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Investigation of the twinning mode in a compressed Mg-10Gd-2Y-0.5Zr alloy assisted by Rietveld refinement

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Abstract. This paper investigated the twinning mode in a homogenized Mg-10Gd-2Y-0.5Zr ingot compressed at 300 ^{o}C and 1 s^{-1} using transmission electron microscopy observation and schematic method. Details about the primary twinning mode was studied based on the minimum sear criterion by comparing the values of the four major twinning modes in the magnesium alloys. The results show that the twins are formed first by $\{10\bar{1}1\}$ primary twinning being step characteristics, and then the secondary twins are formed later around the step by $\{10\bar{1}2\}$ secondary twinning. The results also show that the XRD Rietveld refinement method is an effective means to obtain the lattice parameter and to calculate the twinning shear that has important effect on the primary twinning mode in a h.c.p alloy.

Introduction

It is believed that deformation twinning plays an important role in maintaining a generalized plastic flow of polycrystals with hexagonal closed-packed (h.c.p) [1, 2]. The role of deformation twinning in strengthening and ductility of h.c.p metals has been the subject of a number of investigations [3-5]. Experimentally, it is observed that deformation twinning can effectively strengthen a material under some circumstances and weaken it under others. This complexity results mainly attributes to the activated twinning modes. For magnesium and its alloys, although different twinning modes have been observed by a number of authors, it is quite common for twinning to occur on the $\{10\bar{1}1\}$ plane [6, 7]. In many cases, this is followed by "retwinning" or "secondary" twinning on the $\{10\bar{1}2\}$ plane [3, 8]. This is known as double twinning. Previous works used mainly schematics based on the data for pure magnesium to investigate the double twinning in the magnesium alloys [3, 9]. Little work was paid on the double twinning characteristic by microstructure observation, such as by transmission electron microscopy (TEM). Besides, most of the works about the twinning mode in the magnesium alloys used mainly the data for pure magnesium [10, 11]. It might be validity for those magnesium alloys whose *c*/*a* axial ratio is similar to that for pure magnesium. However, compared with those magnesium alloys, the *c*/*a* axial ratio for the Mg-Gd-Y alloys with higher Gd and Y contents might be different greatly to pure magnesium because of the larger atom radius of the Gd and Y elements. Therefore, the relative values of the twinning shear that is only the function of *c*/*a* axial ratio [2] for some candidate twinning modes in the Mg-Gd-Y alloys with higher Gd and Y contents might be also changed. Obviously, it is a lack of convincing to use the data for pure magnesium to show the twinning mode in the Mg-Gd-Y alloy with higher Gd and Y contents.

It was reported that the twinning shear of the activated twinning mode was commonly smaller than that of the complementary twinning modes [12-15] (minimum shear criterion) under a certain deformation condition. Therefore, it can be proposed that if the twinning shear for some candidate twinning modes in a given alloy could be calculated and compared. The primary twinning mode in this alloy might be predicted.

Nevertheless, little published works have been paid to study the effect of alloy elements, such as Gd and Y, on the *c*/*a* axial ratio, the twinning shear and the twinning mode in the magnesium. In this work, the twinning characteristics and twinning mode in one texture-free Mg-10Gd-2Y-0.5Zr alloy compressed at 300 ^{o}C and 1 s^{-1} were investigated by TEM techniques and schematic methods. More details about the relative values of the twinning shear that can be calculated by the *c*/*a* axial ratio for four major twinning modes in the magnesium alloys was obtained and compared using X-ray diffraction (XRD) Rietveld refinement method to obtain the lattice parameters *a* and *c*. Therefore, the primary twinning in the texture-free Mg-10Gd-2Y-0.5Zr alloy was investigated based on the minimum shear criterion.

Experimental materials and procedures

The alloy used in this work was a homogenized Mg-10Gd-2Y-0.5Zr alloy ingot. The cylindrical samples with Φ10 mm×15 mm dimension were compressed to 50% height on a Gleeble-1500 thermo mechanical simulator at 300 ^{o}C and 1 s^{-1} in the air and immediately cooled to room temperature.

