(a) Article title:

Crystal plasticity analysis of texture development in magnesium alloy during extrusion

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(d) Abstract:

The texture development mechanism during the extrusion of magnesium alloy is investigated by experimental observation and numerical analysis. First, we perform a finite element analysis of a full extrusion process using a phenomenological constitutive equation, and it is confirmed that the loading condition of the extrusion process near the central axis of the billet is approximated by an equi-biaxial compression mode. Then, the equi-biaxial compression problem is adopted as a simplified boundary value problem to be solved using a crystal plasticity model to clarify the detailed texture development mechanism during the extrusion process. The crystal plasticity analysis of equi-biaxial compression successfully reproduces the texture development from an initial random texture to the final experimentally observed texture. The effects of the

deformation modes (i.e. slip and twinning systems) implemented in the calculation and the reference stress ratio of basal to nonbasal slip systems on texture development are studied in detail. Finally, the mechanism of texture development during the extrusion process is discussed in terms of the lattice rotation caused by the activated slip systems.

(e) Keywords:

Magnesium, Texture, B. Crystal plasticity, C. Finite element analysis, A. Twinning

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1. Introduction

The application of lightweight materials with high strength and formability to mechanical components is expected to contribute to the abatement of global warming and the reduced use of fossil fuels, because the energy consumed in their manufacture and operation is less than that of conventional heavier structural materials such as steels. Therefore, considerable attention has been focused on magnesium, the lightest structural metal.

Extensive research on magnesium alloys indicates that their strength and ductility can be simultaneously improved by severe plastic deformation (Chen et al., 2008; Ma et al., 2009). The grain size, which is refined through forming processes, has a significant effect on material properties, especially in magnesium alloys. The slope of the Hall-Petch relation for magnesium alloys that have the hexagonal close-packed (HCP) crystal structure is larger than those for other metallic materials with cubic crystal structures (Mabuchi and Higashi, 1996). Thus, the mechanical properties of magnesium

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3 55 alloys can be significantly improved through severe forming processes. Meanwhile,
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5 56 processes such as rolling and extrusion generally induce strong textures in magnesium
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7 57 alloys (e.g., Wang and Huang, 2007; Liang et al., 2008; Al-Samman and Gottstein, 2008).
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9 58 Magnesium alloys with strong texture exhibit significant anisotropy including
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11 59 tension-compression asymmetry (e.g., Lee et al., 2009; Chino et al., 2008a; 2008b).
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13 60 Both the strong texture and the significant anisotropy of magnesium originate from the
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15 61 HCP crystal structure with low symmetry. That is, nonequivalent deformation modes
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17 62 realized by different types of slip systems and frequently activated twinning are
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19 63 considered to be essential causes of the development of the strong texture and
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21 64 anisotropy in magnesium. Since each deformation mode has different value of the
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23 65 critical resolved shear stress (CRSS) (e.g., Yoshinaga and Horiuchi, 1963a), the active
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25 66 deformation mode cannot be specified only from the Schmid factors for each deformation
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27 67 mode. In addition, deformation twinning has a loading direction dependence (polarity
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29 68 of twinning), which is the main cause of the tension-compression asymmetry (Chino et
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31 69 al., 2008a, 2008b; Mayama et al., 2009). These complicated deformation mechanisms
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33 70 make it difficult to determine the anisotropy and texture development mechanism in
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35 71 magnesium.

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39 72 Recently, a number of studies on HCP metals have been carried out using
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41 73 crystal-plasticity-based simulations (Staroselsky and Anand, 2003; Graff et al., 2007;
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43 74 Mayeur and McDowell, 2007; Beausir et al., 2007; Capolungo et al., 2009). Because the
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45 75 crystal plasticity model explicitly considers deformation mechanisms at the scale of the
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47 76 crystal structure, the activation of nonequivalent deformation modes is systematically
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49 77 calculated. Therefore, crystal-plasticity-based simulations are a powerful tool for
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51 78 determining the complicated deformation mechanism in magnesium alloys (e.g., Agnew
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53 79 et al., 2003; Mayama et al., 2009; Neil and Agnew, 2009; Proust et al., 2009; Choi et al.,
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55 80 2010). Although several investigations of texture development in magnesium alloys in
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57 81 terms of plane strain compression, rolling and equal-channel angular extrusion
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processes have been reported (e.g., Agnew et al., 2001; Styczynski et al., 2004; Agnew et al., 2005. Bohlen et al., 2007; Beausir et al., 2008; Li et al., 2008; Biswas et al., 2010), the number of computational studies on texture development in a conventional extrusion process using the crystal plasticity model has been limited.

In the present study, to determine the mechanisms of texture development during the extrusion of a magnesium alloy, we conduct experiments and crystal-plasticity-based analyses on commercial magnesium alloy AZ31. The microstructural evolution and texture development are observed using a scanning electron microscope (SEM) with electron back scattering diffraction (EBSD) equipment. Since crystal plasticity simulations of the full extrusion process are rather time-consuming, we first perform a finite element analysis of a full extrusion process using a phenomenological constitutive equation. It is confirmed that the loading condition of the extrusion process near the central axis of the billet can be approximated by an equi-biaxial compression mode. Thus, in simulations to clarify the texture development in detail we adopt a simplified boundary value problem of equi-biaxial compression, which is analyzed using the crystal plasticity model. Using this simplified problem formulation, the effects of the deformation modes implemented in the analysis and the reference stress ratio of the basal slip system to the nonbasal slip system on texture development are investigated. Finally, the texture development mechanism is discussed in terms of lattice rotation caused by the activation of slips.

2. Experimental observation

2.1 Material and experimental method

The texture development of the extruded magnesium alloy AZ31 was experimentally observed. The observations were conducted by using a SEM with EBSD equipment. The chemical compositions of the AZ31 ingot used in this study are 3.0 wt.% Al, 0.9 wt.% Zn, 0.3 wt. % Mn and balance Mg. From the ingot, as-cast AZ31 alloy were prepared by

high-frequency induction melting in an Ar atmosphere. From the as-cast alloy, an extrusion billet with a diameter D_e of 29 mm was machined. The billet without heat-treatment was used for extrusion in this study. Figure 1a shows a schematic diagram of the extrusion setup. The billet was extruded with an extrusion ratio R_e of 10 and an extrusion die half angle θ_e of 30° at a temperature T_e of 623 K under a ram speed V_e of 2.5 mm/s. The extruded material was quenched immediately after extrusion to avoid grain growth. The material remaining in the extrusion die and the extruded material were observed. The positions of observations are schematically illustrated in Fig. 1b. Whereas points A, B and C were located within the material remaining in the die, point D was positioned in the completely extruded material. The distances from the entrance of the extrusion die z , as shown in Fig. 1b, the corresponding extrusion ratios R calculated from the geometry of the extrusion die and the equivalent true strains $\bar{\epsilon}_{\text{true}}$ are listed in Table 1. The equivalent true strains (Hirano et al., in press) are calculated by

$$\bar{\epsilon}_{\text{true}} = \ln(R_e). \quad (1)$$

For the EBSD observation, the surfaces of the samples were polished using a cross-section polisher. Pole figures were generated from the EBSD analysis data by performing a texture calculation using a harmonic series expansion approach with a series rank of 16 (OIM Analysis 5.3, 2007). All pole figures in this paper are visualized in terms of the stereographic projection with the same range in the contour bar.

