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## **Crystal Plasticity Simulation of the AZ31B Alloy Sheet under Uniaxial Deformation Considering Grain Boundary Sliding**

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**Abstract**. The aim of present work is to develop a crystal plasticity modeling approach to integrate slip, dynamic recrystallization (DRX) and grain boundary sliding (GBS) for simulating the deformation and texture evolution of magnesium alloys deformed at the high temperature. A GBS model is developed to evaluate strain and grains' rotation induced by GBS, and implemented into the polycrystal plasticity framework VPSC. The VPSC-DRX-GBS model can well reproduce the stress-strain curves and texture evolution. The calculated GBS contribution ratio in tension is obviously higher than in compression due to easier cavity nucleation on grain boundaries under tensile creep-aging conditions. The significantly different texture development in tension and compression deformation due to GBS is well reproduced by the proposed model.

#### 1. Introduction

Magnesium (Mg) alloys have attracted much attention due to their light weight potential especially in the transportation industry in the past two decades. Mg alloy sheets generally exhibit poor ductility at room temperature due to their hexagonal close packed (HCP) crystal structure with limited slip systems. Their ductility can be enhanced at high temperatures which is partially attributed to the dynamic recrystallization (DRX) and grain boundary sliding (GBS) [1].

According to previous experimental research, the GBS involved deformation of Mg alloys usually is accompanied by DRX and includes two stages. In the early stage, the deformation is mainly accommodated by dislocation slip and DRX, through which the grains are refined; in the second stage, GBS plays an important or even dominant role by taking advantage of the already refined grains [2]. The plastic deformation and corresponding texture evolution depend on the combined action of three different mechanisms: dislocation slip, DRX and GBS. Currently, there is no comprehensive modeling method to incorporate the three mechanisms, which can realize the integrated simulation of texture evolution and mechanical response in GBS deformation. The aim of present work is to develop a crystal plasticity modeling approach to integrate slip, DRX and GBS for the first time in order to simulate the deformation and texture evolution of magnesium alloys deformed at the high temperature.

#### 2. Polycrystal plasticity modeling

A commercial AZ31B-H24 alloy sheet was used in the present work, which was previously studied by Zhou et al. [3, 4]. The uniaxial tension and compression tests at 300°C along rolling direction (RD) at a strain rate of 0.0018/s, as well as subsequent optical microscopy (OM) and X-ray diffraction (XRD)



observation have been introduced in detail elsewhere [4]. In this paper, GBS mechanism is incorporated into the visco-plastic self-consistent (VPSC)-DRX framework [5] to develop a polycrystal plasticity based method for simulating the deformation of the AZ31B sheet at 300°C.

## 2.1. Grain rotation mediated by GBS

In the GBS regime, initial basal texture of the rolled and annealed magnesium alloys became more random with the increase of deformation, and strain rate and GBS contribution are critical factors for grains rotation. In the present work, a model to introduce GBS induced grain rotation is proposed as below.

When GBS takes effect, grains affected by GBS are randomly selected to rotate in addition to the rotation induced by dislocation slip. The number of the picked grains is proportional to the ratio of GBS strain rate to total strain rate. Therefore, the expectation of rotated grains  $z_{GBS}$  is determined by

$$z_{GBS} = \sum_{i=1}^{n_g} \eta_g \xi_{GBS,i} \tag{1}$$

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where  $\eta_g$  is a fitting parameter;  $n_g$  is the total grain number;  $\xi_{GBS,i}$  is the GBS contribution ratio for grain *i*.

$$\xi_{GBS,i} = \frac{\dot{\mathcal{E}}_{GBS,i}}{\dot{\mathcal{E}}_{iotal}} \tag{2}$$

where  $\dot{\mathcal{E}}_{GBS,i}$  is the GBS strain rate for the grain *i*,  $\dot{\mathcal{E}}_{total}$  is the total strain rate. The extra random rotation degree of each selected grain should be within 45°.