After deformation, the obtained sample was sectioned in a plane containing the compression direction, ground to 4500 grit SiC, then electropolished using the AC-2 electrolyte (Struers, Denmark) at 20 V and 25 ^{o}C. Optical microscopy was used to obtain the microstructure characteristic of the as-received and the compressed samples. TEM was used to investigate the twin characteristics and twinning modes in the compressed sample. XRD analysis was conducted on the homogenized and the compressed samples. XRD data were received using a Rigaku D/MAX-3B diffractometer with Cu Kα radiation. The XRD profiles were then analyzed with the Rietveld refinement method.

Results and analysis

Fig. 1a shows the typical optical microstructure of the homogenized sample. It can be found that the sample possesses nearly equiaxed grains with grain size of ~50 μm, and the obvious residual intermetallic compounds cannot be found. Comparing to the homogenized sample, the deformation microstructures and the obvious twins with morphology of thick lines can be found clearly in the compressed sample, as shown in Fig. 1b.

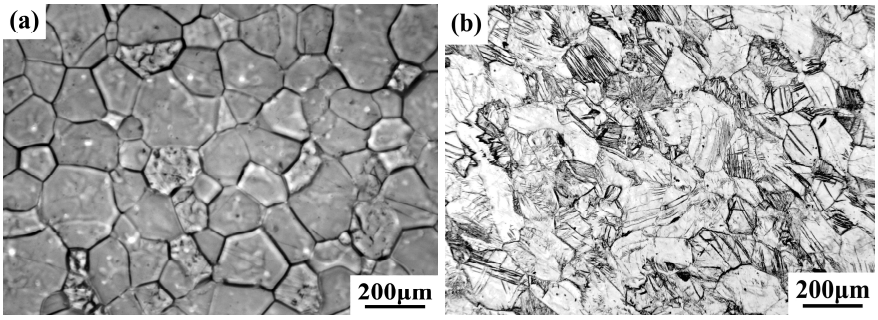

Fig. 1. Microstructure of the Mg-10Gd-2Y-0.5Zr alloy: (a) homogenized; (b) compressed at 300 ^{o}C and 1 s^{-1}

The XRD Rietveld refinement result verifies further that the single hexagonal magnesium phase exists in the two samples, as shown in Fig. 2. Besides, it can be obtained from the XRD Rietveld refinement that the lattice parameters *a* and *c* for magnesium phase in the homogenized sample are 0.32290±0.00003 nm and 0.52159±0.00004 nm, respectively. Therefore, the axial ratio being ~1.6153 that is smaller than that in pure magnesium being ~1.6240 [16] and the ideal axial ratio being ~1.6330 for h.c.p crystals can be obtained. Therefore, twins might form in the compressed samples under a certain condition, especially at low temperature and high strain rates [1, 3, 17]. The optical micrograph shown in Fig. 1b gives evidence that the obvious twins exist in the compressed sample.

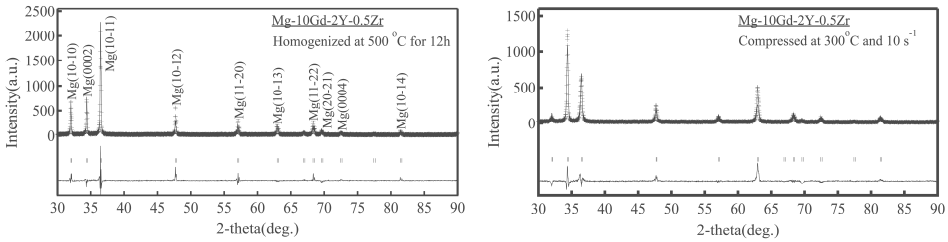

Fig. 2. X-ray diffraction Rietveld refinement results of the Mg-10Gd-2Y-0.5Zr alloy: (a) homogenized; (b) compressed at 300 ^{o}C and 1 s^{-1}