2.2 Result of observation

Figs. 2a-d show the inverse pole figure maps at positions A-D defined in Fig. 1b, respectively. The direction of observation is perpendicular to the extrusion direction (ED) as shown in Fig. 2. Therefore, the horizontal direction in Figs. 2a-d corresponds

to the extrusion direction. In Fig. 2a (position A), several lenticular regions in the coarse grains are seen, and they are identified as the $\{10\bar{1}2\}\langle 10\bar{1}1\rangle$ tensile twin judging from the misorientation angle between the lenticular region and the neighboring grains. In Fig. 2b (position B), bands of fine grains between coarse grains are observed. It is considered that these fine grains were formed owing to grain subdivision during the extrusion process (e.g., Ion et al., 1982; Bohlen et al., 2005; Yi et al., 2006). At position C (Fig. 2c), coarse grains elongated in the extrusion direction are seen, although the area fraction of fine grains is increased from that in Fig. 2b. A microstructure similar to that at position C is observed at position D (Fig. 2d). The type of heterogeneous microstructure observed in Fig. 2d has also been reported in the literature (e.g., Bohlen et al., 2005; Yi et al., 2006). (0001) and $\{10\bar{1}0\}$ pole figures were generated from the inverse pole figure maps shown in Figs. 2a-d, as shown in Fig. 3. These pole figures are stereographic projections on the TD-ND plane. The very high maximum intensity (as indicated by “Max. = ***” in Fig. 3) observed in Fig. 3a (position A), even at the smallest strain level, is a consequence of the generation of the pole figure from the small number of coarse grains observed in Fig. 2a owing to the narrow EBSD observation area. Nevertheless, we consider that the overall texture development during extrusion has been captured in Figs. 3b-d.

3. Numerical procedure

3.1 Finite element analysis of the extrusion process

In the present study, we aim to capture the texture development in the extrusion process using a crystal plasticity finite element method. However, direct simulation of the full extrusion process using this method may be time-consuming owing to a huge computational load. Thus, a finite element analysis of the full extrusion process is first carried out using a phenomenological constitutive equation to obtain a simplified boundary condition for crystal plasticity simulations.

The explicit finite element code DYNA3D is used for the simulation of the full extrusion process. Fig. 4 shows the analysis model¹. The geometry of the extrusion billet and the angle of the extrusion die are set to be the same as those in the experimental setup shown in Fig. 1, but a smaller extrusion ratio of 5 is used to avoid failure of analysis caused by unreasonable mesh-distortion due to the lack of re-meshing feature in the code. The purpose of this analysis is not a quantitative prediction of the extrusion process up to an extrusion ratio of 10 but an estimation of the overall loading condition during the extrusion. To evaluate the difference in the dependence of the loading condition on the position, the changes in the strain components are collected at three different radial positions, X_1 , X_2 and X_3 , as shown in Fig. 4a. As shown in Fig. 4b, the extrusion billet is modeled on a sector-shaped column with dimensions one-twentieth of those of the original extrusion billet. Considering the symmetries of deformation, the circumferential displacements of the billet are fixed as shown in Fig. 4c. The extrusion billet is discretized using 7440 eight-node brick elements. The following linear hardening equation is used:

$$\bar{\sigma} = \sigma_Y + F \bar{\epsilon}^p, \quad (2)$$

where $\bar{\sigma}$, σ_Y , F and $\bar{\epsilon}^p$ are equivalent stress, yield stress, the hardening coefficient and equivalent plastic strain, respectively. The material parameters used in Eq. (2) as well as Young's modulus E , Poisson's ratio ν , density ρ and the friction coefficient μ between the billet and other components used in the calculation are determined as shown in Table 2, referring to experimental results in the literature (e.g., Watanabe et al., 2001; Shi et al., 2007; Agnew et al., 2008; Liang et al., 2009). The dummy block, the container and the extrusion die are assumed to be rigid bodies. The billet is

¹ The present extrusion problem could be treated as an axisymmetric problem. But, we considered a three-dimensional problem as shown in Fig. 4 since axisymmetric analysis is not available in the code used.

processed by translation of the dummy block in the z -direction, as shown in Fig. 4a, at a constant speed of 10 m/s to reduce the computation time. This speed is much larger than that under realistic experimental conditions, but it is confirmed that the calculated kinetic energy is less than 5% of the internal energy throughout the calculation. It was also confirmed that the differences in the calculated results were negligible when the speed is changed to 5 m/s or 1 m/s.

Figs. 5a-c show the calculated relationships between the strain components ε_{xx} , ε_{zz} and ε_{yy} and the stroke of the dummy block at the three different points embedded into the billet as shown in Fig. 4a. Fig. 5a indicates that the shear strain ε_{zx} near the central axis of the billet is negligibly small compared with the normal strains ε_{xx} and ε_{yy} . The shear strain ε_{zx} at the outer positions of the billet (Figs. 5b and c) becomes comparable to the values of the normal strains. From these computational results, it can be concluded that the deformation near the central axis of the billet during the extrusion is well approximated by equi-biaxial compressive straining. Thus, we adopt this boundary value problem for crystal plasticity analysis to evaluate the detailed texture development of the material near the central axis of the billet.

Because the stress-strain relation at high temperatures strongly depends on the strain rate (e.g., Watanabe et al., 2001), it has been confirmed that changes in the yield stress σ_y result in similar trends to those shown in Fig. 5. The computation performed here assumed a low value of the friction coefficient (Liang et al., 2009), since the experiment was carried out using an oil-based lubricant. It was confirmed that a calculation with a higher friction coefficient results in similar trends to those shown in Fig. 5. With an increase in the friction coefficient, whereas values of the shear strain component in the outer regions increase, the shear strain component near the center of the billet is still negligibly small in comparison with the normal stress values.

3.2 Crystal plasticity finite element method

The crystal plasticity finite element method employed here is fundamentally the same as that used in Mayama et al. (2009). In the method, a rate-dependent crystal plasticity model (Pierce et al., 1983) is implemented into each Gauss point in the finite elements. A rate tangent modulus method (Pierce et al., 1983) is used for the numerical integration of the constitutive model.

The shear strain rate $\dot{\gamma}^{(\alpha)}$ for each deformation mode is determined by the resolved shear stress (RSS) $\tau^{(\alpha)}$ as

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \operatorname{sgn}(\tau^{(\alpha)}) \left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right|^{1/m}, \quad (3)$$

where $\operatorname{sgn}(x)=1$ if $x \geq 0$ and $\operatorname{sgn}(x)=-1$ if $x < 0$; m and $\dot{\gamma}_0$ are the slip rate sensitivity parameter and a reference strain rate, respectively, and $g^{(\alpha)}$ is a reference stress that generally depends on both the deformation mode and the loading history. While the experimental results of stress-strain behavior of single crystal AZ31 at high temperature are not available, the experimental and numerical reports for polycrystalline AZ31 and single crystal pure magnesium (Akhtar and Teghtsoonian, 1969a, 1969b; Obara et al., 1973; Agnew et al., 2001; Yin et al., 2005; Graff et al., 2007; Cheng et al., 2008; Al-Samman and Gottstein, 2008; Proust et al., 2009; Neil and Agnew, 2009) indicate that the strain hardening drastically decreases with the increase in testing temperature from 473K to 573K. Based on these reports, the strain hardening at extrusion temperature 623K seems not to be so significant. So, in the present study, work hardening is ignored, and thus constant values of $g^{(\alpha)}$ for each deformation mode are used. Specific values of $g^{(\alpha)}$ are discussed in the following sections. The rate sensitivity parameter is assumed to be $m=0.2$, referring to the literature on experiments on cast AZ31 alloy at high temperatures (e.g., Duygulu and Agnew, 2003; Kim et al., 2008).

