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Crystal plasticity analysis of anisotropic deformation behavior of porous magnesium with oriented pores

T Mayama¹, M Tane², and Y Tadano³

¹ Department of Materials Science and Engineering, Kumamoto University, 2-39-1 Kurokami, Chuo-ku, Kumamoto, 860-8555, Japan

² The Institute of Scientific and Industrial Research, Osaka University, 8-1 Mihogaoka, Ibaraki, Osaka, 567-0047, Japan

³ Department of Mechanical Engineering, Saga University, 1 Honjo-machi, Saga, 840-8502, Japan

E-mail: mayama@kumamoto-u.ac.jp

Abstract. Numerical calculations for porous magnesium with cylindrical oriented pores showed significant influences of active deformation modes in magnesium (Mg) on distinctive "two-stage deformation behavior" during compression. Calculated results also imply that larger grain aspect ratio results in better energy absorption efficiency.

1. Introduction

Several porous metals show high energy absorption capability during compression because of their characteristic deformation process with localization of strain and/or damage [1, 2]. Recently developed porous magnesium with oriented cylindrical pores produced by unidirectional solidification shows very high energy absorption of $\sim 30 \text{ kJ kg}^{-1}$ when the material subjected to compressive loading parallel to elongated direction of pores [3]. This porous magnesium has several distinctive microstructure features including elongated pores and elongated grains in the solidification direction as well as a peculiar crystallographic texture where one of the normal directions of {10-13} planes is closely oriented to the solidification direction. Microstructural observation and numerical analysis in the previous research [3] indicated that different deformation modes were activated depending on loading direction, which leads to strong anisotropy in the deformation behavior. While mechanism of high energy absorption has also suggested in terms of the transition of active deformation modes, the understandings of the relationship between microstructure and mechanical property in the porous magnesium are still limited. There are a number of microstructural parameters which could affect anisotropic deformation behavior and the resultant energy absorption capability. The potentially relevant parameters include single crystal property, crystallographic texture, morphology of grains, pore structure and sample geometry. Numerical analysis which could consider these microscopic parameters helps to gain the detailed understandings of relationship between deformation behavior and the effective parameters, which would be useful for both material design and structural design.

In this study, the influences of active deformation mechanisms and grain aspect ratio on the anisotropic deformation behavior of porous magnesium with oriented pores were numerically investigated by a crystal plasticity finite element method.

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2. Numerical procedure

In this study, a crystal plasticity finite element method was used to consider the geometry of pore structure, crystallographic texture and plastic anisotropy. Analysis model and constitutive model for the present analysis are briefly described as follows.

2.1. Analysis model

Figure 1 shows the analysis model which reproduced pore structure, grain structure and crystallographic texture in an actual porous Mg with directionally oriented cylindrical pores [3]. The analysis model with pores and grains elongated in solidification direction, which is set to be z-axis in the present sample coordinate, is schematically shown in Fig. 1(a). For this model, uniaxial loadings in z-direction are imposed with displacement control both in tension and compression. The initial texture was given to each finite element by Euler angles in accordance with experimentally observed strong fiber texture with a normal direction of {10-13} was oriented to loading direction [3]. The initial (0001) and {10-10} pole figures are shown in Fig. 1(b). In this study, to investigate influence of deformation modes, analyses with deformation modes of FCC structure were also performed. The initial {001} and {110} pole figures for FCC structure are shown in Fig. 1(c), where the initial texture was given by using the same initial Euler angles to Mg model.

2.2. Crystal plasticity constitutive model

A rate-dependent crystal plasticity constitutive model proposed by Peirce et al. [4] was adopted in the present calculation. Slip rate $\dot{\gamma}^{(i)}$ for deformation mode "*i*" was estimated by following power law type equation which depends on resolved shear stress $\tau^{(i)}$ for deformation mode "*i*".

$$\dot{\gamma}^{(i)} = \dot{\gamma}_0 \operatorname{sgn}\left(\tau^{(i)}\right) \left|\tau^{(i)} / g^{(i)}\right|^{1/m} \tag{1}$$

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Here, $\dot{\gamma}_0$ and *m* are a reference shear strain rate and a strain rate sensitivity exponent. In Eq. (1), the evolution equation of reference stress $g^{(i)}$ for deformation mode "*i*" was simply assumed as

$$\dot{g}^{(i)} = \sum_{j} h \left| \dot{\gamma}^{(j)} \right|, \tag{2}$$

where h is a strain hardening rate.

The deformation mechanisms implemented in the present numerical method are basal slip, prismatic slip, second order pyramidal $\langle \mathbf{c}+\mathbf{a}\rangle$ slip and $\{10-12\}$ tensile twinning systems. For twinning, a multiple twin scheme originally proposed by Kalidindi [5] is adopted to evaluate slip activities within all twin variants and the parent region. Material parameters, which had been identified in the previous study [3], were used. For FCC structure, $\{111\}<110>$ slip system was taken into account. For FCC structure, the initial reference stress was set to be 10 MPa while the other material parameters including elastic constants were assumed to be the same to those for Mg. The above crystal plasticity constitutive model was implemented into a finite element code.