Fig. 3a shows the TEM observations of the compressed sample. The slip lines distributed parallel on the deformation matrix (white zone) and the lath microstructure (dark zone) that angled to the white zone can be found clearly. The typical twin characteristic can be obtained from the corresponding selected area diffraction (SAD) patterns of the circle area (interface between the dark and the white zones shown in Fig. 3a), as shown in Fig. 3b. The indexed result of the SAD patterns shows that the slip lines are the trace of the (0002) basal dislocations. The lath microstructure is the twin that was formed by the basal rotation with angle of ~38^{o} around $[\bar{1}2\bar{1}0]$. This angle is similar to that in pure magnesium and the other magnesium alloys twinned by forming $\{10\bar{1}1\}$ primary twin first, after which $\{10\bar{1}2\}$ twin propagated within the primary twins [3, 9].

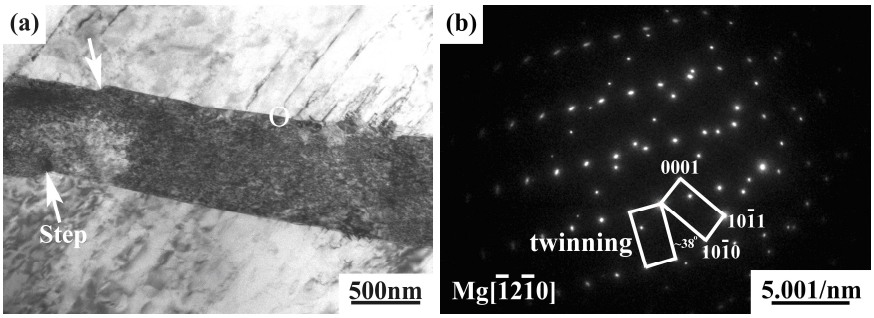

Fig. 3 Morphology of the twin (a) and the SAD patterns for the circle zone (b) of the Mg-10Gd-2Y-0.5Zr alloy compressed at 300 ^{o}C and 1 s^{-1}

Besides, it can also be found from Fig. 3a that the obvious step characteristic exists in the twin boundary. From the molecular dynamic simulation [18] and the high-resolution electron microscopy (HREM) observation [7] about the twin formed by $\{10\bar{1}1\}$ twinning mode, it is reasonable to predict that the twins in the texture-free Mg-10Gd-2Y-0.5Zr alloy compressed at 300 ^{o}C might be formed first by $\{10\bar{1}1\}$ twinning mode and second by $\{10\bar{1}2\}$ twinning mode.

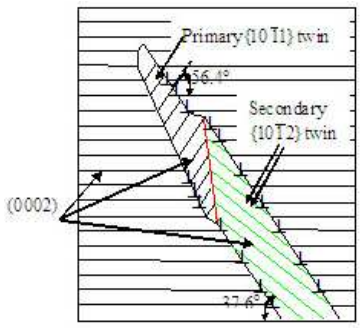

Fig. 4 Schematic of twinning process by primary $\{10\bar{1}1\}$ twinning and secondary $\{10\bar{1}2\}$ twinning in the texture-free Mg-10Gd-2Y-0.5Zr alloy compressed at 300 ^{o}C and 1 s^{-1}. The crosshatching lines correspond to basal plane traces and the image zone axis is a $<1\bar{2}10>$ axis. $\perp$ is the dislocations on the twin boundary

The twinning process in the homogenized Mg-10Gd-2Y-0.5Zr alloy compressed at 300 ^{o}C can be explained schematically by the reorientation angle of the basal plane [3, 5, 9]. This reorientation of the basal plane was illustrated elegantly by Barnett et al. [3] and we have reproduced a version of their diagram including the step characteristic and the dislocations around the twinning boundary, as shown in Fig. 4.