3.3 Deformation mode and CRSSs in magnesium

To ensure realistic calculations, deformation modes and reference stresses for each deformation mode should be carefully chosen. According to previous extensive research, there are several possible deformation modes in pure magnesium single crystal (Read-Hill and Robertson, 1957; Hirsch and Lally, 1965; Yoshinaga and Horiuchi, 1963b; Obara et al., 1973; Miura et al., 2005), i.e., basal, prismatic, first-order pyramidal (pyramidal-1) and second-order pyramidal (pyramidal-2) slip systems. Deformation twinning is also one of the main deformation modes in magnesium. In previous studies (Yoshinaga and Horiuchi, 1963a; Christian and Mahajan, 1995; Barnett et al., 2008), the activation of several different twinning systems has been reported. In the present study, only the twinning system $\{10\bar{1}2\}$ is considered, since our experimental observation (Fig.2) suggested that only this twinning system was activated. These deformation modes are specified in Table 3. In the literature, however, somewhat different active deformation modes and their CRSSs have been reported. Furthermore, experimental data for CRSSs in commercial magnesium alloys are not available since it is difficult to produce single crystals of these alloys with sufficiently large dimensions for mechanical testing. Consequently, the CRSSs for magnesium alloys have been estimated through indirect methods. Barnett (2003) determined the CRSSs for AZ31 by fitting a Taylor model simulation result to his experimental results. In his paper, the CRSSs for the prismatic and pyramidal-2 slip systems were proposed to be as follows:

$$\tau_{prismatic} = 2.5 \ln(Z) - 38 \text{ MPa}, \quad (4)$$

$$\tau_{\langle a+c \rangle} = 2.1 \ln(Z) - 32 \text{ MPa}, \quad (5)$$

where the Zener-Hollomon (Z) parameter is defined as $Z = \dot{\epsilon} \exp(Q/RT)$, while the CRSSs for the basal slip and tensile twinning systems were reported to have constant values of 5 and 32 MPa, respectively. The value of Z in the present study is determined from the gas constant R , the activation energy Q in the literature (Barnett, 2003),

the extrusion temperature T_e assuming no increase in temperature during the extrusion and the average strain rate $\dot{\varepsilon}$ (Hirano et al., in press) during extrusion, calculated by

$$\dot{\varepsilon} = \frac{6V_e \ln R_e \tan \theta_e}{D_e (1 - 1/R_e \sqrt{R_e})}. \quad (6)$$

Consequently, the reference stresses for the basal, prismatic and pyramidal-2 slip systems and the tensile twinning system are set to 5, 32.01, 26.81 and 30 MPa, respectively. Although the CRSS for the pyramidal-1 slip system was not discussed in Barnett (2003), the reference stress for the pyramidal-1 slip system is assumed to be the same as that for the prismatic slip system when it is taken into account in the present application.

3.4 Incorporation of deformation twinning

Among several proposals for the incorporation of twinning into numerical simulations (Van Houtte, 1978; Tome et al., 1991; Staroselsky and Anand, 2003; Graff et al., 2007; Proust et al., 2009), the method proposed by Van Houtte (1978) is used in this study. Details of the numerical procedure for the twinning model are described in Mayama et al. (2009). The followings are the brief explanation of numerical method.

Assuming that the twinning plane normal vector and the shear direction vector by twinning are equivalent to the slip plane normal and the slip direction vectors, respectively, they are incorporated into the crystal plasticity model. Shear strain rate is calculated in the same manner as that for slip deformation by using Eq.(3), except that $\{10\bar{1}2\}$ twinning is not activated by a c-axis compression. Therefore, the shear strain rate must be zero if c-axis compression loading is imposed.

The lattice rotation caused by twinning is evaluated by different method used in slip deformation. An occurrence of lattice rotation by twinning leads to an increase in the

number of grains. Incorporating such unlimited grain subdivisions into the analysis is not feasible. Therefore, in the method proposed by Von Houtte (1978), the number of grains is kept unchanged throughout the analysis. The followings are procedure of calculation of lattice rotation by twinning.

The pseudo-volume fraction of the twin due to twinning system α in each grain is defined by

$$V^{(\alpha)} = \gamma^{(\alpha)} / \gamma_{\text{twin}} . \quad (7)$$

where $\gamma^{(\alpha)}$ is the accumulated shear strain of twinning system α calculated by $\gamma^{(\alpha)} = \int |\dot{\gamma}^{(\alpha)}| dt$, and γ_{twin} is the shear strain due to $\{10\bar{1}2\}$ twinning given by the following equation (Yoo, 1981):

$$\gamma_{\text{twin}} = \sqrt{3} / \frac{c}{a} - \frac{c}{a} / \sqrt{3} . \quad (8)$$

Here, $\frac{c}{a}$ is the lattice parameter ratio. In this study, $\frac{c}{a} \cong 1.62$ is used for magnesium. That is, there is no twinning region in the grain when $V^{(\alpha)} = 0$, and the entire grain is twinned when $V^{(\alpha)} = 1$. Lattice rotations due to the occurrence of twinning are computed by the following procedure:

1. Before the analysis, a threshold value for each twinning system at each integration point is set between 0.3 and 1.0 (Staroselsky and Anand, 2003) using a pseudo-random generator.
2. During deformation, the pseudo-volume fraction of each twinned region is calculated by Eq.(7) using the accumulated shear strain $\gamma^{(\alpha)}$.
3. The calculation is continued if $V^{(\alpha)} < V_{\text{th}}^{(\alpha)}$, the entire grain is rotated according to a specific twinning geometry; i.e., the lattice rotation tensor $\mathbf{R}^{\text{tw}}$ (Staroselsky and Anand, 2003) corresponding to the occurrence of twinning is given by

$$\mathbf{R}^{\text{tw}} = -\mathbf{I} + 2\mathbf{m}^{(\text{twin})} \otimes \mathbf{m}^{(\text{twin})} . \quad (9)$$

where $\mathbf{I}$ and $\mathbf{m}^{(\text{twin})}$ are the unit tensor and the activated twinning plane

normal vector, respectively.

4. The accumulated shear strain $\gamma^{(\alpha)}$ of all twinning systems in the grain subjected to the twinning rotation are reset to zero. Return to step 2.

The procedure given above is incorporated into the crystal plasticity analysis method introduced in Section 3.2.

3.5 Crystal plasticity analysis model

As shown in section 3.1, the equi-biaxial compression mode can approximate the deformation behavior near the central axis of the extrusion billet. In the present study, the equi-biaxial compression problem is adopted as a simplified boundary value problem in crystal plasticity analysis to investigate texture development during the extrusion process because the experimental observation shown in Fig. 2 was conducted near the central axis. A schematic diagram of the crystal plasticity analysis model is shown in Fig. 7. Here, the boundary condition of top surface for extrusion direction (ED) is set to be stress free. A cubic region is uniformly divided into $7 \times 7 \times 7$ elements. Each element is a 20-node brick element with eight Gauss points. Initial crystal orientations are randomly determined using a pseudorandom number generator for each element. Therefore, the model has 343 initial random orientations. Since the lattice rotation is evaluated at every Gauss point, a total of 2744 orientations are considered. The Young's modulus and Poisson's ratio in Table 2 are used in the crystal plasticity simulations.

The number of grains in the material greatly increases during the extrusion process due to grain refinement as shown in Fig. 2. The present crystal plasticity analysis does not take grain refinement into account, i.e., the number of grains is fixed throughout the computation. The effect of this simplification will be discussed in the next section.

4. Results and discussion

4.1 Effect of implemented deformation modes

In this section, to evaluate the effect of the implemented deformation modes, calculations with four sets of reference stress values for each deformation mode, as shown in Table 4 are considered. Calculations using the sets of reference stress values are denoted as ALL, No-PRI, No-PY1 and No-TW. Here, ALL consider basal, prismatic, pyramidal-1 and pyramidal-2 slip system as well as twinning system while No-PRI, No-PY1 and No-TW does not consider prismatic slip, pyramidal-1 slip or twinning system, respectively. Fig. 8 shows the calculated (0001) and $\{10\bar{1}0\}$ pole figures after equi-biaxial compression up to an equivalent true strain of 2.3, which corresponds to an extrusion ratio of 10. In all cases, the intensity of the (0001) poles is high at the circumferential region and the intensity of the $\{10\bar{1}0\}$ poles is high at the center and in a ring-shaped region around the center. These features are qualitatively similar to the experimental observations shown in Fig. 3d, although the maximum intensities in Fig. 3d are higher than those in the computational results. These textures were computed assuming a constant number of grains, while the actual number of grains increased owing to grain refinement during the extrusion as shown in Fig. 2. This agreement between the observed and calculated textures seems to suggest that the subdivision of grains in magnesium during extrusion does not affect the overall texture development. However, the physical reason for this lack of sensitivity to grain subdivision was not clarified in the present study.

