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Crystal plasticity based constitutive modeling of ZEK100 magnesium alloy combined with *in-situ* HEXRD experiments

H J Bong[1,2,*], X Hu[2,3], X Sun[3], Y Ren[4] and Raj K Mishra[5]

[1] Aluminum Department, Korea Institute of Materials Science, Gyeongnam 51508, South Korea
[2] Computational Engineering, Pacific Northwest National Laboratory, WA 99354, USA
[3] Energy and Transportation Science Division, Oak Ridge National Laboratory, TN 37831, USA
[4] X-ray Science Division, Argonne National Laboratory, Argonne, IL 60439, USA
[5] General Motors Research & Development, MI 48090, USA

Abstract. In the current works, both micro- and macro-mechanical properties of a hexagonal close-packed (HCP) polycrystalline ZEK100 magnesium alloy were investigated. In the experimental perspective, *in-situ* high energy X-ray diffraction (HEXRD) from a synchrotron source was conducted during the uniaxial tension along the rolling direction (RD) and the transverse direction (TD) to measure the lattice strain evolutions and stress-strain behaviors. In the modeling perspective, crystal plasticity finite element (CPFE) model was developed incorporating the deformation twinning for the HCP-structured metals. The HEXRD experiments and crystal plasticity models were then coupled to characterize the constitutive behaviors of the ZEK100 alloy. The lattice strain data representing the microscopic behavior of the material and the macroscopic stress-strain behavior were then tied together as objective values to estimate the critical resolved shear stress (CRSS) and hardening parameters of available slip and twin systems of the ZEK100 alloy using the developed CPFE model. The stress-strain behavior as well as the lattice strain variation during the uniaxial tension tests are presented using the CPFE model and compared with the actual HEXRD data.

1. Introduction

The magnesium alloys are potential candidates as structural materials for lightweighting vehicles due to their high strength-to-density ratio. However, the HCP-structured magnesium alloy possesses anisotropic and complex slip/twin systems, and the fact hinders the accurate material modeling for such metals. Various crystal plasticity models considering such slip/twin systems in meso-scale have been reported in the open literature [1–4]. However, precise determination of the constitutive parameters for such a large number of slip/twin system is challenging due to the lack of direct measurement techniques. This can sometimes lead to multiple sets of constitutive parameters if one determines them by back-fitting to macroscopic stress-strain behavior [5].

The high-energy X-ray diffraction (HEXRD) can be a plausible approach to solve aforementioned issue since it can quantify the microstructural behavior by means of measuring lattice strain. The HEXRD, whose typical energy is orders of magnitude higher than conventional XRD using Cu-Kα, enables volumetric diffraction measurement by penetrating the entire sheet metal thickness, commonly in millimeter length scale, while conventional X-ray can only gather the reflected diffraction information near the sample surface. Therefore, much more accurate statistical measurement compared with the

* Corresponding author: hjbong@kims.re.kr

conventional XRD can be attained. Moreover, the HEXRD does not require long collection time [2,6] and enables the continuous diffraction measurement during loading without stopping if sufficiently low loading speed is imposed. Therefore, simultaneous measurement of the microstructural property in terms of lattice strain and macroscopic stress-strain behavior can be made.

In this work, both micro- and macro-mechanical properties of ZEK100 alloy were investigated. At first, the *in-situ* HEXRD tension tests were conducted to measure the lattice strain evolutions and stress-strain curves during the tension along the rolling direction (RD) and transverse direction (TD). The aforementioned *in-situ* HEXRD tension data was coupled with the CPFE model. The CPFE simulations were seeded with initial grain orientations measured from the HEXRD. The critical resolved shear stress (CRSS) and hardening parameters for the various slip/twin systems were identified by fitting to the lattice strain and stress-strain data, simultaneously. Using the determined set of constitutive parameters, the fidelity of proposed approach was examined.

2. Modeling

The description below is intended to provide very brief introduction of crystal plasticity formulation. The interested reader is directed to the detailed reference [7]. In the current work, the rate-dependent crystal plasticity is adopted. The deformation twinning was assumed as pseudo slip obeying the Schmid law [8,9] and well-known predominant twinning reorientation (PTR) model [10] was adopted. The shear rate on the slip system α or the twin system β is expressed as:

$$\dot{\gamma}^{(\alpha \text{ or } \beta)} = \dot{\gamma}_0 \left(\frac{\tau^{(\alpha \text{ or } \beta)}}{\tau_c^{(\alpha \text{ or } \beta)}} \right)^{(1/m)} sign\left(\tau^{(\alpha \text{ or } \beta)}\right) \tag{1}$$

where $\dot{\gamma}_0$ denotes a reference shear rate, m is strain rate sensitivity exponent, $\tau^{(\alpha \text{ or } \beta)}$ and $\tau_c^{(\alpha \text{ or } \beta)}$ are the resolved shear stress and instantaneous CRSS of the α^{th} slip system (or β^{th} twin system), respectively. $\dot{\gamma}_0$ and m is set as 0.0001/s and 0.02, respectively.

