinement assuming an axisymmetric texture, as presented in [18]. Axisymmetric textures can be represented using the axial distribution function (ADF), which is a cut through the pole figure at a line from the center to the perimeter. From the ADF, one can calculate the twin volume fraction (see Fig. 3) by integrating the area under the ADF [18]. Fig. 3 demonstrates that above 1% of applied strain the TVF is larger in compression by ~ 25%.

The intensity changes for selected parent peaks, which are directly proportional to the TVF [11], are shown in Fig. 4. The selected grain orientation families and the corresponding maximal value of the Schmid factor for extension twinning are listed in Table 1.

Table 1. Selected grain orientations and their maximal SF for tension and compression, respectively.

<i>Tension</i>							
Reflection	0002	10 $\bar{1}4$	10 $\bar{1}3$	11 $\bar{2}4$	10 $\bar{1}2^2$	20 $\bar{2}3^2$	
SF _{max}	0.50	0.40	0.34	0.30	0.22	0.14	
<i>Compression</i>							
Reflection	10 $\bar{1}0$	20 $\bar{2}1$	21 $\bar{3}0$	21 $\bar{3}1$	11 $\bar{2}0^2$	10 $\bar{1}1^2$	11 $\bar{2}2^2$
SF _{max}	0.50	0.45	0.45	0.42	0.37	0.31	0.16

It is obvious that for tension (Fig. 4a) the twinned volume fraction decreases proportionally with the decreasing value of maximal SF. In compression (Fig. 4b), this dependence is less clear. Many grain orientations behave similarly to the favorably oriented {10 $\bar{1}$ 0} reflection, i.e. these grains have almost the same twinned volumes. However, grains with orientations {10 $\bar{1}$ 1} and {11 $\bar{2}$ 2} exhibit significantly lower twinned volume.

Figure 5 shows a comparison between tension and compression for grain families with similar maximum SF. It can be seen that in some cases the curves overlap but in others they do not. The difference between tension and compression is clearly

² These peaks may include twin daughters, but their nucleation is highly improbable due to the low SF

orientation dependent. Elucidation of the physical background of this behavior is presented in what follows.

4. Discussion

The present results raise three interesting questions:

- Why is the overall twinned volume fraction larger in compression than in tension?
- Why is there a direct proportion between the maximum SF and the twinned volume only in the tension? Further, why do some grains, having almost the same maximum SF, exhibit similar twinned volumes in both tension and compression, while others do not?
- Can EPSC modeling capture these observations?

4.1 Loading mode dependence of the overall twin volume

Using the calculations listed in the appendix a statistical distribution of SF in a randomly oriented polycrystal can be determined (Fig.6). It is obvious that *in tension* there is larger fraction of grains having a positive SF. However, the majority of them have low SF. Only 10% of grains in tension have $SF > 0.4$, while the same criterion is met by 25% of grains in compression. We can also observe decreasing numbers of grains with increasing SF value in tension and increasing number of grains with increasing SF value in compression. The median value of SF is 0.10 in tension and 0.24 in compression.

As reported elsewhere [5, 19], high SF twins tend to be thicker than those with low SF, because the driving force for twin boundary migration scales linearly with the SF [20]. Thus, *the larger overall twin volume in compression* can be elucidated in terms of a larger number of grains with a high SF for twinning.

4.2 Dependence of the twinned volume fraction on the Schmid factor for extension twinning

In tension, the TVF for a given orientation monotonically decreases with the deviation angle from the ideal orientation. Further, it is obvious from Fig 7, that there is a linear dependence of the twinned volume on the *maximal* value of SF for a given orientation. The interpretation of compression data is more difficult. The correlation between maximal SF and twinned volume is not as strong. We see a higher correlation when we plot TVF against average SF (Fig. 8). This reflects the importance of the number of high SF systems in each orientation. For example, it can be seen in Tables 2 and 3 that all six twin systems have SF=0.5 for (0002) in tension but for $\{10\bar{1}0\}$ in compression only two systems have SF=0.5. The number of favorably oriented systems within a grain is clearly an important determinant of the TVF, not just the value of the SF. This can explain why, despite similar values of maximal SFs, $\{10\bar{1}0\}$ orientations in compression display lower TVFs than (0002) in tension (Fig. 5a).

