Crystal plasticity modelling of shear band deformation and its effect on the formability of Mg–3Al–1Zn sheets

Shuai-Feng Chen1,2, Hong-Wu Song1, Shi-Hong Zhang1*

1 Institute of Metal Research, Chinese Academy of Sciences, Shenyang, 110016, China
2University of Chinese Academy of Sciences, Beijing 100049, China
E-mail address: shzhang@imr.ac.cn

Abstract. Shear bands is a kind of typical microstructure in magnesium alloy which has drawn much attention during recent years. The formation of shear bands during the isothermal differential speed rolling of Mg–3Al–1Zn sheets is analysed by experimental methods. In addition, results of Erichsen and tensile tests indicate that the shear bands have an obvious effect on the anisotropic fracture behaviour and formability of magnesium alloy. A represent volume element (RVE) method combined with crystal plasticity model is established to investigate the effect of shear bands on the anisotropic fracture behaviours systematically by considering the grain size, texture, width, and tilted angle. The simulation results disclose the above factors can induce discontinuous strain and stress between the shear band regions (SBRs) and non-shear band regions (NSBRs), but the grain size and tilted angle have much bigger effect than that of texture and width, leading to the fracture at the interface SBR and NSBR.

Keywords: Magnesium alloy, Crystal plasticity, Shear bands, RVE, Anisotropy, Formability

1. Introduction
Shear band is a kind of typical microstructure during different deformation processes, which is mainly caused by plastic instability (or plastic strain localization) [1]. Many efforts have been paid to characterize the microstructure features of shear bands [2], and to investigate its formation and effect on the fracture of the material [3-5]. Thus, the shear bands formed in the cubic-structured metals like Al, Al-Li and Cu were well understood for their simple deformation modes.

The formation of shear bands in magnesium (Mg) and its alloys is more complex than that of cubic-structured metals because of various deformation modes in hexagonal close-packed (HCP) metals, which is closely related to the initial texture, deformation temperature and process [6]. There have been some reports for the formation mechanism of shear bands and its effect on the ductility. Shear band mainly origins from the strain localization caused by contraction twinning \{101\} or secondary twinning \{10\1\I\}–\{10\1\2\} [7], and its extension is controlled by subsequent recrystallization process [8]. Shear strain induced during forming process plays an important role to promote the formation of shear bands by accelerating recrystallization process [9]. Moreover, features of shear bands such as the formation mechanism incline angle and grain orientations are greatly effected by the initial texture of...
the magnesium alloy [10]. For the effects of shear bands, it can be divided into two aspects: one is the strain localization inside shear bands leading to final fracture [11], and on the other hand, the recrystallized grain inside shear bands can act as an effective way to refine the grain size [12]. However, till now, effect of the shear bands on the formability of Mg sheets should be further clarified, especially, the anisotropy and fracture behaviour of Mg sheets.

Special attention is paid to elucidate the shear band formation under different rolling temperature. In addition, the effect of shear band formed during the rolling process on the anisotropy and fracture is studied by experimental and simulation methods.

2. Experimental procedures

Commercial twin-rolled cast (TRC) Mg–3Al–1Zn sheets with 4000 mm (rolling direction, RD) × 150 mm (transverse direction, TD) × 3 mm (normal direction, ND) were annealed at 673 K for 1 hour in a resistance furnace followed by air cooling. Then, 7 passes differential speed rolling (DSR) were conducted at 423 K, 473 K and 523 K (noted as DSR-423 K, 473 K, 523 K) at speed ratio 1:1.33 realized by upper roller 60mm and lower roller 80mm with a rolling speed 70 mm s⁻¹. Prior to the DSR Process, the sheets were heated to rolling temperature held for 20 minutes, and rollers were also heated to same temperature by heating oil to the RD (noted as 0° tension, 45° tension, 90° tension) with a strain rate 0.001 s⁻¹. To investigate the effect of the shear bands on the formability, Erichsen tests are conducted with deformation temperatures being 293 K, 373 K, 443 K and 503 K respectively.