To model the $\tau_c^{(\alpha \text{ or } \beta)}$ in Eq. (1), the extended Voce hardening law is adopted as follows:

$$\tau_c^{(\alpha \text{ or } \beta)} = \tau_0^{(\alpha \text{ or } \beta)} + \left(\tau_1^{(\alpha \text{ or } \beta)} + \theta_1^{(\alpha \text{ or } \beta)} \cdot \Gamma\right)\left[1 - \exp\left(-\frac{\theta_0^{(\alpha \text{ or } \beta)} \cdot \Gamma}{\tau_1^{(\alpha \text{ or } \beta)}}\right)\right] \tag{2}$$

where Γ is the total accumulated shear strain over the all slip system α or twin system β, $\tau_0^{(\alpha \text{ or } \beta)}$, $\tau_1^{(\alpha \text{ or } \beta)}$, $\theta_0^{(\alpha \text{ or } \beta)}$, and $\theta_1^{(\alpha \text{ or } \beta)}$ are material parameters. The evolution of $\tau_c^{(\alpha)}$ in time derivative form is given by:

$$\dot{\tau}_c^{(\alpha \text{ or } \beta)} = \frac{d\tau_c^{(\alpha \text{ or } \beta)}}{d\Gamma} \sum_{i=1}^{N} \boldsymbol{h}_{ij} \dot{\gamma}^{(j)} \tag{3}$$

where N is total number slip and twin systems, $\boldsymbol{h}_{ij}$ is a hardening coefficient represented by

$$\boldsymbol{h}_{ij} = h_j\left(q + (1-q)\delta_{ij}\right) \tag{4}$$

where q represents the ratio between the latent-hardening to the self-hardening, assumed as 1.0 in the current work.

3. Results

Three slip systems and one twin system were considered: (1) $\{0001\}<11\bar{2}0>$ basal slip, (b) $\{10\bar{1}1\}<11\bar{2}0>$ prismatic slip, (c) $\{11\bar{2}2\}<11\bar{2}3>$ pyramidal slip <a+c>, and (d) $\{10\bar{1}2\}<\bar{1}011>$ tensile twin. The elastic stiffness constants for magnesium [11] were adopted as C_{11}=58, C_{12}=25, C_{13}=20.8, C_{33}=61.2, C_{44}=16.6 GPa.

Using the developed CPFE model seeded with the measured initial texture of the ZEK100 shown in Figure 1, the constitutive parameters of the extended Voce hardening law for available slip/twin systems of ZEK100 was identified by fitting to both microscopic lattice strain and macroscopic stress-strain data measured by the HEXRD. The identified constitutive parameters are listed in Table 1.

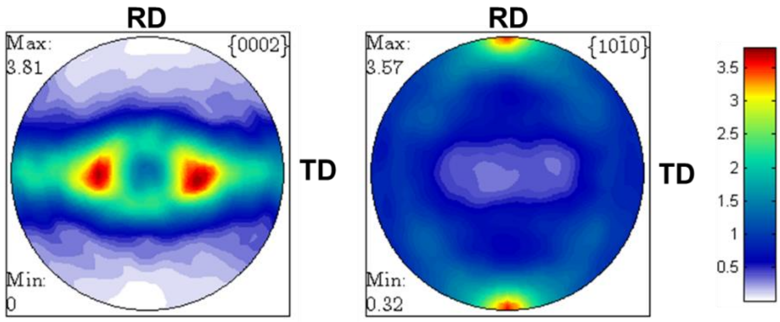

Figure 1. Initial texture of ZEK100 represented by pole figures

Table 1. Identified constitutive parameters of extended Voce hardening law for available slip/twin systems of ZEK100

Slip/twin system	τ_0 (MPa)	τ_1 (MPa)	θ_0 (MPa)	θ_1 (MPa)
Basal	8	10	90	21
Prismatic	92	10	1000	21
Pyramidal <a+c>	102	40	2500	45.5
Tensile Twin	40	15	35	35

The CPFE predicted and HEXRD measured stress-strain curves are compared in Figure 2. The results reveal that the CPFE well predicts the anisotropic stress-strain behavior as well as the ductility during the tension along the two different loading directions, the RD and TD.