Table 2. SF for all six twin variants in tension.

Reflection	0002	$10\bar{1}4$	$10\bar{1}3$	$11\bar{2}4$	$10\bar{1}2$	$20\bar{2}3$
$\Delta\theta$	0°	25°	32°	39°	43°	51°

ϕ	0°	0°	0°	30°	0°	0°
(10 $\bar{1}2$)	0.50	0.30	0.19	0.13	0.00	-0.14
(1 $\bar{1}02$)	0.50	0.37	0.31	0.30	0.19	0.10
(0 $\bar{1}12$)	0.50	0.40	0.34	0.17	0.22	0.13
($\bar{1}012$)	0.50	0.34	0.24	0.17	0.06	-0.08
($\bar{1}102$)	0.50	0.40	0.34	0.30	0.22	0.13
(01 $\bar{1}2$)	0.50	0.37	0.31	0.12	0.19	0.10

Table 3. SF for all six twin variants in compression.

Reflection	10$\bar{1}0$	20$\bar{2}1$	21$\bar{3}0$	21$\bar{3}1$	11$\bar{2}0$	10$\bar{1}1$	11$\bar{2}2$
$\Delta\theta$	0°	15°	0°	11°	0°	28°	31°
ϕ	0°	0°	19°	19°	30°	0°	30°
(10 $\bar{1}2$)	0.50	0.45	0.45	0.42	0.37	0.30	0.16
(1 $\bar{1}02$)	0.13	0.09	0.02	0.00	0.00	0.00	-0.14
(0 $\bar{1}12$)	0.13	0.08	0.29	0.25	0.37	-0.02	0.11
($\bar{1}012$)	0.50	0.42	0.45	0.40	0.37	0.26	0.11
($\bar{1}102$)	0.13	0.08	0.02	0.00	0.00	-0.02	-0.14
(01 $\bar{1}2$)	0.13	0.09	0.29	0.26	0.37	0.00	0.16

According to [4], the nucleation of an additional twin variant in a grain besides that having the highest SF depends on the ratio of SF_i/SF_{max} . We have calculated SF for all 6 twin variants (see [13]) and the ratio between the best variant and the others (see IPF in the appendix Fig.B1). These IPFs show a completely different behavior in

compression. The effect is clear in Tables 2 and 3. In compression, the SF of 3rd ranked system is always less than 0.4, the 5th twin variant is always less than 0.2. In compression the probability of activation of all six twin variants within a grain will be very low. We can thus conclude that in tension the probability of activation of multiple twin variants within a grain is considerably higher than in compression. If we plot the number of variants with SF higher than 90% of the best variant (Fig.9) against maximal SF, we can observe this difference quite clearly. In tension, the high SF grains have the highest number of high SF variants. On the contrary, in compression, there is no direct correlation between number of twin variants and maximal SF.

In Figure 5, the orientation pairs $\{10\bar{1}0\}_C - (0002)_T$ and $\{10\bar{1}1\}_C - \{11\bar{2}4\}_T$, show larger TVF in tension. These two pairs show different number of high SF variants in Figure 9. In case of the other orientation pairs in Figure 5 $\{11\bar{2}0\}_C - \{10\bar{1}3\}_T$, $\{21\bar{3}1\}_C - \{10\bar{1}4\}_T$ and $\{11\bar{2}2\}_C - \{20\bar{2}3\}_T$ the TVF is similar. These pairs show similar numbers of high SF variants in Figure 9. Thus, *the different behavior of TVF dependence on SF is due to the difference in the number of high SF variants. In tension*, with increasing $\Delta\theta$ both the value of $SF_{\max}$ and the number of high SF twin variants proportionally decrease. *In compression*, this dependence is not straightforward, since not only the deviation from the ideal orientation but also the rotation around the c-axis (ϕ) is an important parameter.

4.3 EPSC modeling

Finally, the deformation behavior was modeled using an Elasto-Plastic Self-Consistent (EPSC) model to verify that it could capture the present findings [18]. The reason for

that was the capability of the EPSC for predicting the number of twin variants, which are nucleated within a particular grain.

