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# Full length article On the role of anomalous twinning in the plasticity of magnesium Konstantin D. Molodov \*, Talal Al-Samman, Dmitri A. Molodov, Günter Gottstein

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## ABSTRACT

Specially oriented Mg single crystals were deformed at ambient and elevated temperatures in channeldie compression with the *c*-axis inclined at 45° to the compression direction and  $\langle 10\bar{1}0 \rangle$  parallel to the lateral constraint direction. The specimens deformed by basal slip, entailing a rotation of the *c*-axis towards the compression direction. At room temperature, starting already during early stages of deformation, macroscopic bands comprising a mesh of anomalous  $\{10\bar{1}2\}$  extension twins formed parallel to the constraint direction. These twins were characterized by a *negative* Schmid factor and produced a strain opposite to the imposed deformation. At the final true strain of -1, a significant volume fraction of the matrix was consumed by twins, causing a reorientation of the *c*-axis farther away from the compression direction, and hence delaying the formation of a hard basal texture component. An analysis of the displacement gradient tensors for the six possible extension twin variants showed that the selected twin variants, of which the bands were composed, involved a lattice rotation opposite to the one caused by basal slip. Less twinning was observed at elevated temperatures with the macroscopic bands disappearing at 370 °C. The obtained results are discussed with respect to deformation heterogeneity and the role of anomalous twinning for the deformation behavior of magnesium.

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#### 1. Introduction

Much attention has been paid to the elucidation of the deformation behavior of magnesium and its alloys, in particular with respect to deformation twinning in order to successfully predict the microstructure evolution and texture development of this hcp metal. The {1012} extension twins in Mg, which cause an extension along the *c*-axis, provide a crucial deformation mechanism for strain out of the basal plane. Moreover, the {1012} extension twins are known to grow during progressive deformation and to consume the parent grain, which entails a reorientation of the parent matrix by 86°  $\langle 1120 \rangle$ , giving rise to a dramatic change of the texture compared to slip. A comprehensive understanding of the twin variant selection is therefore of key importance for avoiding the formation of a hard basal component and thus, for enhancing the ductility of the material by texture softening.

 $\{10\overline{1}2\}$  extension twins typically obey the Schmid criterion, i.e. the twin variants with the highest Schmid factor (SF) are activated first in a fashion similar to slip and therefore govern texture evolution [1-3]. In a previous study on magnesium single crystals [4], aligned for *c*-axis extension during channel-die compression, we have shown that these high Schmid factor twins consumed the whole sample in an event of profuse twinning, whereas the

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lower SF variants made up only a negligibly small volume fraction. After reorientation by twinning, further deformation was mostly determined by the orientations of these high Schmid factor twins. In the case of another orientation of the single crystal specimen, when twinning caused a rotation of the initial matrix towards a hard basal orientation [5], the sample failed prematurely during deformation at ambient temperature, owing to a suppression of basal slip. Although we have observed a strict Schmidtype behavior of primary  $\{10\overline{1}2\}$  twinning in our own work on single crystals, it must be pointed out that the high SF twin variants were also optimally compliant with the imposed strain during channel-die compression.

In violation of this rule, there is however, also a very prominent example of deviation from the Schmid-type behavior. Extension twins within contraction twins, i.e.  $\{10\overline{1}1\} - \{10\overline{1}2\}$  double twins, do not conform to the Schmid-type behavior as the 38°  $\langle 11\overline{2}0 \rangle$  variant typically occurs more frequently. This circumstance was explained by self-strain compatibility and ease of growth [6,7] as well as external strain accommodation during rolling [8].

Besides the well-known double twins, there is further indication that  $\{10\overline{1}2\}$  twins do not always obey the Schmid criterion. Examining the activation of extension twins on a grain by grain basis, along with high SF twins, Pei et al. [9] found a number of additional twin variants, which did not conform to the Schmid factor ranking. Yang et al. [10] conducted channel-die experiments on AZ31 alloy and concluded that the extension twin variant which was activated first was the one fitting the externally imposed strain best.





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Furthermore, Nave and Barnett [11] found evidence for  $\{10\overline{1}2\}$  extension twinning after *c*-axis compression of textured polycrystalline samples in a channel-die. This was attributed to unloading or local anomalous stress states. In that case the Schmid type behavior was not only violated in terms of ranking but the twins even produced a strain opposite to the externally imposed one. Koike et al. [12] performed experiments, focusing in particular on anomalous  $\{10\overline{1}2\}$  twinning with the twinning strain directed opposite to the external strain. They found good agreement between the basal slip activity and the tendency for  $\{10\overline{1}2\}$  twinning and concluded that the  $\{10\overline{1}2\}$  twins formed as a consequence of strain accommodation, originating from localized basal slip; i.e. anomalous twins formed when basal slip activity in the twinning grain was higher than in its surrounding grains.

