

Kink formation and concomitant twin nucleation in Mg–Y



L. Wang^{a,*}, J. Sabisch^{a,b}, E.T. Lilleodden^a

^a Institute of Materials Research, Helmholtz-Zentrum Geesthacht, 21502 Geesthacht, Germany

^b Department of Materials Science and Engineering, University of California, Berkeley, CA 94709, USA

ARTICLE INFO

Article history:

Received 22 June 2015

Revised 13 August 2015

Accepted 16 August 2015

Available online 25 August 2015

Keywords:

Magnesium alloys

Tensile testing

Kink band

Twinning

ABSTRACT

During in situ tensile loading of a Mg–2.5 wt%Y alloy, a large kink band was observed. The orientation of the kink band varies continuously with a maximum misorientation angle of 18° with respect to the matrix grain. The formation of the kink band is accompanied by the nucleation of numerous $\{10\bar{1}2\}$ twins at the kink boundaries. A mechanistic model is proposed to account for this unique kink band and concomitant twin nucleation via dissociation of basal dislocations. This mechanism is aided by the presence of Y, which suppresses $\{10\bar{1}2\}$ twinning and simultaneously decreases the stacking fault energy.

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Mg is considered a promising structural material for automobile and aerospace industries due to its high specific strength compared with Al and steels. A critical technical barrier against a widespread application of Mg alloys, however, is the lack of ductility and poor formability [1]. At room temperature, the deformation of Mg is dominated by basal slip and $\{10\bar{1}2\}$ tensile twinning, while other slip or twin systems are generally suppressed due to their much higher critical resolved shear stresses (CRSSs) [2–6]. One approach to alleviate this problem is by adding a small amount of solute rare earth elements, which have been shown to affect both relative CRSS and stacking fault energy (SFE). Stanford et al. [7] estimated the CRSS of basal slip, pyramidal $\langle c+a \rangle$ slip, and $\{10\bar{1}2\}$ twinning in Mg–2.2 wt%Y by coupling in situ neutron diffraction experiment and elastoplastic self-consistent (EPSC) simulation. The result suggests that Y hardens all three deformation modes, but the hardening effect is stronger for $\{10\bar{1}2\}$ twinning than for slip modes. Sandlöbes et al. [8] used transmission electron microscopy (TEM) to examine the deformation microstructure in Mg–3 wt%Y and pure Mg after cold rolling. A high density of I_1 stacking faults were found, which served as nucleation sites for $\langle c+a \rangle$ dislocations. It suggests that Y reduces the stacking fault energy (SFE) in Mg, as was subsequently verified by first-principles studies [9,10]. In a more recent study, Stanford et al. [11] reported the observation of $\{11\bar{2}1\}$ twins in a single-phase Mg–10 wt%Y alloy after compression. While this twin mode has been frequently observed in other hexagonal materials such as Ti [12,13] ($c/a = 1.587$), Zr

[14,15] ($c/a = 1.593$), Re [16] ($c/a = 1.614$), and Co [17] ($c/a = 1.628$), it is rarely observed for Mg ($c/a = 1.623$). A general argument for the surprising observation of this twin in a Mg–Y alloy is that Y hardens the primary $\{10\bar{1}2\}$ twin mode which leads to the preferential nucleation of $\{11\bar{2}1\}$ twins, but details of the twin nucleation process is still unclear because the characterization was made ex situ.

Here, we present the results from an in situ straining study of a coarse-grained Mg–Y alloy, using grain-level characterization of the deformation-induced microstructural evolution. An unexpected kink band was observed to form in a grain whose c -axis was almost parallel to the tensile direction. Basal slip lines were found crossing the kink, and small $\{10\bar{1}2\}$ twins were identified in the vicinity of the kink. Based on the observed microstructure evolution, a dislocation reaction model is proposed to account for the kink formation.

A binary Mg–2.5 wt%Y solid solution alloy was produced by casting at the Magnesium Innovation Centre (MagIC) of Helmholtz-Zentrum Geesthacht. To achieve a homogeneous composition distribution, the melt was taken to 700 °C for 10 min before casting. A relatively small cylinder die ($D = 18$ mm, $H = 100$ mm) was used. The as-cast piece of cylinder material was cut into two half-cylinders by electrical discharge machining (EDM). Dog-bone tensile specimens with a gauge dimension of 5 mm \times 2 mm \times 1 mm ($L \times W \times T$) were extracted from one half-cylinder, with the tensile axis being parallel to the vertical direction of the half-cylinder. The specimen to be tested was close to the top of the half-cylinder. The surface was prepared using conventional grinding and polishing procedures. The final thickness was reduced to ~ 0.4 mm. An EBSD scan of the initial

* Corresponding author.

E-mail addresses: wly857@gmail.com, leyun.wang@hzg.de (L. Wang).

microstructure close to the gauge center was performed using a Zeiss Gemini Ultra 55 scanning electron microscope (SEM). Grain sizes range from 100 μm to more than 1 mm. The specimen was deformed by tensile test using a MICROTTEST 200N (Deben, UK Limited) module at a constant crosshead speed of 0.2 mm/min, which corresponds to a nominal strain rate of $6.67 \times 10^{-4} \text{ s}^{-1}$. The microstructure evolution during the loading was monitored using an Olympus SZX10 optical microscope connected with a video recording system. Fig. 1 shows the engineering stress–strain curve of the test at a strain of about 10%, along with the microstructure evolution near the gauge center associated with points A–H labeled on the stress–strain curve. Based on the initial EBSD measurement, crystallographic orientations of four large grains ($d > 500 \mu\text{m}$) as well as the approximate grain boundaries between them were overlaid on the micrograph of the initial structure prior to loading (point A). Grain 3 (Euler angles = $(181^\circ, 83^\circ, 5^\circ)$) is a large grain with its c -axis almost parallel to the tensile axis. This is a favorable condition for $\{10\bar{1}2\}$ twin nucleation, and our initial focus was on the 1–3 grain boundary in order to observe potential slip transfer induced twin nucleation events [18]. During the loading, slip lines were first observed in Grain 1 and Grain 2, favorably oriented grains for basal and prismatic slip, respectively. At an applied stress of 70 MPa (point C), slip lines appeared inside Grain 3. Using the standard trace analysis [18], these slip lines were found to correspond to basal slip, as marked by the white dashed line in the micrograph for C. At point D, a lenticular kink band, evidenced by the bright contrast, quickly developed in Grain 3 from the region where basal slip lines had concentrated. The original basal