The Voce parameters used for fitting are shown in Table 4. The match between the experimental data and the theoretical curve is satisfying (Fig. 10).

Table 4. Voce parameters for compression test

	$\tau_0[MPa]$	$\tau_1[MPa]$	$\theta_0[MPa]$	$\theta_1[MPa]$
Basal	13	7	100	50
Prismatic	25	5	120	15
2nd order pyramidal	120	90	200	100
Twinning	8	0	0	0

The EPSC model gives further information about the texture changes, which can be utilized for calculation of theoretical diffraction patterns. From the output of the EPSC we calculated the relative intensity changes of diffraction peaks measured also by neutron diffraction (see above). It is evident from Fig. 11 that the EPSC model predicts similar behavior shown in Figure 4.

Our assumption is that nucleation of more variants that provides different strain direction is an important parameter for twinned volume. Twin variants $(10\bar{1}2)[\bar{1}011]$ and $(\bar{1}012)[10\bar{1}1]$ provides mirror symmetric strain. From the point of view of EPSC model there is not a big difference between them and they can be considered together. Similarly, we can make pairs from the other four variants. Therefore, we have 3 variant pairs with different straining. Figs. 12 display the orientations of those grains, which

according to the EPSC model undergo twinning. The colors represent number of nucleated twin variants within the grains having a particular orientation, predicted by the model. The calculations clearly illustrate that there is a significant difference between the tension and compression case, respectively. And the EPSC modeling results are in excellent agreement with the theoretical calculations presented in Fig. 9.

In Figure 12a the data for tension show for $\Delta\theta < 30^\circ$ (red area) grains that exhibit nucleation of at least three variants. For $\Delta\theta > 30^\circ$ nucleation of only two (blue area) or one variant (green area) is observed.

In compression (Figure 12b), at most two variants are predicted to form. The number of variants depends on the ϕ angle, this is on the rotation of the grain around the c -axis.

The EBSD observations support these conclusions. The presence of all six variants can be observed in grain T1 in Fig. 6. The orientation of T1 grain is almost ideal for extension twinning *in tension*, (SF: 0.46, 0.48, 0.48, 0.48, 0.49, 0.47). However, we can also observe twin nucleation in grains, which are highly deviated from ideal orientation. The deviation of grain T2 (Fig. 2a) is $\theta = 77^\circ$, $\phi = 25^\circ$ and SF in tension are (-0.35, -0.28, **0.02**, -0.37, -0.30, **0.02**). Despite the low SF, the EBSD proved nucleation of the variants with positive SF. The twinned volume in this particular grain is not high, but owing to the high number of such oriented grains, their contribution to the overall TVF is not negligible. In contrast, grain C1 is almost ideally oriented for twinning *in compression*

(SF: 0.41, 0.09, 0.06, 0.44, 0.11, 0.05). However, the SF_i/SF_{max} ratio for $i > 2$ is small. Consequently, nucleation of two variants (more precisely a pair of twin variants) is observed – exactly, as the EPSC model predicts. The C2 grain is deviated by the

$\phi = 25^\circ$ (SF: 0.29, 0.22, -0.05, 0.32, 0.25, -0.06). All four high SF variants are nucleated which is again in good agreement with the EPSC results.

We thus conclude that the results of EPSC modeling are in good agreement with measured data and theoretical results. The EPSC well predict the anomalous SF dependence of TVF and provides better insight on twin variants selection.

The analysis presented above demonstrates, how the twinned volume fraction can depend on the SF. However, the twin nucleation and growth are influenced also by other microstructural parameters as e.g. the orientation of the neighboring grains [21], stress gradients across the grain [5] or interaction of twin boundaries with dislocations [22]. In order to get a complex picture about the twinning in magnesium alloys, these factors have to be taken also into account. However, such analysis is out of scope of the present paper.