Fig. 9 shows the calculated results of texture development in the case of ALL. The pole figures in Figs. 9a-d correspond to the experimental ones shown in Figs. 3a-d. Gradual texture development was predicted by the computation. The experimental result in Fig. 3a exhibited very high maximum intensities due to the effect of a small number of large grains in the narrow observation window as pointed out in section 2.2. In the computation, the maximum intensity in Fig. 9a is very low compared with that in

Fig. 3a because the texture in Fig. 9a did not develop from the initial random orientations.

Here, the relative activity is defined as the fraction of the shear strain increment $d\gamma^{(\text{mode})}$ of the each equivalent deformation mode. In the computation, the increment $d\gamma^{(\text{mode})}$ is obtained from summing up the shear strain increments $d\gamma^{(\alpha)}$ of each equivalent deformation mode in all grains within the analysis model. Figs. 10a-d show the relative activity of each deformation mode during equi-biaxial compression in the cases of ALL, No-PRI, No-PY1 and No-TW. Whereas the deformation modes considered in the four cases are different, the activity of the basal slip system is predominant throughout the deformation in all cases. In addition, the pyramidal-2 slip system exhibits almost the same activity in all four cases. This is because only the pyramidal-2 slip system, except for the twinning system whose activity is limited to the beginning of deformation as shown in Figs. 10a-c, accommodates the deformation in the c -axis direction. The slip directions of all other slip systems are on the (0001) plane, and they thus make no contribution to c -axis deformation, as shown in Fig. 6. The second largest contribution depends on the implemented deformation mode. In the case of ALL, the pyramidal-2 system provides the second largest contribution, while the pyramidal-1 slip system and the prismatic slip system are the second largest contributions in the cases of No-PRI and No-PY1, respectively.

Next, the effect of twinning on texture development is considered. Here, to evaluate the texture development quantitatively, an angle θ is defined as the angle between the $[0001]$ direction and the extrusion direction, as schematically shown in Fig. 11a. Fig. 11b shows changes in the average θ value and the standard deviation of θ in the cases of ALL, No-PRI, No-PY1 and No-TW. The lines show the results for ALL, No-PRI and No-PY1, in which twinning is considered. The circles indicate the result for No-TW, in which twinning is not considered. Almost the same relationships for the cases with consideration of twinning can be seen in Fig. 11b, but the curves for

the case without twinning are clearly different from the other curves. The change in the average θ value is greater in the cases with twinning than in the case without twinning, although the final values of the average θ at an equivalent true strain of 2.3 are similar in all cases. These results suggest that deformation twinning accelerates the texture development in the early stage of the extrusion process.

4.2 Effect of reference stress ratio

The experimental results for magnesium single crystals (Read-Hill and Robertson, 1957; Yoshinaga and Horiuchi, 1963a; 1963b) show that CRSSs for nonbasal slip systems are significantly dependent on temperature while the temperature dependences of CRSSs for basal slip and twinning systems are relatively small (Sheely and Nash, 1960). In extrusion, the temperature in deformed billet depends on both the extrusion temperature and the extrusion speed. From this viewpoint, it is important to examine the relationship between the reference stress ratio of the basal slip system to the nonbasal slip system and texture development to determine how extrusion conditions affect texture development. In this section, the effect of the reference stress ratio on texture development is studied.

The reference stresses used in this section are shown in Table 5. All deformation modes shown in Fig. 6 are implemented in the calculations. For simplicity, the same value of reference stress for all nonbasal slip systems τ_{nonbasal} is assumed. The reference stresses for the basal slip and twinning systems are fixed to $\tau_{\text{basal}} = 5$ and $\tau_{\text{twin}} = 30$ MPa, respectively, because the CRSSs for the basal slip and twinning systems are less sensitive to temperature than those for the nonbasal slip systems (Barnett, 2003).

Fig. 12 shows (0001) and $\{10\bar{1}0\}$ pole figures after equi-biaxial compression up to an equivalent true strain of 2.3. While pole figures similar to those in Fig. 8 are obtained in Figs. 12c and d, qualitatively different textures are presented in Figs. 12a

and b. The annular high intensity region in the (0001) pole figures tends to move toward the center with decreasing reference stress ratio, and the maximum intensity appears at the center of the (0001) pole figures in Fig. 12a. In addition, two ring-shaped high-intensity regions emerge in the $\{10\bar{1}0\}$ pole figures shown in Figs. 12a and b. The reason for this texture development is discussed in the next section.

Fig. 13 shows the relationships between the relative activity of each deformation mode and the equivalent true strain during equi-biaxial compression. The pyramidal-1 and pyramidal-2 slip systems are the two dominant deformation modes in Fig. 13a. In contrast, in the other cases the basal slip system is dominant. This is similar to the tendency shown in Fig. 10. With decreasing reference stress ratio, the activity of the basal slip and twinning systems decreases. The decrease in activity of the twinning system results in the increase in the activity of the pyramidal-2 slip system, because the strain in the c -axis direction must be accommodated by the activity of the pyramidal-2 slip and twinning systems.

4.3 Texture development mechanism

The normal direction to the slip plane of the activated slip system rotates towards the compressive direction (e.g., Taylor, 1927). In the present crystal plasticity model, the changes in the slip direction $\mathbf{s}^{(\alpha)}$ and the direction normal to the slip plane $\mathbf{m}^{(\alpha)}$ are calculated by

$$\dot{\mathbf{s}}^{(\alpha)} = \mathbf{W}^* \mathbf{s}^{(\alpha)} \quad \text{and} \quad \dot{\mathbf{m}}^{(\alpha)} = \mathbf{W}^* \mathbf{m}^{(\alpha)}, \quad (10)$$

where $\mathbf{W}^*$ is the nonplastic (i.e., elastic and rigid body) spin tensor given by

$$\mathbf{W}^* = \mathbf{W} - \mathbf{W}^p. \quad (11)$$

In Eq. (11), $\mathbf{W}$ and $\mathbf{W}^p$ are the continuum and plastic spin tensors, respectively. Here, for simplicity, assuming that the deformation mode is homogeneous equi-biaxial compression mode based on the result obtained in section 3.1, $\mathbf{W}$ at each material point is negligible. In this case, Eq. (11) becomes

$$\mathbf{W}^e = -\mathbf{W}^p. \quad (12)$$

In crystal plasticity theory, $\mathbf{W}^p$ is given by

$$\mathbf{W}^p = \sum_{\alpha} \frac{\dot{\gamma}^{(\alpha)}}{2} (\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)} - \mathbf{m}^{(\alpha)} \otimes \mathbf{s}^{(\alpha)}) = \sum_{\alpha} \dot{\gamma}^{(\alpha)} \mathbf{w}^p{}^{(\alpha)} \quad (13)$$

with

$$\mathbf{w}^p{}^{(\alpha)} = \frac{1}{2} (\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)} - \mathbf{m}^{(\alpha)} \otimes \mathbf{s}^{(\alpha)}). \quad (14)$$

From Eqs. (10) and (12)-(14), the axis of lattice rotation due to the activation of each slip system is given by the direction perpendicular to both the slip direction and the normal direction to the slip plane. Table 6 shows the axis of rotation due to the activation of each slip system. In addition to rotations caused by slip, the crystal lattice orientation is changed by the activation of twinning. The axis of lattice rotation caused by twinning is $\langle 11\bar{2}0 \rangle$ owing to the geometry of the $\{10\bar{1}2\}$ twin (e.g. Barnett et al., 2008). In the following the No-PY1 case is considered, for simplicity. As pointed out in section 4.1, the consideration of twinning has only a small effect on the overall texture development. Thus, twinning is not taken into account in the following. The rotations about the $\langle 10\bar{1}0 \rangle$ axis caused by basal and pyramidal-2 slip systems change the normal direction of the (0001) plane. In contrast, the rotation about the $[0001]$ axis caused by the prismatic slip system does not change the direction normal to the (0001) plane, while it changes the direction normal to the $\{10\bar{1}0\}$ plane. Therefore, the development mechanisms of (0001) and $\{10\bar{1}0\}$ pole figures are separately considered below.