The more favorable alignment of the basal slip plane is shown: so too is the development of secondary $\{10\bar{1}2\}$ twinning in the primary $\{10\bar{1}1\}$ interior. The primary $\{10\bar{1}1\}$ twinning reorients the basal plane by ~56.2^{o} around a $<1\bar{2}10>$ axis; in this case, the secondary $\{10\bar{1}2\}$ twinning rotates the basal pole "back" by ~86^{o} around the same axis and the net result is a reorientation of the original basal plane by ~37.6^{o} around the $<1\bar{2}10>$ axis.

Nevertheless, it is more persuasive if the twinning process, especially to the primary twinning mode in the homogenized Mg-10Gd-2Y-0.5Zr alloy can be explained from the theoretical point of view. Several theories have been made to study the primary twinning mode in the crystalline materials. The two most classical theories were applied commonly [19]. The first theory was made to determine twinning elements of crystalline materials from the knowledge of crystal structure, because of their importance for insight into possible twinning modes and resultant orientation relationships of twinned crystals in the context of microstructural manipulation. The second theory was based on the minimum shear criterion. It is valid for all crystal structures with a known twinning shear. Based on the obtained lattice parameters for magnesium phase in the homogenized sample, the minimum shear criterion was used to determine the primary twinning mode in the homogenized alloy compressed at 300 ^{o}C and 1 s^{-1}. The calculated twinning shear for four dominant twinning modes in the magnesium alloys is shown in Table 1.

Table 1 Dominant twinning modes and twinning shear in the texture-free Mg-10Gd-2Y-0.5Zr alloy

Twinning modes	$\{10\bar{1}1\}<10\bar{1}2>$	$\{10\bar{1}2\}<10\bar{1}\bar{1}>$	$\{11\bar{2}2\}<11\bar{2}3>$	$\{11\bar{2}1\}<\bar{1}\bar{1}26>$
Twinning shear [2]	$s=\frac{4\gamma^2-9}{4\gamma\sqrt{3}}$	$s=\frac{\gamma^2-3}{\gamma\sqrt{3}}$	$s=\frac{2(\gamma^2-2)}{3\gamma}$	$s=\frac{1}{\gamma}$
	0.12842	-0.13965	0.25146	0.61907

It can be seen from Table 1 that the twinning shear being ~0.12842 for $\{10\bar{1}1\}<10\bar{1}2>$ mode is lower than those for the other three modes. According to the minimum shear criterion [19], the primary twinning is formed in the texture-free Mg-10Gd-2Y-0.5Zr alloy by the $\{10\bar{1}1\}<10\bar{1}2>$ mode. Because the step characteristic that was the result of the coalescence of the zonal dislocations [18] exists in the twin boundary formed by the primary twinning, the higher density dislocations and the local stress concentration exist around the step. The local stress concentration might cause the secondary twinning to coordinate the plastic deformation or lead to crack nucleation [2]. In present work, the secondary twinning formed by $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ mode minimize the compatibility strain [3] then might improve the plastic deformation of the homogenized Mg-10Gd-2Y-0.5Zr alloy.

Conclusion

In conclusion, the obvious twins exist in the homogenized Mg-10Gd-2Y-0.5Zr alloy compressed at 300 ^{o}C and 1 s^{-1}. The twins were formed in the compressed alloy by $\{10\bar{1}1\}$ primary twinning, and then the secondary twin occurred interior the primary twin by $\{10\bar{1}2\}$ secondary twinning. The step characteristic exists on the twin boundary between the deformation matrix and the $\{10\bar{1}1\}$ primary twin. Theoretical investigation of the primary twinning mode in the homogenized Mg-10Gd-2Y-0.5Zr alloy (texture-free) using the minimum shear criterion shows that the XRD

Rietveld refinement method is a valid tool to obtain the lattice parameters then to calculate and compare the values of the twinning shear for some candidate twinning modes in a given texture-free h.c.p alloy.

Acknowledgements

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