Effect of twin thickness-length ratio on twin-induced dynamic recrystallization of coarse-grained Mg alloys

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Abstract

In the current study, based on the disclination quadrupole, the thermodynamic process of the necklace-like TDRX structures with smooth and straight boundaries is theoretically modeled. The influence of the applied shear stress and the twin thickness-length ratio on the misorientation angle between TDRX and matrix grain and the volume ratio of TDRX to parent twin band are numerically analyzed and experimentally validated by the electron back-scatter diffraction characterization. The results show that: (1) the misorientation angle increases with increasing applied shear stress; (2) The greater the thickness-length ratio is, the lower the volume ratio of TDRX to parent twin is; (3) The elevation of the applied shear stress can clearly escalate the volume ratio of TDRX to parent twin. Based on the above results, some strategies regulating TDRX are given based on the control of the applied shear stress and twin thickness-length ratio.

1. Introduction

Compared with Al alloys and steels\([1, 2]\), magnesium and its alloys have a lower density and a higher specific strength. Their lightweight applications have attracted widespread attention. However, at low temperatures independent slip systems in the HCP structure of magnesium and its alloys are insufficient, which leads to poor formability. As a major deformation coordination mechanism, twinning is capable to re-arrange the crystal lattice and favor slip\([2, 3]\), playing a vital role in the plastic deformation of magnesium alloys.

Generally, the twinning within the coarse grains gradually evolves into the necklace-like twin-induced dynamic recrystallization (TDRX)\([4, 5]\) with smooth and straight boundaries during the severe plastic deformation processes, such as rolling, forging, extrusion, and so on. TDRX typically leads to grain refinement and orientation optimization\([6]\), dropping the strain hardening rate sharply and improving the strength and toughness of the material\([7–9]\). During the plastic deformation process, TDRX is the predominant softening mechanism within the coarse grains of as-cast magnesium alloys\([10–12]\). It was experimentally found that the gliding and rearrangement of the dislocations within twin bands can construct low-angle grain boundaries. As deformation continues, the misorientation angle gradually increases after the subgrains absorb the accumulated energy, the low-angle grain boundaries evolve into the large-angle grain boundaries, and new grains form\([13, 14]\). Compared with the parent twinning, the new grain has a softer orientation and can release the stress concentration. Therefore, the TDRX is crucial to continuing plasticity and avoiding brittle fracture of the coarse-grained magnesium alloy.

TDRX in magnesium alloys has been widely reported in the range of low (below 523 K), medium (523 K–623 K), and high temperatures (above 623 K)\([6]\). Xu et al\([15]\) found that compared with 400 °C, 300 °C is more favorable for TDRX. This implied that compared with the discontinuous and continuous DRXs that are strongly dependent on temperatures, TDRX is not very sensitive to temperatures, but mainly depends on stresses\([12, 15]\). In addition, it was reported that age hardening at 150 °C can induce fine and dense precipitates, thereby increasing the number of twins...
and reducing the size and total volume fraction of twins \[16\]. The morphology of twin bands can significantly influence twin intersection and double twinning in Mg alloys \[17\], however its effect on TDRX have been rarely reported. The effect of the morphology of twin bands on TDRX might be critical and promising in material design and property optimization of Mg alloys.

Disclinations \[18, 19\], which were originally introduced in the defect mechanics of solids, are the special sources of local stresses. Disclinations are characterized by its typical singularity and the property of multi-value fields of displacement and rotation associated with the defects. At present, the structure and concept of the disclinations quadrupole have been successfully used to model the grain boundary gliding and migration \[20–22\], grain rotation \[23\], deformation twins \[24–26\], microband \[27–29\], and so on. The TDRX is on the basis of the partition of twin bands by the large-angle grain boundaries originated from gliding and rearrangement of dislocations. Therefore, based on the equivalence of dislocation walls and disclination dipoles, the disclination quadrupole that is equivalent to a deformed band can fully account for the TDRX. In the current study, the effect of temperatures can be ignored in the thermodynamic simulation process of TDRX, and the deformation bands with smooth boundaries, specific geometry and misorientation can be modeled by the elastic energy-driven disclination quadrupole (the elastic deformation is larger than the plastic deformation or cannot be ignored in the early deformation stage within coarse grains).