First, the development mechanism of the (0001) pole figure during extrusion is considered. In the case of No-PY1, only the basal and pyramidal-2 slip systems affect the development of the (0001) pole figure except for a minor contribution from twinning. Figs. 14a-d show schematic diagrams of the lattice rotation caused by the activation of the basal and pyramidal-2 slip systems. Thick lines show the activated slip systems. With the activation of the basal slip system, the direction normal to the basal plane rotates towards the compressive direction as shown in Figs. 14a and b. In

the case of extrusion, the compressive direction is perpendicular to the extrusion direction. The direction normal to the (0001) plane is aligned with that perpendicular to the extrusion direction when the basal system is predominantly activated. This leads to an increase in the intensity at the circumferential region of the (0001) pole figure as shown in Figs. 3, 8 and 9. By contrast, the activation of the pyramidal-2 slip system is expected to yield the opposite lattice rotation as shown in Fig. 14d. Eventually, the lattice rotations caused by the basal and pyramidal-2 slip systems may become balanced as shown in Fig. 14c. In reality, the crystal orientation schematically illustrated in Fig. 14c depends on the CRSS ratio of the basal slip system to the pyramidal-2 slip system. Both slip systems are activated simultaneously when the resolved shear stresses (RSSs) for both the slip systems reach their critical values, i.e. CRSS. This is a reason why qualitatively different pole figures were predicted depending on the reference stress ratio of the basal slip system to nonbasal slip systems as shown in Fig. 12.

Next, the development mechanism of the $\{10\bar{1}0\}$ pole figure during extrusion is considered. The purpose of the consideration is to clarify the reason why not the direction normal to the $\{11\bar{2}0\}$ plane but that normal to the $\{10\bar{1}0\}$ plane aligns with the extrusion direction. For simplicity, only the activity of the prismatic slip system when the (0001) plane is parallel to the compressive direction is considered. The justification of this simplification is inductively shown by crystal plasticity analysis in the final part of this section. Fig. 15a shows a schematic diagram of the loading direction, crystal orientation and ϕ , defined as the angle between the compressive direction and the $[1\bar{1}00]$ direction. Fig. 15b shows the relationship between the Schmid factors for the three prismatic slips and ϕ . The Schmid factors for each prismatic slip vary with the loading direction. Fig. 15c shows schematic diagrams indicating crystal orientations, active slip systems and the directions of lattice rotation. In Figs. 15b and c, s_1 , s_2 and s_3 indicate the $(10\bar{1}0)[\bar{1}2\bar{1}0]$, $(01\bar{1}0)[\bar{2}110]$ and

$(\bar{1}100)[\bar{1}\bar{1}20]$ slips, respectively. In Fig. 15c, the slip planes with the highest Schmid factor for each direction are highlighted by thick lines. Only when the compressive direction coincides with the $\langle 10\bar{1}0 \rangle$ or $\langle 11\bar{2}0 \rangle$ direction ($\phi = -30^\circ$, $\phi = 0^\circ$ or $\phi = 30^\circ$ in Fig. 15c), two prismatic slips are activated simultaneously owing to the same Schmid factor for the two prismatic slips. For these crystal orientations, the opposite tendencies of lattice rotation caused by a pair of prismatic slips are balanced with each other. Thus, overall lattice rotation does not occur as a result of prismatic slip. In contrast, when the compressive direction deviates from the $\langle 10\bar{1}0 \rangle$ or $\langle 11\bar{2}0 \rangle$ direction ($-30^\circ < \phi < 0^\circ$ or $0 < \phi < 30^\circ$ in Fig. 15c), the Schmid factor of one prismatic slip becomes higher than those of the other slips as shown in Fig. 15b, which induces a single slip of the prismatic slip. As a result of this single slip, the lattice rotates around the $[0001]$ axis. This rotation aligns the $\langle 11\bar{2}0 \rangle$ direction with the compressive direction ($\phi = -30^\circ$ or $\phi = 30^\circ$ in Fig. 15c) because the direction normal to the activated slip system rotates toward the compressive direction and the rotation stops at $\phi = \pm 30^\circ$. In the case of equi-biaxial compression, the alignment of the $\langle 11\bar{2}0 \rangle$ direction with the compressive direction results in the alignment of the $\langle 10\bar{1}0 \rangle$ direction with the ED direction in Fig. 7. Therefore, during extrusion, the $\{10\bar{1}0\}$ plane tends to become oriented in the extrusion direction.

In contrast, if the virtual $\{11\bar{2}0\}\langle 10\bar{1}0 \rangle$ slip system is considered instead of prismatic slip system, the lattice rotation is expected to be different from that discussed above. Fig. 15d shows schematic diagrams of lattice rotation due to the activation of the $\{11\bar{2}0\}\langle 10\bar{1}0 \rangle$ system. The relationship between the Schmid factors for each slip system and angle ϕ in Fig. 15b is also valid for this case upon redefining s_1 , s_2 and s_3 as $(\bar{1}2\bar{1}0)[\bar{1}010]$, $(2\bar{1}\bar{1}0)[01\bar{1}0]$ and $(11\bar{2}0)[\bar{1}100]$ slips, respectively. In this case, when the compressive direction coincides with the $\langle 10\bar{1}0 \rangle$ or $\langle 11\bar{2}0 \rangle$ direction ($\phi = -30^\circ$, $\phi = 0^\circ$ or $\phi = 30^\circ$ in Fig. 15d), two of the $\{11\bar{2}0\}\langle 10\bar{1}0 \rangle$ slips are activated simultaneously because of the same value of the Schmid factor for these two

systems. However, in this case, when the compressive direction deviates from the $\langle 10\bar{1}0 \rangle$ or $\langle 11\bar{2}0 \rangle$ direction ($-30^\circ < \phi < 0^\circ$ or $0 < \phi < 30^\circ$ in Fig. 15d), the activation of a single slip of the virtual $\{11\bar{2}0\}\langle 10\bar{1}0 \rangle$ system aligns the $\langle 10\bar{1}0 \rangle$ direction with the compressive direction ($\phi = 0^\circ$ in Fig. 15d). This is the opposite lattice rotation from that in the case of a prismatic slip as shown in Fig. 15b. During extrusion, therefore, it is expected that the $\{11\bar{2}0\}$ plane aligns with the extrusion direction owing to the activation of the virtual $\{11\bar{2}0\}\langle 10\bar{1}0 \rangle$ slip system.

Finally, the above mentioned mechanism of the $\{11\bar{2}0\}$ pole figure development is confirmed by the crystal plasticity analysis of equi-biaxial compression considering the virtual $\{11\bar{2}0\}\langle 10\bar{1}0 \rangle$ slip system without consideration of the prismatic slip system. The reference stresses for the basal, $\{11\bar{2}0\}\langle 10\bar{1}0 \rangle$ and pyramidal-2 slip systems are 5, 32.01 and 26.81, respectively. The pyramidal-1 slip system and tensile twinning system are not considered in this calculation. Fig. 16 shows (0001) and $\{10\bar{1}0\}$ pole figures of the developed texture after equi-biaxial compression up to an equivalent true strain of 2.3. These pole figures have a qualitatively different distribution from those in Fig. 8. The $\{10\bar{1}0\}$ pole figure in Fig. 16 indicates that the $\{11\bar{2}0\}$ plane aligns with the extrusion direction. This result suggests that the alignment of the $\{10\bar{1}0\}$ plane in the extrusion direction is due to lattice rotation caused by the activity of the nonbasal slip system with the $\langle 11\bar{2}0 \rangle$ slip direction.

5. Conclusions

In this study, texture development during extrusion in the magnesium alloy AZ31 was investigated by experimental observation and numerical analysis. To clarify the texture development mechanism in the magnesium alloy during extrusion the effects of each deformation mode and the reference stress ratio of the basal slip system to the nonbasal slip systems on texture development were studied by crystal plasticity analysis. Consequently, the following conclusions were obtained.