Optical microscopy (OM) of microstructure at the centre of ND×RD plane etched with a solution consisting of picric acid (4.8 g), acetic acid (10 ml), water (10 ml) and ethanol (70 ml) was carried out by using Zeiss Observation Z1m optical microscope. Specimens for Electro Backscattered Diffraction (EBSD) analysis were prepared by electro-polishing with 10 % perchloric aid and 90 % ethanol at voltage 15 V and temperature 238 K. EBSD data and fracture morphology were acquired on the Hitachi S3400N scanning electron microscope (SEM, with Oxford Instrument HKL channel 5 system).

3. Results and discussion

3.1 Shear band formation under different rolling temperatures

Fig. 1 shows the OM microstructure of as-rolled sheets with the thickness 2.2 mm and 1.0 mm. From the Fig. 1(a) and 1(b), it can be seen that the twinning fraction decreases dramatically with the increasing of rolling temperature for decreasing of the critical resolved shear stress (CRSS) of the non-basal slip modes[13]. Meanwhile, twinning morphology evolves from the intersection type (Fig. 1(a)) to the parallel type (Fig. 1(b)) and the narrow shear bands are mainly formed inside the big grains with the direction along the twinning lamellas. When the rolling temperature rises to 523 K, it is hard to observe the activation of twinning in Fig. 1(c), which agrees with the results that the activation of pyramidal <c+a> can accommodate the compression strain along the ND when the deformation temperature is higher than 503 K. Thus, there is no observation of shear band in the DSR-523 K sheet.

As shown in the Fig. 1(d), (c) and (f), the numbers and morphology of the shear band present great difference between different final as-rolled sheets. There are numerous shear bands (marked with red dash line) with an average width about 5 μm and intersection shape in the Fig. 1 (d). Moreover, abundant residual twinning is still observed inside big matrix grains, and the average size of recrystallized grain is just about 1 μm nearly the same with width of twinning lamellas. For the DSR-473 K sheets in Fig 1(e), the final width of shear bands is about 20 μm which is a factor of 4 higher than that of shear bands in DSR-423 K. These shear bands are nearly parallel with each other and the microstructure is full of recrystallized grains with no observation of residual twinning (Fig. 1 (b)). The
microstructure of the as-rolled sheet of DSR-423 K and DSR-473 K consists of shear band regions (SBRs) and non-shear band regions (NSBRs). However, for the final DSR-523 K sheets, there is still no formation of shear bands thought the thickness reduction has been 66.7 %.

Fig. 1. OM microstructure of as-rolled sheets with thickness 2.2 mm (a) DSR-423 K (b) DSR-473 K (c) DSR-523 K; with thickness 1.0 mm (d) DSR-423 K (e) DSR-473 K (f) DSR-523 K.

3.2 Effect of shear band on the mechanical properties

Table 1 presents the magnitude of the effect of shear bands on mechanical properties of annealed sheets stretched along different directions to the RD. For annealed DSR-423 K sheets, the average yield stress $\sigma_{YS}$ and ultimate tensile stress $\sigma_{UTS}$ are 219 MPa and 280 MPa, respectively. The maximum difference of the uniform elongation $\delta_{UE}$ and total elongation $\delta_{TE}$ along different direction tension are just 0.9 % and 0.3%. Otherwise, it is different for the annealed DSR-473 K sheets where the biggest difference of the uniform elongation $\delta_{UE}$ and total elongation $\delta_{TE}$ can reach 2.3% and 3.5% with the relative error being 14.7 % and 16.3 % respectively. Meanwhile, the relative deviation of yield stress $\sigma_{YS}$ and ultimate tensile stress $\sigma_{UTS}$ is only 3 % and 2.5 %. So, it is necessary to highlight the effect of shear band on the strength and fracture behaviour individually. In other words, the shear bands considered can cause obviously anisotropic fracture behaviour, but has little influence on the strength of Mg sheets which is mainly determined by average grain size [14].