Conclusion

The evolution of the $\{10\bar{1}2\}$ extension twinning during tension and compression testing of Mg-2 wt.% Al alloy was studied *in-situ* by neutron diffraction measurements and theoretically by elasto-plastic self-consistent modeling. The following conclusions may be drawn:

- The overall twinned volume is larger in compression owing to the larger number of grains favorably oriented for nucleation of twins with high Schmid factor for twinning,
- *In tension*, the twinned volume fraction decreases with increasing deviation of the given grain from the ideal orientation for extension twinning.
- *In compression*, not only the deviation from the ideal orientation, but also the grain rotation around the c-axis plays an important role. The latter parameter

determines the probability of the activation of further twin variants. Therefore, the ideally oriented and deviated, but properly rotated grains can exhibit the same twinned volume, owing to the higher number of twin variants nucleated in the latter grains.

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Appendix

A. Calculation of the loading mode dependence of the Schmid factors for extension twinning (Fig A.1)

Generally, the Schmid factor, giving proportion between the critically resolved shear stress (τ) on a slip plane and the stress applied to the material (σ) is given by:

$$m = \cos \varphi \cos \lambda \quad (\text{A.1})$$

where φ is angle between loading direction ($\vec{F}$) and slip plane normal ($\vec{n}$) and λ is angle between loading direction and slip direction ($\vec{s}$).

We did the calculation in Cartesian coordinates system selecting the loading direction aligns with the z -axis ($\vec{F} = |F|\vec{e}_z$) and using Euler angles and Bunge notation ($\phi_1\theta\phi_2$) to define the grain orientation. In the initial state configuration ($0^\circ 0^\circ 0^\circ$) the basal plane (0001) is perpendicular to z -axis and prismatic plane ($10\bar{1}0$) is perpendicular to the y -axis. Therefore the θ rotation is around the x -axis, which is the $\langle 1\bar{2}10 \rangle$ direction. The ϕ_1 rotation takes place around the z axis (=loading direction). Thus, it does not influence the angle between loading direction and slip direction. Therefore and we can set it as 0° and simplify an expression for Euler angles as $(\theta\phi)$. Using the vector algebra, we can write the Schmid law as follows:

$$m = (\vec{e}_n(\theta\phi) \cdot \vec{e}_z)(\vec{e}_s(\theta\phi) \cdot \vec{e}_z) \quad (\text{A.2})$$

There are six twinning planes and each of them has one twinning direction. The following calculation is done for the $(10\bar{1}2)[10\bar{1}\bar{1}]$ variant. The ϕ angle for the other variants can be expressed as $\phi = \phi' + k \cdot 60^\circ$, where $k \in \{0,1,2,3,4,5\}$. The plane

normal vector and slip direction are expressed as a combination of the initial state and the rotation matrix.

$$\vec{n} = (0, c/a, \sqrt{3}) \quad (\text{A.3})$$

$$\vec{s} = (0, -\sqrt{3}, c/a) \quad (\text{A.4})$$

Since we needn't take into account the ϕ_1 rotation, there are only two rotation matrices.

$$C(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & \sin \theta \\ 0 & -\sin \theta & \cos \theta \end{pmatrix} \quad (\text{A.5})$$

$$B(\phi) = \begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (\text{A.6})$$

The transformation from the coordinate system connected with the crystal to base fixed to the loading direction is:

$$\vec{n}(\theta\phi) = (B(\phi)C(\theta))^{-1} \vec{n}_0 \quad (\text{A.7})$$

$$(B(\phi)C(\theta))^{-1} = \begin{pmatrix} \cos \phi & -\sin \phi & 0 \\ \cos \theta \sin \phi & \cos \theta \cos \phi & -\sin \theta \\ \sin \theta \sin \phi & \cos \phi \sin \theta & \cos \theta \end{pmatrix} \quad (\text{A.8})$$

From eq. (A.2)-(A.8) we get:

$$m = \left((B(\phi)C(\theta))^{-1} \vec{e}_{n_0} \cdot \vec{e}_z \right) \left((B(\phi)C(\theta))^{-1} \vec{e}_{s_0} \cdot \vec{e}_z \right) \quad (\text{A.9})$$

Since $\vec{e}_z = (0,0,1)$, we are only interested about the z projection of $\vec{e}_n, \vec{e}_s$.

$$m = \frac{1}{(c/a)^2 + 3} (\cos \phi \sin \theta c/a + \cos \theta \sqrt{3}) (-\cos \phi \sin \theta \sqrt{3} + \cos \theta c/a) \quad (\text{A.10})$$

Using the relation between trigonometric functions

$$\cos(\phi + 60^\circ) = (\cos \phi - \sqrt{3} \sin \phi)/2 \text{ and } \cos(\phi + 120^\circ) = (-\cos \phi - \sqrt{3} \sin \phi)/2$$

we can calculate SF for all variants.