Figure 1. Analysis model. (a) Model geometry for porous metal with directionally oriented cylindrical pores. (b) Initial pole figures for Mg (HCP crystal). (c) Initial pole figures for FCC crystal.

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3. Results and discussion

Previous researches on porous metals with directionally oriented cylindrical pores [3, 6, 7] showed qualitatively different stress-strain curves depending on materials. To clarify the origin of material dependence of deformation, influences of deformation modes and grain aspect ratio were studied.

3.1. Influence of active deformation modes.

Influence of active deformation mode on stress-strain behavior was studied by tensile loading and compressive loading analysis with deformation modes in Mg and FCC crystal. Red and blue lines in Fig. 2(a) show calculated stress-strain curves with deformation modes in Mg and FCC crystal, respectively. The stress-strain curves of Mg in tension and compression, which is denoted by red solid and broken lines, were significantly different. In compression of Mg, the initial rapid strain hardening was followed by gradual increase in stress (hereafter "two-stage hardening behavior"), which lead to high energy absorption efficiency, whereas tensile loading exhibited low strain hardening rate throughout deformation. On the other hand, FCC model shows insignificant asymmetry between tension and compression, which denoted by blue solid and broken lines.

The reason for the significant deformation asymmetry in Mg was considered in terms of active deformation modes based on the relative activity during deformation in Fig. 2(b). Contribution of basal slip system, which is dominant deformation mode at the beginning of deformation, decreases to ~0.6 for both tension and compression. Conversely, activity of Pyramidal-2<c+a> increased until $\varepsilon =$ ~20% in compression while the activity of prismatic slip system kept increasing up to $\varepsilon = 30\%$. Furthermore, during tensile loading, contribution of twin system was more than 0.1 until $\varepsilon = ~15\%$ while activity of twin system was much smaller during compressive loading. These differences and transitions of active deformation mode with significantly different reference stresses probably lead to pronounced deformation asymmetry and "two-stage hardening behavior" in Mg. This was confirmed by additional calculations with the same initial reference stress of 10MPa for all slip system without twinning for HCP structure (hereafter HCP equi model). The calculated results are denoted by gray lines in Fig. 2(a). The calculated stress-strain curves for FCC model and HCP equi model are similar, which indicates that non-equivalent deformation mode in Mg is indispensable for appearance of pronounced deformation asymmetry and "two-stage hardening behavior" during compression.



Figure 2. Tension/compression asymmetric deformation behavior. (a) Influences of crystal structure and loading direction on stress-strain curves. (b) Relative activity in Mg model.

3.2. Influence of grain aspect ratio.

Influence of grain aspect ratio on deformation behavior in porous Mg subjected to compressive loading was studied. Calculated compressive loading behavior by three analysis models with different

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grain aspect ratios (1:1, 1:2 and 1:5) as schematically shown in Fig. 3(a) and original aspect ratio (1:10) in Fig. 1(a) were compared. All the models were divided into 640 finite elements. The stress-strain curves in Fig. 3(b) exhibit that larger aspect ratio tend to show more significant decrease in strain hardening rate at $\varepsilon = \sim 20\%$, which results in more pronounced "two-stage hardening behavior". From the viewpoint of energy absorption capability, larger decrease in strain hardening rate increase energy absorption efficiency.

(0001) pole figures at $\varepsilon = 35\%$ in Fig. 3(c) indicate clear difference depending on grain aspect ratio. With larger grain aspect ratio, (0001) pole distribution is deviated from axial symmetry about z-axis. In other words, larger grain aspect ratio lead to larger deviation from ideal fiber texture. This difference in texture development implies that larger fraction of boundary region in the model with smaller grain aspect ratio would lead to more uniform deformation.



Figure 3. Influence of grain aspect ratio on compressive loading in Mg model. (a) Schematic diagrams of grain structure. (b) Effect of grain aspect ratio on stress-strain curve. (c) Influence of grain aspect ratio on (0001) pole figure at compressive strain of 35%.

4. Conclusions

The present numerical calculations were summarized by following conclusions.

1. Comparison between numerical results of deformation modes for Mg (HCP structure) and FCC structure implied that anisotropy of active deformation modes in Mg is indispensable for significant deformation asymmetry and "two-stage hardening behavior" in compression, which is characterized by initial rapid hardening followed by significant decrease in strain hardening rate.

2. In compressive loading of porous Mg, larger grain aspect ratio contributes to "two-stage hardening behavior", which results in larger energy absorption efficiency.

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