Although a large number of experiments have found that TDRX occurs at multiple temperatures and revealed its physical mechanism, the effect of twin thickness-length ratio on TDRX, which may facilitate and broaden the application of TDRX in microstructural design to enhance the formability of coarse-grained Mg, is still unclear. The goal of the current study is to unmask the effect of the twin specific ratio on the profuse TDRX within coarse-grained Mg alloys.

2. Materials and experiments

2.1. Materials and hot rolling
The commercial AZ31 Mg alloy used was received in the form of as-cast. The as-cast magnesium alloy was selected to ensure the profuse twinning and TDRX extensively exist within the coarse grains during the following rolling process. The coarse-grained Mg alloy with a random texture has an average grain diameter of 245.5 μm, and no twinning is present within the coarse grains. The slabs, with initial dimensions of 123.44 mm in length, 90.8 mm in width, and 12.5 mm in thickness, were preheated to 573 K and held for 10 min before rolling. The diameter and speed of the both rollers were 90 mm and 19 r min\(^{-1}\), respectively. The slabs were rolled using a single rolling pass with a thickness reduction ratio of 17.3%\%. Single pass rolling can avoid grain refinement excessively to ensure the clear observation the twinning and TDRX. The temperature of 573 K was selected to avoid brittle cracking and ensure the profuse twinning and TDRX within coarse grains. The average strain rate of 1.72 s\(^{-1}\) during the rolling was close to the industry processes and limited by the rolling equipment. To avoid the influence of static recrystallization, the slabs were water quenched immediately after the hot rolling.

2.2. Electron back-scatter diffraction measurements
Microstructures on the transverse direction (TD) cross-sections were measured by the electron back-scatter diffraction (EBSD) technique using a Hitachi SU5000 scanning electron microscope equipped with an Oxford...
AZtec Nordlys Max data acquisition system. Prior to the EBSD measurements, the specimens were first ground to 1200 grit using SiC papers and then were mechanically polished with diamond paste through the sequence of W3.5, W2.5, W1, W0.5 and W0.25, after which they were etched in a solution of 10 ml HNO3, 30 ml acetic acid, 40 ml H2O and 120 ml alcohol. The EBSD samples were prepared in triplicate. The scanning field area was 800 \( \mu m \times 956 \mu m \), and the grains with a large amount of twin bands were selected as subsets.

3. Modelling

The subgrain boundaries formed by dislocation slip and piling up can eventually evolve into large angle grain boundaries with continuous deformation. Then new recrystallized grains are formed within the parent twin band with a strength of \( \omega_0 \) (rotational angle), achieving grain refinement and orientation softening. In the disclination theory, the magnitude of the Frank vector (rotation vector) has the meaning of the disclination strength in the same way as the magnitude of the Burgers vector characterizes the dislocation strength [30]. Two disclination quadrupoles are employed to model the evolution of TDRX from a twin band. In this process, the smooth and straight grain boundary formed by the rearrangement of the dislocations can be modeled by a disclination dipole, and the new grain can be modeled by a disclination quadrupole with a strength of \( \omega_1 \).

The schematic diagram (figure 1) shows that the TDRX is modeled by the nucleation of the disclinations quadrupole within the 2D twin band of Mg crystal (x-axis is along the <10–11> direction, and the xoz plane is the \(-1012\) twin plane), the angle \( \alpha \) equal to 43.15 degree represents the angle between the twinning plane (black line) and the basal plane of the twin band (red lines) or matrix (blue lines), and the angle \( \beta \) represents the angle between the twin plane and the basal plane of recrystallized grain (green lines). In state I, only a twin, with a length of \( L \) and a thickness of \( S \), occurs in the grain. In state II, TDRX, with a length of \( d \) and the same thickness as its parent twin, is formed within the twin band and assumed to initiate from the left end. Both the twin band and the recrystallized grain with different misorientation angles can be modeled by disclination quadrupoles with strengths of \( \omega_0 \) and \( \omega_1 \), respectively.

Referring to [25, 31], the rotational angle \( \omega \) caused by local deformation by twin or recrystallization can be calculated by the following equation:

\[
\omega = 2 \arctan \left( \frac{e^T}{2} \right) \tag{1}
\]

where \( e^T \) is the shear transformation, which is the measure of the rotation of recrystallized grain from its parent phase.