slip lines were redirected by about 12° relative to their initial direction at point C, suggesting an orientation rotation inside the kink band. In addition, small features show up at the upper boundary of the kink band, which are later identified as newly nucleated $(\bar{1}012)$ $[10\bar{1}1]$ twins. With further straining (from E–H), the kink grew laterally and more $(\bar{1}012)$ twins were found in its vicinity, and a few $(\bar{1}102)$ $[1\bar{1}01]$ twins with dark contrast were identified in the left part of Grain 3 (point F). The video recording the microstructure evolution during loading can be found in the [Supplementary material \(loading.mp4\)](#).

After the peak load was reached, the sample was gradually unloaded at the same displacement rate, and the unloading process was recorded in a second video ([unloading.mp4](#)). Detailed EBSD characterization was subsequently performed for the kink in Grain 3, as shown in Fig. 2. From the optical micrograph, the kink band grew across the entire Grain 3. There are also some small kinks parallel to the big kink, as evidenced by their bright contrast. The direction of basal slip lines are deviated when crossing these kinks. Furthermore, twins are observed adjacent to the kink boundary, having likely nucleated from the upper boundary of the big kink. These are marked by red arrows in the figure. According to EBSD based misorientation analysis (Fig. 2(b)), as well as twin plane trace analysis (Fig. 2(c)), they belong to the twin system $(\bar{1}012)$ $[10\bar{1}1]$ with a Schmid factor of 0.482. Likewise, twins that nucleated from the grain boundary between Grains 3 and 4 (Fig. 1, point F) were identified as $(\bar{1}102)$ $[1\bar{1}01]$ twins with a Schmid factor of 0.493.

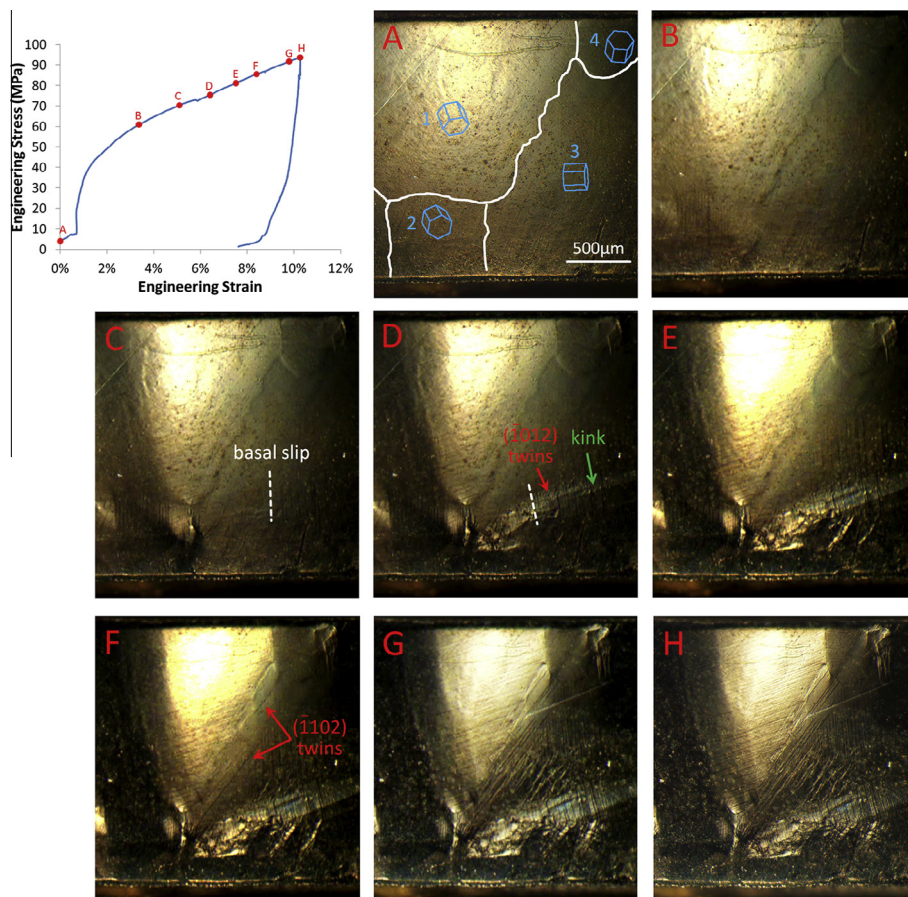


Fig. 1. Engineering stress–strain curve of the tensile test. Optical microscopy tracks the microstructure evolution. Basal slip lines first appeared in Grain 3 (C), followed by the formation of a large kink band (D). $(\bar{1}012)$ twins nucleated from the upper boundary of the kink. With further straining, the kink grew laterally and more $(\bar{1}012)$ twins are found in its vicinity. A few $(\bar{1}102)$ twins also developed in the left part of Grain 3 (F).

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