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3 566 1. The crystal plasticity analysis of equi-biaxial compression with consideration of the
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5 567 prismatic or pyramidal-1 slip system results in very similar texture development to that
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7 568 with consideration of both systems although the activity of each deformation mode
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9 569 depends on the deformation mode implemented in the calculation.
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11 570 2. Analysis without the consideration of twinning also reproduces a similar texture to
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13 571 that with the consideration of twinning. However, a comparison of the calculated
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15 572 results suggests that deformation twinning in magnesium accelerates texture
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17 573 development during extrusion.
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19
20 574 3. Calculations with smaller reference stress ratios of the basal slip system to the
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22 575 nonbasal slip systems lead to a qualitatively different texture owing to the change in
23
24 576 the activity of each deformation mode.
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26 577 4. From the comparison of a calculation using real slip systems in magnesium with a
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28 578 calculation using a virtual slip system, it is suggested that the lattice rotation caused by
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30 579 a nonbasal slip system with the $\langle 11\bar{2}0 \rangle$ slip direction is the predominant mechanism
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32 580 for the alignment of the $\{10\bar{1}0\}$ plane in the extrusion direction.
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36 582 Acknowledgements

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38
39 583 The work of T.M. was partially supported by a Grant-in-Aid for Scientific Research from
40
41 584 the Ministry of Education, Culture, Sports, Science and Technology of Japan
42
43 585 (KAKENHI: No.21760082) and the Kumamoto Prefecture Collaboration of Regional
44
45 586 Entities for the Advancement of Technological Excellence from Japan Science and
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47 587 Technology Agency.
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49 588 50 589 References

51
52
53 590 Agnew, S.R., Yoo, M.H., Tomé, C.N., 2001. Application of texture simulation to
54
55
56 591 understanding mechanical behavior of Mg and solid solution alloys containing Li or Y.
57
58 592 Acta Mater. 49, 4277-4289.
59
60
61
62
63
64
65

- 1
2
3 593 Agnew, S.R., Tomé, C.N., Brown, D.W., Holden, T.M., Vogel, S.C., 2003. Study of slip
4
5 594 mechanisms in a magnesium alloy by neutron diffraction and modeling. *Scripta Mater.*
6
7 595 48, 1003-1008.
8
9 596 Agnew, S.R., Mehrotra, P., Lillo, T.M., Stoica, G.M., Liaw, P.K., 2005. *Acta Mater.* 53,
10
11 597 3135-3146.
12
13 598 Agnew, S.R., Dreyer, C.E., Polesak, F.J., Chiu, W.V.III., Neil, C.J., Rodriguez, M., 2008.
14
15 599 Constitutive behavior of four wrought magnesium alloys under warm forming
16
17 600 conditions. *Magnesium Technol.* 2008, 159-164.
18
19 601 Akhtar, A., Teghtsoonian, E., 1969a. Solid solution strengthening of magnesium single
20
21 602 crystals-I alloying behaviour in basal slip. *Acta Metall.* 17, 1339-1349.
22
23 603 Akhtar, A., Teghtsoonian, E., 1969a. Solid solution strengthening of magnesium single
24
25 604 crystals-II the effect of solute on the ease of prismatic slip. *Acta Metall.* 17, 1351-1356.
26
27 605 Al-Samman, T., Gottstein, G., 2008. Room temperature formability of a magnesium
28
29 606 AZ31 alloy: Examining the role of texture on the deformation mechanisms. *Mater. Sci.*
30
31 607 *Eng. A* 488, 406-414.
32
33 608 Al-Samman, T., Gottstein, G., 2008. Dynamic recrystallization during high temperature
34
35 609 deformation of magnesium. *Mater. Sci. Eng. A* 490, 411-420.
36
37 610 Barnett, M.R., 2003. A Taylor model based description of the proof stress of magnesium
38
39 611 AZ31 during hot working. *Metall. Mater. Trans. A* 34, 1799-1806.
40
41 612 Barnett, M.R., Keshavarz, Z., Beer, A.G., Ma, X., 2008. Non-Schmid behaviour during
42
43 613 secondary twinning in a polycrystalline magnesium alloy. *Acta Mater.* 56, 5-15.
44
45 614 Beausir, B., Tóth, L.S., Neale, K.W., 2007. Role of strain-rate sensitivity in the crystal
46
47 615 plasticity of hexagonal structures. *Int. J. Plasticity* 23, 227-243.
48
49 616 Beausir, B., Suwas, S., Tóth, L.S., Neale, K.W., Fundenberger, J.-J., 2008. Analysis of
50
51 617 texture evolution in magnesium during equal channel angular extrusion. *Acta Mater.*
52
53 618 56, 200-214.
54
55 619 Biswas, S., Dhinwal, S.S., Suwas, S., 2010. Room-temperature equal channel angular
56
57
58
59
60
61
62
63
64
65

620 extrusion of pure magnesium. *Acta Mater.* 58, 3247-3261.
 621 Bohlen, J., Yi, S.B., Swiostek, J., Letzig, D., Brokmeier, H.G., Kainer, K.U., 2005.
 622 Microstructure and texture development during hydrostatic extrusion of magnesium
 623 alloy AZ31. *Scripta Mater.* 53, 259-264.
 624 Bohlen, J., Nürnberg, M.R., Senn, J.W., Letzig, D., Agnew, S.R., 2007. The texture and
 625 anisotropy of magnesium-zinc-rare earth alloy sheets. *Acta Mater.* 55, 2101-2112.
 626 Capolungo, L., Beyerlein, I.J., Kaschner, G.C., Tomé, C.N., 2009. On the interaction
 627 between slip dislocations and twins in HCP Zr. *Mater. Sci. Eng. A* 513-514, 42-51.
 628 Chen, B., Lin, D.-L., Jin, L., Zeng, X.-Q., Lu, C., 2008. Equal-channel angular pressing
 629 of magnesium alloy AZ91 and its effects on microstructure and mechanical properties.
 630 *Mater. Sci. Eng. A* 483-484, 113-116.
 631 Chen, Y.Q., Zhang, H., Chen, Z.H., Xian, K.F., 2008. Flow stress equation of AZ31
 632 magnesium alloy sheet during warm tensile deformation. *J. Mater. Proc. Tech.* 208,
 633 29-34.
 634 Chino, Y., Kimura, K., Hakamada, M., Mabuchi, M., 2008a. Mechanical anisotropy due
 635 to twinning in an extruded AZ31 Mg alloy. *Mater. Sci. Eng. A* 485, 311-317.
 636 Chino, Y., Kimura, K., Mabuchi, M., 2008b. Twinning behavior and deformation
 637 mechanisms of extruded AZ31 Mg alloy. *Mater. Sci. Eng. A* 486, 481-488.
 638 Christian, J.W., Mahajan, S., 1995. Deformation twinning. *Prog. Mater. Sci.* 39, 1-157.
 639 Choi, S.-H., Kim, D.H., Park, S.S., You, B.S., 2010. Simulation of stress concentration in
 640 Mg alloys using the crystal plasticity finite element method. *Acta Mater.* 58, 320-329.
 641 Duygulu, O., Agnew, S.R., 2003. The effect of temperature and strain rate on the tensile
 642 properties of textured magnesium alloy AZ31B sheet. *Magnesium Technology 2003*,
 643 237-242.
 644 Graff, S., Brocks, W., Steglich, D., 2007. Yielding of magnesium: From single crystal to
 645 polycrystalline aggregates. *Int. J. Plasticity* 23, 1957-1978.
 646 Hirano, M., Yamasaki, M., Hagihara, K., Higashida, K., Kawamura, Y., 2010. Effect of