3.1. Potential energy difference before and after TDRX

Taking parent twinning as the initial system, the free energy of state I is expressed by the elastic energy \( E_1 \) of the disclination quadrupole itself and the interaction between disclinations [19]:

\[
E_1 = \frac{D \omega_0^2 S^2}{2} - \frac{D S^2}{2} [h^2 \ln (h^2) - (1 + h^2) \ln (1 + h^2) + 1] \omega_0^2 + 2\gamma_1 L \tag{2}
\]

where \( D = \mu / [2\pi(1 - \nu)] \), \( \mu \) represents the shear modulus, \( \nu \) represents Poisson’s ratio, \( h = L / S \) represents length-thickness ratio of parent twin band, \( \gamma_1 \) represent the twin boundary energy per unit area.

Taking the completion of TDRX within the parent twin band as the current system, the elastic energy \( E_2 \) results from three disclination dipole themself and their interaction.

\[
E_2 = \frac{D \omega_0^2 S^2}{4} + \frac{D \omega_1^2 S^2}{2} + \frac{D \omega_0^2 S^2}{2} [(1 + t^2) \ln (1 + t^2) - t^2 \ln (t^2) - 1] + \frac{D \omega_0^2 \omega_1 S^2}{2} [1 + (h - t)^2] \ln [1 + (h - t)^2] - (h - t)^2 \ln [(h - t)^2] - 1] + \frac{D \omega_0^2 \omega_1 S^2}{2} [h^2 \ln (h^2) - (1 + h^2) \ln (1 + h^2) + 1] + 2\gamma_1 L + \gamma_2 S \tag{3}
\]

where \( t = d / S \) represent the length-thickness ratio of TDRX grain, \( d = mL \), \( m \) represents the volume ratio of TDRX to parent twin band, \( \gamma_2 \) represents the large-angle grain boundary energy per unit area.

In addition, the total free energy per unit thickness of state II also includes the energy dissipated by the dislocation slip resistance \( \Pi_{\text{DISs}} \) (generated by the external work by resistance) and the energy changed by the applied shear stress in the process of TDRX \( \Pi_{\text{EXT}} \) (generated by the external work by applied force):
where $\tau_R$ represents the lattice resistance to dislocations in the TDRX process, and $\tau_{APPL}$ is the applied shear stress, $e_2^T$ represents the shear transformation of the recrystallized grain.

Finally, the change of the total free energy per unit thickness $\Delta \Pi_{TDRX}$ associated with the TDRX process from state I and II can be formulated as follows:

$$\Delta \Pi_{TDRX} = E_2 - E_1 + \Pi_{DISS} + \Pi_{EXT}$$  \hspace{1cm} (6)$$

To better demonstrate the influence of twinning thickness-length ratio on the TDRX within coarse grains, the thickness-length ratio $\eta = 1/h$ was substituted into equation (6).
Figure 4. (a) EBSD IQ diagrams of twinning and TDRX within a coarse-grained AZ31 magnesium alloy. The blue numbers 1–77 are the labels of two twin variants with the same twin boundaries \{10−12\} <−1011>, the black lines represent the high-angle grain boundaries, the yellow lines represent the \{10−12\} ETW boundaries (other twinning systems are rarely present), the silver areas represent substructures, the aqua areas represent deformed areas, the red areas encompassed by yellow lines represent TDRXs, and DRXed grains A, B and C are not the TDRX grains. (b) Pole figure and Inverse pole figure, where x, y and z represent the normal, rolling, and transverse directions of the hot rolled plate, respectively.
4. Results and discussion

For coarse-grained magnesium alloys, TDRX is very common at the low strain stage. It is the key to avoiding brittle fracture and continuing plastic deformation. Figure 2 shows the influence of different applied shear stress and recrystallization orientation angle on the relationship between total free energy change and twin thickness-length ratio. It can be seen that the free energy change of the entire system first decreases with increasing thickness-length ratio of the twin band until it reaches the lowest point, which is the stable equilibrium state, and then it gradually rises with increasing thickness-length ratio. The system equilibrium positions of all curves correspond to the same thickness-length ratio, which means that with the same twin thickness-length ratio, the greater the applied shear stress is, the greater the shear transformation after TDRX. It indicates that the elevation of the applied shear stress can increase the misorientation angle between the recrystallized grain and the matrix grain, realizing the orientation softening [6].