Table 1 Mechanical properties of annealed sheets under different rolling temperatures stretched along different directions

| Rolling temperatures | Tensile directions to RD(°) | $\sigma_{YS}$ (MPa) | $\sigma_{UTS}$ (MP a) | $\delta_{UE}$ (%) | $\delta_{TE}$ (%) |
|----------------------|-----------------------------|---------------------|----------------------|------------------|------------------|
| 423K                 | 0                           | 220                 | 280                  | 17.7             | 23.4             |
|                      | 45                          | 223                 | 289                  | 16.8             | 23.5             |
|                      | 90                          | 215                 | 272                  | 17.3             | 23.2             |
| 473K                 | 0                           | 193                 | 251                  | 15.3             | 19.5             |
|                      | 45                          | 198                 | 256                  | 17.6             | 23               |
|                      | 90                          | 200                 | 253                  | 17.8             | 23.5             |

Fig. 2 shows the photos of the Erichsen tests with deformation temperatures being 293 K, 373 K, 443 K and 503 K. The depth of the punch in test dentation in the specimen expressed in millimeteres.
is the so-called Erichsen index (IE) displayed in Fig. 3 which indicates that the DSR-423 K sheets possess the best formability. Both of DSR-423 K and DSR-523 K have better formability than that of DSR-473 K, so the anisotropic fracture behaviour induced by the shear bands can decrease the formability.

![Fig. 2. The photos of the Erichsen tests: (a) DSR-423 K (b) DSR-473 K (c) DSR-523 K (1-293 K, 2-373 K, 3-443 K, 4-503 K)](image)

![Fig. 3. The IE values of the Erichsen tests of annealed DSR-423 K, DSR-473 K and DSR-523 K.](image)

### 3.3 Simulation results of shear band parameters on fracture behaviours

Fig. 4 shows typical shear bands (marked by red lines) of the annealed DSR-423 K sheets identified by EBSD method. In Fig. 4(a), two shear bands are detected with width W (W₁ = 20 μm, W₂ = 25 μm) and tilted angle θ (θ₁ = 30.6°, θ₂ = 31.4°). To investigate the effect of grain size and texture of shear band, a critical grain size 5μm is chosen to separate the SBRs and NSBRs with average grain size d being 8μm and 3.6μm respectively shown in Fig. 4(b) and (c). The intensity I₀ of basal texture of two kinds of regions (Fig. 4(d) and (e)) is 10.93 and 9.97. It is worthy to say that the basal texture of NSBRs presents two peaks with angle of deviation from ND being about 10° and SBRs shows one peak with just about 4° deviation angle.

![Fig. 4. EBSD data of annealed 1.0 mm DSR-473 K sheet, inverse pole figure of (a) whole area (b) NSBRs (d≥5 μm) (c) SBRs (d<5 μm) with label 100 μm; basal pole figure of (d) NSBRs and (e) SBRs.](image)
To model the effects of shear bands parameters (\(W, \theta, d\) and \(I_b\)) quantitatively, Viscous-plasticity self-consistent (VPSC) model [20] and finite element method (FEM) are adopted. For the grain size effect, the effective Hall-Petch relationship is used to estimate the CRSS difference between SBRs and NSBRs by the following equation:

\[
\tau_s = \tau_0 + k(d_1^{-1/2} - d_2^{-1/2})
\]

where, the \(\tau_s\) is the CRSS of basal slip, \(k\) is effective Hall-Petch slope obtained by \(k=K/M\). The \(K\) is Hall-Petch slope with large range. The value 225 MPa \(\cdot\) \(\mu m^{1/2}\) is adopted for the average grain size is less than 10 \(\mu m\) [15], \(M\) is Taylor factor, 2.45 [16]. Moreover, the mixture hardening law shown in equation (2) is employed to obtain the accurate hardening parameters by fitting the experimental data of annealed DSR-473K sheets along different directions tension:

\[
\sigma = (1 - f)\sigma_{NSBRs} + f\sigma_{SBRs}
\]

in the above equation, the \(f\) is area fraction of SBRs, 15\%, \(\sigma_{NSBRs}\) and \(\sigma_{SBRs}\) are the stress of NSBRs and SBRs. \(\sigma\) is the mixture stress of the mixture hardening law.

Eqs. (1) and (2) combined with VPSC model form a new model to consider the difference between grain size and texture types of SBRs and NSBRs. Fig 5 shows the stress-strain curves of SBRs, NSBRs and mixture of SBRs and NSBRs predicted by the new model. The good agreement between stress-strain of the prediction of mixture hardening law and experiment data indicates that the new model can estimate the mechanical properties of the SBRs and NSBRs reasonably.