Under GBS dominated deformation, the compatible conditions (five slip systems needed for compatible and homogeneous deformation under plastic deformation) are not necessary to be fulfilled, and grain rotation will randomize the deformation texture. In uniaxial tension of the present AZ31B sheet, the c-axis will rotate toward the sheet normal by basal slip, while prismatic slip rotates the grain around c-axis to the balance position. After the onset of GBS, the grain will rotate about c-axis by a random angle with no specific balance direction.

#### 2.2. VPSC-GBS-DRX model

The GBS method is implemented into the VPSC-DRX framework. Figure 1 shows the flowchart of the proposed VPSC-DRX-GBS approach. The computational procedures are as follows:

1. If strain is less than the critical strain for initiating GBS,  $\varepsilon_{GBS}$  (0.2 for the present AZ31B alloy), the status of a given aggregate, including stress, strain and orientation, is updated by the VPSC model, and the total strain rate  $\dot{\mathbf{\epsilon}}_{total,i}$  for a grain *i* is equal to the plastic strain rate  $\dot{\mathbf{\epsilon}}_{i}$ .

2. When the critical dislocation density for DDRX initiation is achieved, new DRX grains will nucleate,

2. When the critical dislocation density for DDRX initiation is achieved, new DRX grains will nucleate, followed by growth through boundary migration.

3. If strain reaches  $\mathcal{E}GBS$ , the GBS strain rate for the grain *i* is calculated by

$$\dot{\varepsilon}_{GBS,i} = \frac{6bv_D}{d_i} \sinh(v \frac{\sigma_i}{K_B T (1 - D_{c,i})}) \exp(\frac{-\Delta F}{RT})$$
(3)

where  $\upsilon_D$  is a typical lattice vibrational frequency, and  $\upsilon_D \approx 10^{13}$ ;  $d_i$  is the grain size;  $\nu$  is the activation volume, taken as  $\overline{b}^3$ ;  $\sigma_i$  is the effective stress of grain *i*;  $K_B$  is the Boltzmann's constant (1.38×10<sup>-23</sup> J/K); *T* is the temperature;  $\Delta F$  is the activation energy for grain boundary diffusion (92 kJ/mol for Mg alloys); *R* is the gas constant (8.314 J/(mol·K)).

The cavitation damage parameter  $D_c$  is introduced to characterize the process of void nucleation, growth and coalescence during high-temperature deformation. For a grain *i*,  $D_{c,i}$  is determined by the rupture strain  $\mathcal{E}$  and GBS strain rate as below, considering the difference in tension and compression.

$$\begin{cases} D_{c,i} = 0, \, \sigma_{m,i} < 0\\ \dot{D}_{c,i} = \frac{1}{3\varepsilon_f} \dot{\varepsilon}_{GBS,i}, \, \sigma_{m,i} \ge 0 \end{cases}$$

$$\tag{4}$$

where  $D_{c,i}$  is permanently set to zero in compression, and the hydrostatic pressure  $\sigma_{m,i} = \frac{1}{3}(\sigma_{1,i} + \sigma_{2,i} + \sigma_{3,i}).$ 

4. Update the macroscopic plastic strain rate  $\dot{\mathbf{\epsilon}}$ , in which the weighted average of the plastic strain rate over the aggregate has to coincide with the macroscopic counterpart, i.e.

$$\dot{\boldsymbol{\varepsilon}} = \left\langle \dot{\boldsymbol{\varepsilon}}_i \right\rangle = \left\langle \dot{\boldsymbol{\varepsilon}}_{total,i} - \dot{\boldsymbol{\varepsilon}}_{GBS,i} \right\rangle \tag{5}$$

where  $\dot{\mathbf{\epsilon}}_{GBS,i}$  and  $\dot{\mathbf{\epsilon}}_i$  represent strain rates of grain *i* due to GBS and dislocation slip respectively and the bracket " $\langle \rangle$ " denotes the average over grains, weighted by associated volume fractions. 5. Calculate stress and strain by using the macroscopic plastic strain rate in the framework of VPSC,

and update effective stress  $\sigma_i$  for grains.