The influence of different volume ratios of recrystallization to parent twin on the relationship between total free energy change and twin thickness-length ratio is also given (figure 3). As shown in the figure, the lowest

| Table 1. Thickness-length ratio of twin variant I without recrystallization. |
| Twin band label | Thickness-length ratio | Twin band label | Thickness-length ratio | Twin band label | Thickness-length ratio | Twin band label | Thickness-length ratio |
|-----------------|------------------------|-----------------|------------------------|-----------------|------------------------|-----------------|------------------------|
| 2               | 23.4%                  | 3               | 10.7%                  | 4               | 23.5%                  | 5               | 31.6%                  |
| 6               | 22.2%                  | 7               | 30.5%                  | 8               | 19%                    | 9               | 12.7%                  |
| 10              | 30%                    | 11              | 10.4%                  | 12              | 25.2%                  | 13              | 17.9%                  |
| 15              | 11.9%                  | 16              | 15.6%                  | 17              | 10.8%                  | 18              | 15%                    |
| 19              | 22.9%                  | 20              | 10.3%                  | 21              | 9.3%                   | 22              | 9.6%                   |
| 23              | 9.8%                   | 26              | 21.6%                  | 27              | 24.2%                  | 29              | 14.5%                  |
| 31              | 11.1%                  | 33              | 10.6%                  | 34              | 19.9%                  | 35              | 15.5%                  |
| 36              | 14.8%                  | 37              | 14.1%                  | 38              | 24%                    | 40              | 20%                    |
| 41              | 12.3%                  | 42              | 26.2%                  | 43              | 13.2%                  | 47              | 12.9%                  |
| Arithmetic mean | 17.4%                  | Standard deviation | 0.0652 |

| Table 2. Thickness-length ratio of twin variant I with recrystallization. |
| Twin band label | Thickness-length ratio | Twin band label | Thickness-length ratio | Twin band label | Thickness-length ratio | Twin band label | Thickness-length ratio |
|-----------------|------------------------|-----------------|------------------------|-----------------|------------------------|-----------------|------------------------|
| 1               | 7.5%                   | 14              | 8.7%                   | 24              | 4.5%                   | 25              | 4%                     |
| 28              | 7.1%                   | 30              | 5.6%                   | 32              | 6.1%                   | 39              | 10.9%                  |
| 44              | 9.3%                   | 45              | 4.3%                   | 46              | 4%                     | 48              | 8.8%                   |
| 49              | 8.5%                   |                |                         |                |                        |                |                        |
| Arithmetic mean | 6.9%                   | Standard deviation | 0.022 |

| Table 3. Thickness-length ratio of twin variant II without recrystallization. |
| Twin band label | Thickness-length ratio | Twin band label | Thickness-length ratio | Twin band label | Thickness-length ratio | Twin band label | Thickness-length ratio |
|-----------------|------------------------|-----------------|------------------------|-----------------|------------------------|-----------------|------------------------|
| 50              | 37.9%                  | 51              | 21.5%                  | 52              | 12.5%                  | 53              | 25.2%                  |
| 54              | 24.9%                  | 55              | 32%                    | 56              | 11.7%                  | 57              | 28.6%                  |
| 58              | 23.1%                  | 59              | 85.2%                  | 60              | 67.1%                  | 61              | 20.4%                  |
| 62              | 21.3%                  | 63              | 41%                    | 65              | 15.8%                  | 67              | 13.9%                  |
| 68              | 26.5%                  | 69              | 26.8%                  | 72              | 13.1%                  | 73              | 29.4%                  |
| 74              | 14.2%                  | 75              | 18.9%                  |                |                        |                |                        |
| Arithmetic mean | 27.77%                 | Standard deviation | 0.1735 |