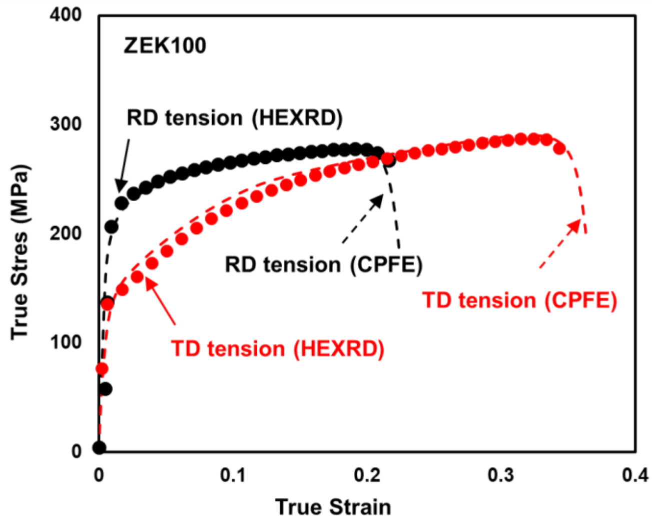

Figure 2. CPFE-predicted and HEXRD-measured stress-strain curves of ZEK100 under two different loading directions, RD and TD.

The CPFE predicted and HEXRD measured lattice strains are compared in Figure 3. Regardless of the loading direction, the results reveal that the CPFE can also capture the microscopic behavior of the ZEK100 alloy in terms of the lattice strain. The results in Figures 2 and 3 showing the excellent agreement of the CPFE predictions and the HEXRD measurements in both micro-and macro-scales validate the fidelity of the current approach and the identified constitutive parameters for each slip/twin system.

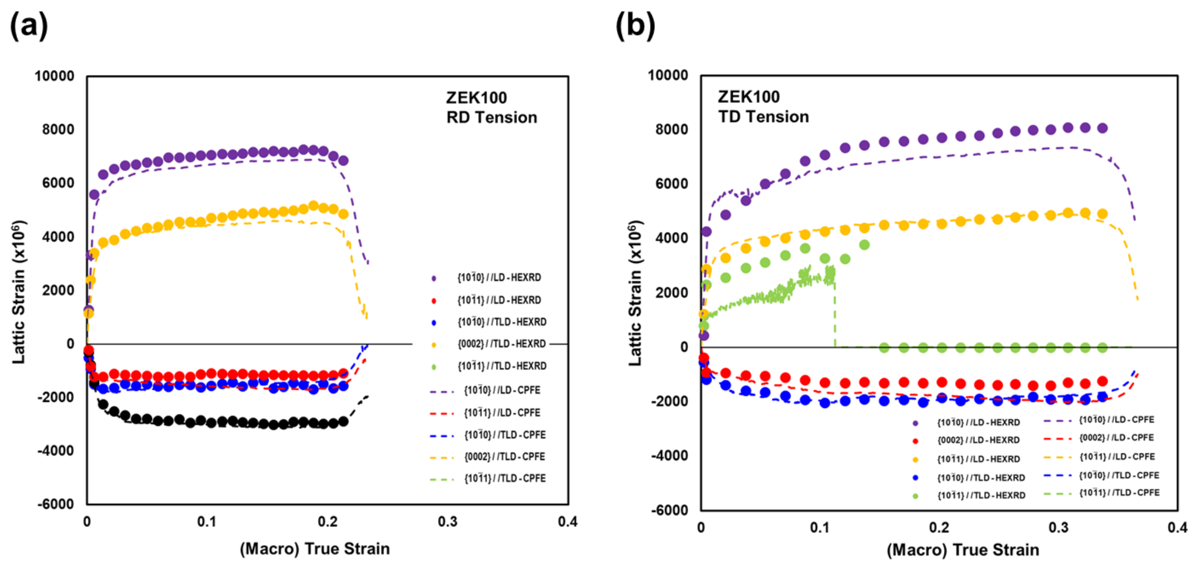

Figure 3. CPFE-predicted and HEXRD-measured lattice strain evolutions as a function of macroscopic true strain under the tension along (a) RD, and (b) TD

4. Conclusions

From the CPFE based modeling of ZEK100 alloy coupled with the *in-situ* HEXRD, following conclusions could be reached:

- The CPFE model was able to predict the anisotropic stress-strain behavior of ZEK100 in macroscale as well as the lattice strain evolutions measured from the *in-situ* HEXRD.

- The approach could enable the accurate constitutive parameter identification of the HCP-structured metals with multiple and anisotropic slip/twin systems.

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