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Simulation of texture evolution and macroscopic properties in Mg alloys using the crystal plasticity finite element method

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ABSTRACT

A crystal plasticity finite element method (CPFEM), considering both crystallographic slip and deformation twinning, was used to simulate texture evolution and macroscopic properties of AZ31 Mg alloys. To capture grain reorientation due to deformation twinning in twin-dominated deformation, a predominant twin reorientation (PTR) model was considered. The validity of the proposed theoretical framework was demonstrated through comparison of simulated results, such as texture evolution and macroscopic properties, with the experimental results and measurements. The simulation of texture evolution and macroscopic properties of AZ31 Mg alloys was shown to be in good agreement with the corresponding experimental results.

1. Introduction

The various deformation modes, such as basal $\langle \mathbf{a} \rangle$ slip, prismatic $\langle \mathbf{a} \rangle$ slip, pyramidal $\langle \mathbf{a} \rangle$, pyramidal $\langle \mathbf{c}+\mathbf{a} \rangle$ slip and tensile twinning, complicate the deformation behavior of hexagonal close packed (HCP) polycrystalline Mg alloys. It is known that critical resolved shear stress (CRSS) of non-basal slip systems at near room temperature (RT) is much higher than that of a basal slip system [1–3]. The limited number of operative slip systems at near RT, is responsible for the poor formability of Mg alloys. Therefore, a high temperature and a low strain rate have been used to improve the formability of Mg alloys. Modification of crystallographic texture is another method to improve the formability of Mg alloys. A sharp basal fibre texture has been characterized as the main texture component in wrought Mg alloys. It was reported that the addition of alloy elements into Mg alloys induces spreading of the basal poles in the rolling direction (RD) [2,4]. The studies reveal that spreading of the basal plane enhances the activation of basal slip during plastic deformation. As the c/a ratio of the hexagonal Mg lattice (1.624) is less than $\sqrt{3}$, a tensile twin is easily activated by c-axis tension [5,6]. Deformation twinning can affect the evolution of deformation texture and macroscopic properties [1,7–11]. To understand texture evolution in Mg alloys during plastic deformation, a number of simulation studies have been conducted in various length scales. In particular, many studies have been conducted in an attempt to understand the effect of twin reorientation on the evolution of texture and macroscopic properties during plastic deformation. A predominant twin reorientation (PTR) model [12] has been suggested to explain the reorientation of the crystallographic orientation by deformation twinning. In the PTR model, twinning is considered to be a pseudo-slip mechanism and a grain is allowed to reorient rapidly if a specific accumulated value reaches the threshold. The PTR model has been successfully implemented in visco-plastic self-consistent (VPSC) models [13–15] to capture grain reorientation due to deformation twinning [2,15–19]. The VPSC model is reportedly based on a homogenization scheme that can successfully predict macroscopic properties and texture evolution during plastic deformation. However, the VPSC model has limited application to metal-forming simulations due to their complicated geometry. Crystal plasticity finite element methods (CPFEM) based on an inhomogenization scheme have been developed to simulate heterogeneous plastic deformation of hexagonal close packed (HCP) polycrystalline materials [20–23]. A critical issue of the current theoretical framework of CPFEM is the incorporation of a reorientation scheme by deformation twinning into the constitutive equations. A probabilistic approach [21] was used to simulate the texture evolution and stress–strain response of a polycrystalline Mg alloy. In the approach, the orientations of grains were replaced by twin-related orientations only if the twinned volume fraction exceeded a certain random number. A total Lagrangian

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approach [24] was proposed to simulate rolling textures in a polycrystalline Zr alloy. The same theoretical framework was used to simulate the texture evolution and flow stress in high purity α-Ti [23,25]. The PTR model has been used to simulate to simulate earing profiles after deep drawing [26] and texture evolution during hot rolling [27].

In the present work, we present a theoretical framework for including crystallographic slip and deformation twinning in the CPFEM. The PTR model was implemented to capture grain reorientation due to deformation twinning. The validity of the proposed model framework was verified by comparing the predicted texture evolution, twin-volume fraction and macroscopic properties of AZ31 Mg alloys with the measured experimental results.

2. Experimental procedure and theoretical methods

2.1. Materials and microstructure

The present study used strip-cast AZ31 (3 wt.% Al, 1 wt.% Zn, balance Mg) Mg alloy followed by hot rolling. The sheet of 2 mm thick had a grain size of approximately 10.16 μm. To examine macroscopic texture of as-rolled AZ31 Mg alloy sheet, pole figure measurements were carried out using a Rigaku D Max 2500 X-ray diffractometer. The five ((0 0 0 2), (1 0 $\bar{1}$ 0), (1 0 $\bar{1}$ 1), (1 0 $\bar{1}$ 2), and (1 1 $\bar{2}$ 0)) incomplete pole figures (tilting angle: 0–70°) were used to calculate ODF. Based on the five incomplete pole figures, the crystallographic orientation distribution function (ODF) was calculated using the WIMV method [28] and Beartex software. The EBSD technique was used to analyze the microtexture and twin-volume fraction of as-rolled and deformed specimens. The specimens deformed to true strains of 0.05 and 0.1 were cut in the rolling direction (RD)–normal direction (ND) section parallel to the compression axis. The specimens were prepared using colloidal silica as the polishing medium for the intermediate stage. The final specimens were prepared by electro-polishing in AC2 electrolyte for the final stage. Automated EBSD scans were measured in the stage-control mode using TSL data acquisition software. Microtexture and twin-volume fraction were examined by scanning an area of 300 μm × 100 μm at a step size of 0.5 μm. The EBSD data were analyzed using the TSL software to evaluate pole figure, ODF and twin-volume fraction.