| Table 4. Thickness-length ratio of twin variant II with recrystallization. |
| Twin band label | Thickness-length ratio | Twin band label | Thickness-length ratio | Twin band label | Thickness-length ratio | Twin band label | Thickness-length ratio |
|-----------------|------------------------|-----------------|------------------------|-----------------|------------------------|-----------------|------------------------|
| 64              | 14.9%                  | 66              | 11.6%                  | 70              | 20.6%                  | 71              | 13.7%                  |
| 76              | 29.5%                  | 77              | 9.6%                   |                |                        |                |                        |
| Arithmetic mean | 16.65%                 | Standard deviation | 0.0668 |
energy point can be deemed as the stable equilibrium state, and the thickness-length ratio corresponding to this lowest point gradually decreases with increasing volume ratio of recrystallization to parent twin band. It means that when the same shear stress is applied, the greater the twin thickness-length ratio is, the less volume ratio the recrystallized grain possesses, and that the twin band with a greater thickness-length ratio requires a greater driving force to be fully recrystallized. The theoretical prediction is consistent with the experimental observation results in figure 4(a).

The microstructures and texture on TD plane of the hot rolled AZ31 magnesium alloy were measured by EBSD. As shown in the EBSD IQ map which was produced by the EBSD post-processing software Channel 5 with the critical angles of 2° and 15° (figure 4(a)), profuse extension twinning (ETW) and a few TDRXs exist the selected grain (the black line represents the high-angle grain boundary, the yellow line represents the \{10\textendash12\} ETW boundary, and the red area encompassed by yellow lines represents TDRX). It is statistically indicated that TDRX preferentially occurs within the ETW with comparatively small thickness-length ratio. The ETW variant I that is almost vertical in the IQ map are numbered from 1\textendash49, and the arithmetic average method is used to calculate the average thickness-length ratio of recrystallized and non-recrystallized twins. The statistics are listed in tables 1 and 2. The average thickness-length ratio of the twins without recrystallization is much larger than that of the twins with recrystallization. The ETW variant II that is inclined to horizonal line by an angle of around 40° in the IQ map are numbered from 50\textendash77. The statistics are listed in tables 3 and 4. The average thickness-length ratio of the twins without recrystallization is much larger than that of the twins with recrystallization. In figure 4(a), the equiaxed grain labeled by A is actually not a TDRX because it is not encompassed by the yellow twin boundary, the twin band B is incomplete, and C is similar to A. Therefore, these three DRX grains are not counted into the statistics.

Although the thicknesses and lengths directly measured from the IQ map are not equal to the actual values, the ratios are true for the same variant [33] (incomplete twin bands are excluded in the statistics). This experimental result is fully in accordance with the abovementioned theoretical prediction regarding the relationship between the twin thickness-length ratio in figure 3 and the volume ratio of recrystallization to parent twin. Meanwhile, the pole figure and the inverse pole figure in figure 3(b) show that the texture of the selected grain with TDRX obviously deviates from the c-axis texture, and the orientation softening is realized. In addition, figures 2, 5 and 3 give the interrelated conclusions under the same model, and the results of figures 2 and 5 are also in accordance with the works based on different methodologies [6, 12]. Therefore, the results of figures 2 and 5 are considered to be valid.

Figure 5 shows the influence of different applied shear stresses and the volume ratios of recrystallization to parent twin on relationship between total free energy change and twin thickness-length ratio ($\nu = 0.34, L = 50\mu m, \mu = 14.9\text{GPa}, \tau_R = 3\text{MPa}, \gamma_2 = 1.89Jm^{-2}, e_{1T}^c = 0.13,$ and $e_{2T}^c = 0.18$).
5. Conclusions

In this study, the thermodynamic modeling and EBSD characterization of the TDRX within a coarse grain of the as-cast AZ31 magnesium alloy are carried out, and the influence of the applied shear stress and the twin thickness-length ratio on the TDRX are revealed. The disclination quadrupole model used in this study can exquisitely model the deformation bands with lattice mismatch. The results indicate that: The elevation of the applied shear stress can enhance the recrystallization misorientation angle, thereby realizing the orientation softening; Subjected to the same shear stress, a larger twin thickness-length ratio leads to a lower volume ratio of TDRX to parent twin, while the parent twin with a lower thickness-length ratio is prone to be fully recrystallized; The applied shear stress can stimulate TDRX, increasing volume ratio of TDRX to parent twin.

TDRX is of great importance for the plasticity and ductility of the casting magnesium alloy at early deformation stage. The shear stress and the twin thickness-length ratio manipulated by the appropriate processes are capable of optimizing the TDRX activity.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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