In a more recent study, Wang et al. [13] conducted in-situ compression tests on Mg and Mg alloys containing rare-earth elements. They observed non-Schmid behavior of extension twinning in both cases and drew the conclusion that twinning is in line with Schmid's law in orientations, which are favorable for twinning, while in the case where twinning is not favored by the macroscopic stress, the formation of twins can be understood as a mechanism for accommodation of local strain, rather than a response to external strain. The authors effectively employed the Luster–Morris parameter [14] as a criterion for twin variant selection.

By analysis of  $\{10\bar{1}1\}$  contraction twinning in polycrystals, Jonas et al. [15] established a relationship between the twin variant selection and the necessary strain accommodation in neighboring grains. They found that high SF twin variants were less likely if their accommodation required appreciable amounts of prismatic slip in the neighboring grain. The same principle was used by Mu et al. [16] for the variant selection of primary, secondary and tertiary twins.

To add to the point that twin variant selection is not always simply correlated with the SF, molecular dynamics simulations revealed a substantial sensitivity of  $\{10\overline{1}2\}$  twins to non-Schmid stresses [17], indicating that twinning nucleation is heterogeneous in nature.

In contrast to our earlier studies on Mg single crystals [4,5,18,19] the recent work focused on the deformation behavior of single crystals with a 'soft' orientation, i.e., where the *c*-axis was initially inclined at an angle of 45° to the compression direction. Consequently, deformation was expected to employ basal slip only and at a very low flow stress [20], owing to the low critical resolved shear stress for basal slip at room temperature [21]. As reported and discussed in the current paper, this model case provided an opportunity to study deformation heterogeneity and the appearance of anomalous twinning since no twinning was expected to operate under the present conditions. Moreover, the used orientation represented a classic case of a 'soft' grain, which rotates towards a hard

(a)

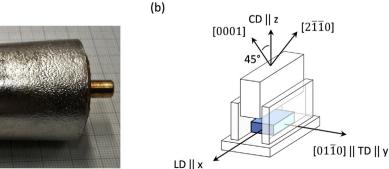
basal orientation as a consequence of basal slip. This slip-induced orientation change is of particular interest, since the emergence of a hard basal texture component accounts for reduced room temperature ductility of polycrystalline Mg in plane strain deformation. Mechanisms for preventing the formation of a hard basal component are therefore highly desired.

#### 2. Experimental

For the growth of single crystals of commercially pure (min. 99.95%) magnesium a stainless steel mold was used. The inside of the mold was covered with a graphite based die coating (Acheson Hydrokollag IP 5). A vertical Bridgeman furnace with argon atmosphere was utilized for the growth process. Specially oriented cylindrical monocrystalline seeds with the *c*-axis parallel to the growth direction were employed. Fig. 1a shows a grown single crystal which was then mounted onto a goniometer with a compound of glue and copper powder to ensure electrical conductivity for electrical discharge machining (EDM). By means of the Laue X-ray back diffraction method [22] the crystallographic axes of the grown single crystals were aligned with respect to the specimen coordinate system. After alignment, smaller specimens for the PSC tests with dimensions of 14 mm  $\times$  10 mm  $\times$  6 mm were cut from the grown single crystals by EDM. The deformation geometry with respect to the PSC coordinate system is illustrated in Fig. 1b. Both the *c*-axis as well as the  $[2\overline{1}\overline{1}0]$  crystal direction were aligned at an angle of 45° to the compression direction. The misalignment between the crystallographic directions of the crystal and the corresponding specimen axes i.e. compression (CD), longitudinal (LD) and transverse direction (TD) of the channel-die were less than 1°. PSC tests were carried out using a conventional screw-driven ZWICK testing machine at ambient and elevated temperatures of 200 °C and 370 °C. The samples were deformed at a constant strain rate of  $10^{-3}$  s<sup>-1</sup> up to a logarithmic strain (referred to as true strain) of  $\varepsilon_t = -1$ ; with  $\varepsilon_t = \ln(1+\varepsilon)$ , where  $\varepsilon$  is the engineering strain. The applied force as well as the displacement in CD was monitored and regulated by a computer equipped with an automated data acquisition system. For tests at ambient temperature lubrication oil was used in order to minimize friction. Some selected tests at ambient temperature were also performed using a thin Teflon film in combination with oil as well as hexagonal boron nitride (h-BN) powder. At elevated temperatures h-BN powder was used exclusively as a lubricant. Both the sample and channel-die were guenched rapidly in water to conserve the PSC microstructure.

The specimens were cut at the mid-surface of the LD-TD plane, metallographically polished and color etched to characterize the microstructure by means of optical microscopy using polarized light. In detail, the sample preparation comprised soft grinding,





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