2.2. Mechanical properties

To measure the macroscopic mechanical properties of hot-rolled AZ31 Mg alloy sheets, tensile specimens were cut from the sheet to the RD. Tensile specimens were prepared by laser cutting in accordance with ASTM standard B557M-94 (gauge length: 25 mm; width: 6 mm). Compressive specimens were machined by laser cutting from the sheet. The initial height and width of the compressive specimens were 4 mm and 10 mm, respectively. The main experimental difficulty encountered during evaluation of in-plane compression was the buckling phenomenon. To avoid buckling, either through-thickness sheet stabilization [29] or a thicker Mg sheet have been used [3]. In the present study, a thicker Mg sheet with a low ratio (=2) of height to thickness was used to avoid the buckling phenomenon. The specimens were installed in a GLEEBLE® 3500C thermo-mechanical simulator and heated by means of an inductive heating device at a rate of 5 °C/s. After holding at 200 °C for 1 min, they were deformed at a strain rate of 0.1 s^{-1}. The loading direction of specimens was parallel to the RD of the sheet and allowed to shrink or expand in the transverse direction (TD) and ND of the sheet. The uniaxial loading tests were interrupted by unloading and, with the aid of a micrometer, the plastic strains were measured relative to the width and thickness directions to determine the *R*-value (i.e., the plastic strain ratio). Taking into account the condition of volume constancy, the *R*-value is defined by [30]

$$R = \frac{\varepsilon_w}{\varepsilon_t} = -\frac{\varepsilon_w}{(\varepsilon_l + \varepsilon_w)} = \frac{\ln(w_f/w_i)}{-\ln(l_f/l_i) - \ln(w_f/w_i)} \tag{1}$$

where ε_l, ε_w and ε_t are the strains in the length, width and thickness directions, respectively; *l*, *w* and *t* represent sample length, width, and thickness, respectively, and *i* and *f* represent the initial and final values. All *R*-value measurements were conducted at true strains of 0.04, 0.08 and 0.1. To capture the effect of strain on the evolution of crystallographic texture and deformation twinning, the tests were stopped at true strains of 0.05 and 0.1. After the plastic deformation, the deformed specimens were cooled in water to maintain their deformed microstructures.

3. Theoretical procedure

Texture evolution and macroscopic properties in HCP polycrystalline Mg alloys was simulated using the finite element code, ABAQUS/Standard [31], with the material model programmed based on continuum crystal plasticity theory. A rate-dependent constitutive relation has been implemented into the user material subroutine UMAT in ABAQUS. The model is fundamentally based on a multiplicative decomposition of the deformation gradient, **F**, into a plastic part characterized by shearing rates on active slip and twin systems, as well as a part that accounts for the rotation and elastic distortion of the crystal lattice.

$$\boldsymbol{F} = \boldsymbol{F}^e \cdot \boldsymbol{F}^p \tag{2}$$

This formula leads to additive decomposition of the velocity gradient into elastic and plastic parts,

$$\mathbf{L} = \mathbf{L}^e + \mathbf{L}^p \tag{3}$$

with the plastic part determined by slip rates, $\dot{\gamma}^\alpha$, on slip/twin planes with normals, $\mathbf{m}^\alpha$, and slip/twin directions, $\mathbf{S}^\alpha$

$$\mathbf{L}^p = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \tag{4}$$

The summation represents all of the deformation modes, N ($=N_s + N_t$), consisting of slip, N_s, and twin systems, N_t.

The plastic part of the velocity gradient is decomposed further into symmetric and antisymmetric parts ($\mathbf{L}^p = \mathbf{D}^p + \boldsymbol{\omega}^p$) to yield the formula

$$\mathbf{D}^p = \frac{1}{2}\sum_{\alpha=1}^{N} \dot{\gamma}^\alpha (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha + \mathbf{m}^\alpha \otimes \mathbf{s}^\alpha) = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha \mathbf{P}^\alpha$$

$$\boldsymbol{\omega}^p = \frac{1}{2}\sum_{\alpha=1}^{N} \dot{\gamma}^\alpha (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha - \mathbf{m}^\alpha \otimes \mathbf{s}^\alpha) = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha \mathbf{W}^\alpha \tag{5}$$

where $\mathbf{D}^p$ is the plastic part of the rate of deformation tensor and $\boldsymbol{\omega}^p$ is the plastic spin. The evolution of the slip/twin directions and slip/twin plane normals can be expressed in terms of the elastic part of the deformation gradient as

$$\boldsymbol{s}^\alpha = \boldsymbol{F}^e \cdot \boldsymbol{s}_o^\alpha \quad \text{and} \quad \boldsymbol{m}^\alpha = \boldsymbol{m}_o^\alpha \cdot \boldsymbol{F}^{e-1} \tag{6}$$

where $\boldsymbol{s}_o^\alpha$ and $\boldsymbol{m}_o^\alpha$ are the slip/twin vectors in the reference orientation of the crystal lattice.

The rate of change of $\mathbf{F}^e$ is given by

$$\dot{\mathbf{F}}^e = \mathbf{L}^e \cdot \mathbf{F}^e = (\mathbf{L} - \mathbf{L}^p) \cdot \mathbf{F}^e \tag{7}$$