The schematic of RVE model and its boundary conditions are presented in Fig. 6. In Fig. 6(a), the RVE models of shear band morphology along different direction tension are displayed. It is interesting that the width (\(W\)) and tilted angle (\(\theta\)) of shear bands will evolve with changing the tension directions. To simulate tension process, the boundary conditions with \(u_x^+ = -u_x^-, u_{yenter}^+ = -u_{yenter}^- = 0\) are set up to the RVE model.

The distribution of the effective plastic strain and effective stress in Fig. 7 displays the heterogeneous deformation of NSBRs and SBRs. The difference between the effective strain at point A, B, C and D at each region indicates that the shear bands have a big effect on the anisotropic fracture of the annealed DSR-473 K. The effective strain of NSBRs is larger than that of SBRs, especially at the interface between the NSBRs and SBRs, which is main reason that leads to the discontinuous deformation. When stretched along the RD (0° tension) in Fig. 7 (a), point B displays the biggest heterogeneity of effective plastic strain which may lead to the final fracture at the interface.
Remarkably, the maximum discontinuity occur at the point C (45° tension) of Fig. 7 (b) with the value being 0.03 which is much smaller than 0.1 of point B. However, for the tension along the TD (90° tension), uniform error with value 0.01 is obtained at the interface of NSBRs and SBRs. Combining with experimental data displayed in Table 1, it can be concluded that fracture correlated with the elongation in Table 1 is mainly determined by the strain discontinuity at the interface of NSBRs and SBRs.

Fig. 6. (a) The schematic of RVE model considering shear band morphology on different direction tension. (b) boundary conditions of RVE model, where the centre of model is fixed along the y direction to simulate the morphology evolution of shear bands during the tension process.

Fig. 7. Simulation results of the RVE model during the different direction tension: effective strain distribution of (a) 0° tension (b) 45° tension (c) 90° tension, effective stress distribution of (b) 0° tension (d) 45° tension (f) 90° tension.

4. Conclusions

According to the experimental observation and simulation results of deformation and effect of shear bands, the following conclusions can be obtained:

1. The formation of shear bands is obviously affected by the rolling temperature. Different rolling temperatures will result in formation of shear bands with different morphologies.

2. A new model considering the shear band parameters is established. The strain discontinuity at the interface of NSBRs and SBRs may be the main reason for the anisotropic fracture and low formability of DSR-423 K sheets.
References

[1] Duggan B J, Hatherly M, Hutchinson W B, Wakefield P T 1978 Metal Sci 12 343.
[2] Peirce D, Asaro R J, Needleman A 1983 Acta Metall 31 1951.
[3] Jia N, Eisenlohr P, Roters F, Raabe D, Zhao X 2012 Acta Metall 60 3415.
[4] Kohlhoff G D, Malin A S, Lücke K, Hatherly M 1988 Acta Metall 36 2841.
[5] Leffers T, Bilde-Sorensen J B. 1991 Acta Metall Mater 38 1917.
[6] Barnett M R, Nave M D, Bettles C J 2004 Mater. Sci. Eng. A 386 205.
[7] Yan H, Xu S W, Chen R S, Kamado S, Honma T, Hana E H 2011, Scripta Mater 64 141.
[8] Zhang Z, Wang M P, Jiang N, Zhu S 2012. J All. Comp 512 73.
[9] Ion S E, Humphreys F J, White S H, 1982 Acta Metall 30 1909.
[10] Chun Y B, Davies C H J 2012 Mater. Sci. Eng. A 556 253.
[11] Kim H L, Lee J-H, Lee C S, Bang W, Ahn S H, Chang Y W 2012 Mater. Sci. Eng. A 558 431.
[12] Fatemi-Varzaneha S M, Zarei-Hanzakia A, Cabrera J M 2011 J All. Comp 509 3806.
[13] Song G S, Zhang S H, Zheng L, L. Q. Ruan 2011 J All. Comp 509 6481.
[14] Del Valle J A, Carreno F, Ruano O A 2006 Acta Metall 54 4247.
[15] Barnett M R, Keshavarz Z, Beer A G, Atwell D 2004 Acta Metall 52 5093.
[16] Jain A, Duygulu O, Brown D W, Tome C N, Agnew S R 2008 Mater. Sci. Eng. A 486 545.