647 extrusion parameters on mechanical properties of $Mg_{97}Zn_1Y_2$ alloys at room and
 648 elevated temperatures. *Mater. Trans.*, 51, 1640-1647.
 649 Hirsch, P.B., Lally, J.S., 1965. The deformation of magnesium single crystal. *Phil. Mag.*
 650 12, 595-648.
 651 Houtte, P.V., 1978. Simulation of the rolling and shear texture of brass by the Taylor
 652 theory adapted for mechanical twinning. *Acta Metall.* 26, 591-604.
 653 Ion, S.E., Humphreys, F.J., White, S.H., 1982. Dynamic recrystallisation and the
 654 development of microstructure during the high temperature deformation of
 655 magnesium. *Acta. Metall.* 30, 1909-1919.
 656 Kim, W.J., Kim, H.K., Kim W.Y., Han, S.W., 2008. Temperature and strain rate effect
 657 incorporated failure criteria for sheet forming of magnesium alloys. *Mater. Sci. Eng.*
 658 A488, 468-474.
 659 Lee, M.G., Kim, S.J., Wagoner, R.H., Chung, K., Kim, H.Y., 2009. Constitutive modeling
 660 for anisotropic/asymmetric hardening behavior of magnesium alloy sheets:
 661 Application to sheet springback. *Int. J. Plasticity* 25, 70-104.
 662 Li, H., Hsu, E., Szpunar, J., Utsunomiya, H., Sakai, T., 2008. Deformation mechanism
 663 and texture and microstructure evolution during high-speed rolling of AZ31B Mg
 664 sheets. *J. Mater. Sci.* 43, 7148-7156.
 665 Liang, S.J., Liu, Z.Y., Wang, E.D., 2008. Microstructure and mechanical properties of
 666 Mg-Al-Zn alloy deformed by cold extrusion. *Mater. Lett.* 62, 3051-3054.
 667 Liang, S.J., Liu, Z.Y., Wang, E.D., 2009. Simulation of extrusion process of AZ31
 668 magnesium alloy. *Mater. Sci. Eng. A* 499, 221-224.
 669 Ma, A., Jiang, J., Saito, N., Shigematsu, I., Yuan, Y., Yang, D., Nishida, Y., 2009.
 670 Improving both strength and ductility of a Mg alloy through a large number of ECAP
 671 passes. *Mater. Sci. Eng. A* 513-514, 122-127.
 672 Mabuchi, M., Higashi, K., 1996. Strengthening mechanisms of Mg-Si alloys. *Acta Mater.*
 673 44, 4611-4618.

- 674 Mayama, T., Aizawa, K., Tadano, Y., Kuroda, M., 2009. Influence of twinning
- 675 deformation and lattice rotation on strength differential effect in polycrystalline pure
- 676 magnesium with rolling texture. *Comput. Mater. Sci.* 47, 448-455.
- 677 Mayeur, J.R., McDowell, D.L., 2007. A three-dimensional crystal plasticity model for
- 678 duplex Ti-6Al-4V. *Int. J. Plasticity* 23, 1457-1485.
- 679 Miura, H., Yang, X., Sakai, T., Nogawa, H., Miura, S., Watanabe, Y., Jonas, J.J., 2005.
- 680 High temperature deformation and extended plasticity in Mg single crystals. *Phil.*
- 681 *Mag.* 85, 3553-3565.
- 682 Neil, C.J., Agnew, S.R., 2009. Crystal plasticity-based forming limit prediction for
- 683 non-cubic metals: Application to Mg alloy AZ31B. *Int. J. Plasticity* 25, 379-398.
- 684 Obara, T., Yoshinaga, H., Morozumi, S., 1973. $\{11\bar{2}2\}\langle\bar{1}\bar{1}23\rangle$ slip system in
- 685 magnesium. *Acta Metall.* 21, 845-853.
- 686 Orientation Imaging Microscopy (OIM) Software Version 5.3 User Manual, 2007.
- 687 TexSEM Laboratories (TSL).
- 688 Peirce, D., Asaro, R.J., Needleman, A., 1983. Material rate dependence and localized
- 689 deformation in crystalline solids. *Acta Metall.* 31, 1951-1976.
- 690 Proust, G., Tomé, C.N., Jain, A., Agnew, S.R., 2009. Modeling the effect of twinning and
- 691 detwinning during strain-path changes of magnesium alloy AZ31. *Int. J. Plasticity* 25,
- 692 861-880.
- 693 Read-Hill, R.E. and Robertson, W.D., 1957. Deformation of magnesium single crystals
- 694 by nonbasal slip. *Trans. Metall. Soc. AIME* 209, 496-502.
- 695 Sheely, W.F., Nash, R.R., 1960. Mechanical properties of magnesium monocrystals.
- 696 *Trans. Metall. Soc. AIME* 218, 416-423.
- 697 Shi, T., Yu, K., Li, W.-X., Wang, R.-C., Wang, X.-Y., Cai, Z.-Y., 2007. Hot-compression
- 698 constitutive relation of as-cast AZ31 magnesium alloy. *Trans. Nonferrous Met. Soc.*
- 699 *China* 17, s336-s341.
- 700 Staroselsky, A., Anand, L., 2003. A constitutive model for hcp materials deforming by

701 slip and twinning: application to magnesium alloy AZ31B. *Int. J. Plasticity* 19,
 702 1843-1864.
 703 Styczynski, A., Hartig, Ch., Bohlen, J., Letzig, D., 2004. Cold rolling textures in AZ31
 704 wrought magnesium alloy. *Scripta Mater.* 50, 943-947.
 705 Taylor G.I., 1927. The distortion of crystals of aluminum under compression. Part II. –
 706 Distortion by double slipping and changes in orientation of crystal axes during
 707 compression. *Proc. Roy. Soc. London A* 116, 16-38.
 708 Tomé, C.N., Lebensohn, R.A., Kocks, U.F., 1991. A model for texture development
 709 dominated by deformation twinning: application to zirconium alloys. *Acta Metall*
 710 *Mater.* 39, 2667-2680.
 711 Van Houtte, P., 1978. Simulation of the rolling and shear texture of brass by the Taylor
 712 theory adapted for mechanical twinning. *Acta Metall.* 26, 591-604.
 713 Wang, Y.N., Huang, J.C., 2007. The role of twinning and untwinning in yielding
 714 behavior in hot-extruded Mg-Al-Zn alloy. *Acta Mater.* 55, 897-905.
 715 Watanabe, H., Tsutsui, H., Mukai, T., Kohzu, M., Tanabe, S., Higashi, K., 2001.
 716 Deformation mechanism in a coarse-grained Mg-Al-Zn alloy at elevated temperatures.
 717 *Int. J. Plasticity* 17, 387-397.
 718 Yi, S.B., Zaefferer, S., Brokmeier, H.-G., 2006. Mechanical behaviour and
 719 microstructural evolution of magnesium alloy AZ31 in tension at different
 720 temperatures. *Mater. Sci. Eng. A* 424, 275-281.
 721 Yin, D.L., Zhang, K.F., Wang, G.F., Han, W.B., 2005. Warm deformation behavior of
 722 hot-rolled AZ31 Mg alloy. *Mater. Sci. Eng. A* 392, 320-325.
 723 Yoo, M.H., 1981. Slip, twinning, and fracture in hexagonal close-packed metals. *Metall.*
 724 *Trans. A* 12, 409-418.
 725 Yoshinaga, H., Horiuchi, R., 1963a. Deformation mechanisms in magnesium single
 726 crystals compressed in the direction parallel to hexagonal axis. *Trans. JIM* 4, 1-8.
 727 Yoshinaga, H., Horiuchi, R., 1963b. On the nonbasal slip in magnesium crystals. *Trans.*