θ - angle between the c -axis and the loading direction

ϕ - is the angle describing rotation of the unit cell around the c-axis

SF	m_{tw}^1	m_{tw}^2	m_{tw}^3	m_{tw}^4	m_{tw}^5	m_{tw}^6
Twinning plane	(10 $\bar{1}$ 2)	(1 $\bar{1}$ 02)	(0 $\bar{1}$ 12)	($\bar{1}$ 012)	($\bar{1}$ 102)	(01 $\bar{1}$ 2)

Table A1. Assignment of SF to the twinning plane

$$m_{tw}^1 = (3 \cos \theta + 2\sqrt{2} \sin \theta \cos \phi)(4\sqrt{2} \cos \theta - 6 \sin \theta \cos \phi)/34 \quad (\text{A.11})$$

$$m_{tw}^2 = (3 \cos \theta + \sqrt{2} \sin \theta (\cos \phi - \sqrt{3} \sin \phi))(4\sqrt{2} \cos \theta - 3 \sin \theta (\cos \phi - \sqrt{3} \sin \phi))/34 \quad (\text{A.12})$$

$$m_{tw}^3 = (3 \cos \theta - \sqrt{2} \sin \theta (\cos \phi + \sqrt{3} \sin \phi))(4\sqrt{2} \cos \theta + 3 \sin \theta (\cos \phi + \sqrt{3} \sin \phi))/34 \quad (\text{A.13})$$

$$m_{tw}^4 = (3 \cos \theta - 2\sqrt{2} \sin \theta \cos \phi)(4\sqrt{2} \cos \theta + 6 \sin \theta \cos \phi)/34 \quad (\text{A.14})$$

$$m_{tw}^5 = (3 \cos \theta - \sqrt{2} \sin \theta (\cos \phi - \sqrt{3} \sin \phi))(4\sqrt{2} \cos \theta + 3 \sin \theta (\cos \phi - \sqrt{3} \sin \phi))/34 \quad (\text{A.15})$$

$$m_{tw}^6 = (3 \cos \theta + \sqrt{2} \sin \theta (\cos \phi + \sqrt{3} \sin \phi))(4\sqrt{2} \cos \theta - 3 \sin \theta (\cos \phi + \sqrt{3} \sin \phi))/34 \quad (\text{A.16})$$

B. Calculation of the ratio between the best variant and the others.

SF of coupled variants (1 – 4, 2 – 5, 3 – 6) are similar, we will work further only with

the variant with higher SF. In compression $m_{tw}^1 > m_{tw}^6 > m_{tw}^2$, in tension $m_{tw}^5 >$

$m_{tw}^3 > m_{tw}^4$.

We plotted the IPF of SF for the best variant and ratio between others variants and the best one (Fig. B.1).

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Figure A.1 Variation of the Schmid factors for extension twinning in a) tension, b) compression in θ - ϕ space calculated using Eqs. 11-16. The blue color represents negative values.

Figure B.1 IPF of Schmid factor for a) tension b) compression and ratio of Schmid factors between the c,d) 3rd, resp. e,f) 5th variant and the best one

Figure 1

Figure 2a

Figure 2b

Figure 3

Figure 4a

Figure 4b

Figure 5a

a)

Figure 5b

Figure 5c

Figure 5d

Figure 5e

Figure 6

Figure 7

Figure 8

Figure 9

Figure 10a

Figure 10b

b)

Figure 11a

a)

Figure 11b

b)

Figure 12a

Twinned grains Tension

Figure 12b

Twinned grains Compression

Figure A.1

Figure B.1