6. Calculate rotation of grains by Eqs. (1) and (2).



Figure 1. Flowchart of VPSC-DRX-GBS model

#### 3. Simulation results

#### 3.1. Flow stress

Figure 2 shows the comparison between the experimental and fitted stress-strain curves. The calculated results by the VPSC-DRX-GBS model agree well with the experimental results of RD tension and RD compression. For comparison, the stress-strain curves without considering GBS are also calculated and shown in Figure 2, by turning the GBS module off. Without consideration of GBS, the stress-strain curve without GBS fits the experimental result for RD compression, while the calculation obviously overestimates the stress after 0.2 strain for RD tension, and cannot reproduce the softening behavior. GBS gives rise to more softening in tension than in compression, because contribution of GBS to deformation is significantly reduced in compression.

Generally, there is no evident difference between tension and compression for the softening by DRX, and the DRX will lead to the grain refinement. In contrast, due to the greater stress softening in tension and stable grain size distribution after 0.2 strain for the AZ31B Mg sheet [4], the softening behavior cannot be attributed to DRX, but GBS after 0.2 strain.



Figure 2. The experimental and fitted stress-strain results of the AZ31B sheets at 300°C. ("w/o GBS" represents "without GBS".)

#### 3.2. Texture analysis

The calculated texture at 0.4 strain in the form of pole figures is compared with experimental results in RD tension and RD compression, as shown in Figure 3. The experimental texture was tested from XRD measurement, and more details about the experimental texture development will be exhibited elsewhere. The predicted texture in RD tension considering GBS is consistent with measurements, and texture intensity with GBS module is evidently reduced compared to that without considering GBS. In RD tension, the dominantly active basal <a> and prismatic <a> slip modes cause the suppression of basal texture in the (0002) pole figure and formation of hexagonal maxima distribution in the (10-10) pole figure. With the enhancement of GBS, random rotation of grains reduces overall texture intensity, which results in more disperse distribution texture in the (0002) pole figure disappears.

The predicted texture in RD compression is also consistent with measurements, while texture intensity is slightly reduced with GBS module. In compression, the texture distributions with and without considering GBS are similar due to less activation of GBS. In RD compression, the activation of the basal slip <a> and prismatic <a> slip modes split the basal texture in the (0002) pole figure and results in two maxima distribution in the (10-10) pole figure [3].

Therefore, RD tension and RD compression show the obvious difference between tension and compression in terms of texture development, which can be attributed to less activation of GBS in compression.



Figure 3. The comparison of texture between simulations and experiments at 0.4 strain: (a) RD tension and (b) RD compression.

#### 3.3. GBS contribution

The calculated mean GBS contribution ratios in RD tension and RD compression, with the proceeding of deformation after 0.2 strain, are presented in Figure 4. The GBS contribution ratio in RD tension is obviously higher than in RD compression. The evolution trends of GBS contribution ratio vary with the loading modes. For RD tension, the value of GBS contribution ratio rises steadily, with increasing strain. For RD compression, the GBS contribution ratio decreases slowly from 0.16 to 0.14, resulting from the stress softening.

The significant reduction of the GBS contribution ratio in the compression mode is calculated by the current VPSC-DRX-GBS model. Much higher tension GBS contribution ratio than compression can be attributed to the easier cavity nucleation on grain boundaries under tensile creep conditions.



Figure 4. The evolution of mean GBS contribution ratio to overall strain rate

#### 4. Conclusions

In this work, a VPSC-DRX-GBS model is developed by introducing GBS model into the VPSC-DRX framework to simulate the deformation and texture evolution of the Mg alloy. The following conclusions can be drawn.

- 1) A polycrystal plasticity based integration modeling method incorporating GBS is developed, and the stress-strain curves and texture evolution can be simultaneously calculated.
- 2) By introducing the cavitation damage parameter  $D_c$  into GBS model, the polycrystal plasticity model can reproduce the tension-compression difference induced by GBS.
- 3) Due to GBS, tension and compression deformation results in significant different texture development. The proposed model for GBS mediated grain rotation can well reproduce the texture development. In RD tension, the random grains' rotation induced by GBS produces more disperse distribution texture in the (0002) pole figure, and hexagonal maxima distribution disappears. In the compression modes, GBS effect is much weaker, which hardly influences texture distribution.

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