1		
2		
3	728	JIM 5, 14-21.
4		
5	729	
6		
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3	730	Figure captions	
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5	731	Fig.1	Schematic diagrams of extrusion experiment
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7	732		(a) Schematic diagram of extrusion setup
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9	733		(b) Schematic diagram of positions of EBSD observation
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13	735	Fig.2	Inverse pole figure maps of each position indicated in Fig. 1(b)
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15	736		(a) Position A
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17	737		(b) Position B
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19	738		(c) Position C
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21	739		(d) Position D
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25	741	Fig.3	Pole figures generated from EBSD analysis
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27	742		(a) Position A
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29	743		(b) Position B
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31	744		(c) Position C
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33	745		(d) Position D
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37	747	Fig.4	Model used for macroscopic extrusion analysis
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39	748		(a) Geometry of analysis model
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41	749		(b) Geometry of billet model
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43	750		(c) Boundary condition for billet
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47	752	Fig.5	Relationship between strain components and stroke of dummy block
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49	753		(a) Position X ₁ (x = 1.62 mm)
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51	754		(b) Position X ₂ (x = 6.86 mm)
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53	755		(c) Position X ₃ (x = 14.3 mm)
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3	757	Fig.6	Deformation modes in magnesium
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7	759	Fig.7	Schematic diagram of model and boundary condition for crystal plasticity
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9	760	analysis	
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13	762	Fig.8	Pole figures after equi-biaxial compression predicted by crystal plasticity
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15	763	analysis	
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17	764	(a) ALL	
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19	765	(b) No-PRI	
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21	766	(c) No-PY1	
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23	767	(d) No-TW	
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28	769	Fig.9	Calculated texture evolution in the case of ALL
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30	770	(a) $\bar{\varepsilon}_{\text{true}} = 0.22$	
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32	771	(b) $\bar{\varepsilon}_{\text{true}} = 0.84$	
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34	772	(c) $\bar{\varepsilon}_{\text{true}} = 1.91$	
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36	773	(d) $\bar{\varepsilon}_{\text{true}} = 2.3$	
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41	775	Fig.10	Relative activity of each deformation mode
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43	776	(a) ALL	
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45	777	(b) No-PRI	
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47	778	(c) No-PY1	
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49	779	(d) No-TW	
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51	780		
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54	781	Fig.11	Effect of consideration of twinning on change in angle between c -axis and
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56	782	extrusion direction	
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58	783	(a) Definition of angle θ	
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(b) Changes in average and standard deviation of θ

Fig.12 Effect of reference stress ratio on texture after equi-biaxial compression

(a) $(\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1:1:6)$

(b) $(\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1:3:6)$

(c) $(\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1:5:6)$

(d) $(\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1:6:6)$

Fig.13 Relative activity of each deformation mode

(a) $(\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1:1:6)$

(b) $(\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1:3:6)$

(c) $(\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1:5:6)$

(d) $(\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1:6:6)$

Fig.14 Lattice rotation caused by activation of basal and pyramidal-2 slip systems

Fig.15 Lattice rotation around c -axis

(a) Definition of angle ϕ

(b) Relationship between Schmid factors of each slip system and angle ϕ

(c) Lattice rotation caused by activation of the prismatic slip system

(d) Lattice rotation caused by activation of the virtual $\{11\bar{2}0\}\langle 10\bar{1}0 \rangle$ slip system

Fig.16 Texture after equi-biaxial compression considering virtual $\{11\bar{2}0\}\langle 10\bar{1}0 \rangle$ slip system instead of prismatic slip system

Fig.1 Schematic diagrams of extrusion experiment
(a) Schematic diagram of extrusion setup
(b) Schematic diagram of positions of EBSD observations

Fig.2 Inverse pole figure maps of each position indicated in Fig. 1(b)

(a) Position A
(c) Position C

(b) Position B
(d) Position D

Fig.3 Pole figures generated from EBSD analysis

(a) Position A
(c) Position C

(b) Position B
(d) Position D

Fig.4 Model used for macroscopic extrusion analysis

- (a) Geometry of analysis model
- (b) Geometry of billet model
- (c) Boundary condition for billet

Fig.5 Relationship between strain components and stroke of dummy block
 (a) Position X_1 ($x = 1.62$ mm) , (b) Position X_2 ($x = 6.86$ mm),
 (c) Position X_3 ($x = 14.3$ mm)

Fig.6 Deformation modes in magnesium

Fig.7 Schematic diagram of model and boundary condition for crystal plasticity analysis

Fig.8 Pole figures after equi-biaxial compression predicted by crystal plasticity analysis

(a) ALL, (b) No-PRI, (c) No-PY1, (d) No-TW

Fig.9 Calculated texture evolution in the case of ALL

(a) $\bar{\epsilon}_{\text{true}} = 0.22$ (b) $\bar{\epsilon}_{\text{true}} = 0.84$
(c) $\bar{\epsilon}_{\text{true}} = 1.91$ (d) $\bar{\epsilon}_{\text{true}} = 2.3$

Fig.10 Relative activity of each deformation mode

- (a) ALL
- (b) No-PRI
- (c) No-PY1
- (d) No-TW

a **b**

Fig.11 Effect of consideration of twinning on change in angle between c -axis and extrusion direction

(a) Definition of angle θ

(b) Changes in average and standard deviation of θ

Fig.12 Effect of reference stress ratio on texture after equi-biaxial compression

(a) $(\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1 : 1 : 6)$ (b) $(\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1 : 3 : 6)$
(c) $(\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1 : 5 : 6)$ (d) $(\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1 : 6 : 6)$

Fig.13 Relative activity of each deformation mode

$$\begin{aligned}
 \text{(a)} \quad & (\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1:1:6) & \text{(b)} \quad & (\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1:3:6) \\
 \text{(c)} \quad & (\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1:5:6) & \text{(d)} \quad & (\tau_{\text{basal}} : \tau_{\text{non-basal}} : \tau_{\text{twin}}) = (1:6:6)
 \end{aligned}$$

Fig.14 Lattice rotation caused by activation of basal and pyramidal-2 slip systems

Fig.15 Lattice rotation around c -axis

- (a) Definition of angle ϕ
- (b) Relationship between Schmid factors of each slip system and angle ϕ
- (c) Lattice rotation caused by activation of the prismatic slip system
- (d) Lattice rotation caused by activation of virtual $\{11\bar{2}0\}\langle 10\bar{1}0\rangle$ slip system

Fig.16 Texture after equi-biaxial compression considering $\{11\bar{2}0\}\langle 10\bar{1}0\rangle$ slip system instead of prismatic slip system

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Table 1 Deformation at each position in SEM/EBSD observation

Position	Distance	Corresponding	Equivalent true strain
	z [mm]	extrusion ratio, R_e	$\bar{\epsilon}_{\text{true}} = \ln R_e$
A	1.7	1.24	0.22
B	8.5	2.3	0.84
C	15.3	6.76	1.91
D	extruded	10	2.30

2

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Table 2 Material parameters used in finite element analysis of extrusion

E [GPa]	ν	F [GPa]	σ_y [MPa]	ρ [kg/m ³]	μ
45	0.35	0.01	50	1740	0.001

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Table 3 Definitions of deformation modes in magnesium

Slip system	Basal	Prismatic	Pyramidal-1	Pyramidal-2	Twinning
Slip plane	(0001)	$\{10\bar{1}0\}$	$\{10\bar{1}1\}$	$\{11\bar{2}2\}$	$\{10\bar{1}2\}$
Slip direction	$\langle 11\bar{2}0 \rangle$	$\langle 11\bar{2}0 \rangle$	$\langle 11\bar{2}0 \rangle$	$\langle 11\bar{2}3 \rangle$	$\langle 10\bar{1}1 \rangle$

7 Table 4 Reference stresses $g^{(\alpha)}$ used for the calculations in section 4.1 (MPa)

Name	Basal	Prismatic	Pyramidal-1	Pyramidal-2	Twinning
ALL	5	32.01	32.01	26.81	32
No-PRI	5	∞	32.01	26.81	32
No-PY1	5	32.01	∞	26.81	32
No-TW	5	∞	32.01	26.81	∞

9 Table 5 Reference stresses $g^{(\alpha)}$ used for the calculation in section 4.2 (MPa)

Reference stress ratio	Basal τ_{basal}	Prismatic $\tau_{\text{non-basal}}$	Pyramidal-1 $\tau_{\text{non-basal}}$	Pyramidal-2 $\tau_{\text{non-basal}}$	Twinning τ_{twin}
1 : 1 : 1	5	5	5	5	30
1 : 3 : 6	5	15	15	15	30
1 : 5 : 6	5	25	25	25	30
1 : 6 : 6	5	30	30	30	30

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Table 6 Axis of lattice rotation when spin tensor $\mathbf{W}$ is ignored				
Slip system	Basal	Prismatic	Pyramidal-1	Pyramidal-2
Axis of lattice rotation	$\langle 10\bar{1}0 \rangle$	$[0001]$	$\langle 10\bar{1}2 \rangle$	$\langle 10\bar{1}0 \rangle$

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