Mesoscale Modeling and Validation of Texture Evolution during Asymmetric Rolling and Static Recrystallization of Magnesium Alloy AZ31B

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The focus of the present research is to develop an integrated deformation and recrystallization model for magnesium alloys at the microstructural length scale. It is known that in magnesium alloys nucleation of recrystallized grains occurs at various microstructural inhomogeneities such as twins and localized deformation bands. However, models need to be developed that can predict the evolution of the grain structure and texture developed during recrystallization and grain growth, especially when the deformation process follows a complicated deformation path such as in asymmetric rolling. The deformation model is based on a crystal plasticity approach implemented at the length scale of the microstructure that includes deformation mechanisms based on dislocation slip and twinning. The recrystallization simulation is based on a Monte Carlo technique that operates on the output of the deformation simulations. The nucleation criterion during recrystallization is based on the local stored energy, and the Monte Carlo technique is used to simulate the growth of the nuclei resulting from local stored energy differences and curvature. The model predictions are compared with experimental data obtained through electron backscatter analysis and neutron diffraction.

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I. INTRODUCTION

WROUGHT magnesium alloys have limited room-temperature (RT) ductility that is closely related to the crystallographic texture that develops during plastic deformation.^[1] For example, during rolling or extrusion, a strong basal texture develops that severely reduces the available deformation modes by slip or twinning. Considerable effort has been made to increase the RT ductility of wrought magnesium alloys by inducing the formation of nonbasal texture components during thermomechanical processing. One set of approaches is based on alloying that induces deformation banding^[2] or particle-stimulated nucleation,^[3] resulting in significant weakening of the basal texture component. Another approach involves designing deformation paths and annealing sequences that weaken the basal texture^[4–6]

such as asymmetric rolling, cyclic extrusion, and compression and electropulsing.

The texture that develops during asymmetric rolling of wrought magnesium alloys is influenced by several variables, including rolling temperature, speed, compression to shear ratio, and the plastic strain. Texture can also be influenced significantly by the components that nucleate and grow during static/dynamic recrystallization that occurs under a given deformation path. Even though micromechanical models that can predict the texture evolution through dislocation slip and twinning during large plastic deformation in magnesium alloys have been under development for a while,^[7–9] microstructural length scale models that can predict the texture evolution under the combined influence of deformation and recrystallization in these alloys are not well developed. The focus of this effort is to develop a coupled deformation and recrystallization model for a wrought magnesium alloy and to validate the model using experimental data. Specifically, the effort involved the investigation of static recrystallization of the magnesium alloy AZ31 using *in situ* neutron diffraction.

The computational approach is based on an extension of previous work by the authors in predicting the texture evolution during thermomechanical processing of aluminum alloys and steels using a coupled deformation and annealing simulation approach.^[10–15] In these models, a crystal plasticity-based approach was used to model the inhomogeneous deformation at the microstructural length scale. The deformation model captured the heterogeneity of the stored energy at various microstructural locations such as grain boundaries,

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triple lines, particle deformation zones, *etc.* A nucleation model based on orientation dependent recovery of the deformation substructure was used along with the deformation data to simulate the nucleation process during recrystallization. The growth of the nuclei in the deformation substructure was simulated using a Monte Carlo (MC) technique assuming misorientation-dependent grain boundary energy and mobility. A kinetic MC scheme was used to model the simultaneous evolution of the structure resulting from both recrystallization and grain growth. The simulations could predict the evolution of cube texture during recrystallization of aluminum alloys and the strengthening of the $\{111\}\langle 112 \rangle$ orientations during recrystallization of iron. In the previous models, large plastic strain was modeled using dislocation slip as the only deformation mechanism. Although this is true for the deformation of many face-centered cubic and base-centered cubic and polycrystals, twinning is a significant deformation mode in hexagonal close-packed polycrystals such as magnesium. The following section describes the crystal plasticity approach that was used to model deformation by slip and twinning.

II. COMPUTATIONAL APPROACH

Simulations of deformation were carried out using the “neighborhood compliance” (NC) model,^[16] which takes into account the influence of the local neighborhood on the deformation of each grain in the microstructure. The constitutive response of the material was modeled using crystal plasticity, and in addition to crystallographic slip, twinning was included in the model as an additional mode of deformation. Neglecting elastic deformations, it is assumed that plastic deformation is accommodated by shear on appropriate slip and twin systems, followed by a rigid rotation of the crystal, which is modeled using the following multiplicative decomposition of the crystal deformation gradient F_c :

$$F_c = R^* F^p \quad [1]$$

where F^p is the deformation gradient caused by shear along the slip and twin systems, and R^* is the rigid rotation of the crystal lattice. When written in rate form, this leads to the following additive decomposition of the crystal velocity gradient L_c :

$$L_c = \dot{F}_c F_c^{-1} = \dot{R}^* R^{*T} + L^p \quad [2]$$

The plastic part of the velocity gradient L^p is given by a linear combination of the shear rates on the various slip and twin systems, which is expressed as follows:

$$L^p = \sum_{\alpha} \dot{\gamma}^{\alpha} (s^{\alpha} \otimes m^{\alpha}) \quad [3]$$

where $\dot{\gamma}^{\alpha}$ is the rate of shear on slip or twin system α , which has a normal m^{α} and a shear direction s^{α} . The velocity gradient L_c can be separated into symmetric and skew-symmetric portions, which can be written as follows in terms of the symmetric and skew-symmetric parts of the Schmid tensor $T^{\alpha} = s^{\alpha} \otimes m^{\alpha}$:

$$D_c = \sum_{\alpha} \dot{\gamma}^{\alpha} P^{\alpha} \quad [4]$$

$$W_c = \dot{R}^* R^{*T} + \sum_{\alpha} \dot{\gamma}^{\alpha} Q^{\alpha} \quad [5]$$

Assuming rate-dependent material response, the shear rate on each slip plane is expressed as follows in terms of the resolved shear stress on that plane:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \left| \frac{\tau^{\alpha}}{\tau_0^{\alpha}} \right|^{1/m} \text{sign}(\tau^{\alpha}) \quad [6]$$

where τ^{α} is the resolved shear stress, τ_0^{α} is the resistance to slip, and $\dot{\gamma}_0^{\alpha}$ is a reference rate of shear. For twin systems, the rate of shear is computed in a similar fashion, with the added condition that the rate of shear is nonzero only for a positive value of τ^{α} . The resolved shear stress is computed from the crystal deviatoric stress as follows:

$$\tau^{\alpha} = \sigma'_c \cdot P^{\alpha} \quad [7]$$

where P^{α} is the symmetric portion of the Schmid tensor T^{α} . By combining Eqs. [4], [6], and [7], and eliminating $\dot{\gamma}^{\alpha}$, the following expression relating the crystal deformation rate and deviatoric stress can be obtained:

$$D_c = \left[\sum_{\alpha} \frac{\dot{\gamma}_0^{\alpha}}{\tau_0^{\alpha}} \left| \frac{\tau^{\alpha}}{\tau_0^{\alpha}} \right|^{\frac{1}{m}-1} P^{\alpha} \otimes P^{\alpha} \right] : \sigma'_c \quad [8]$$

If the deformation rate of the crystal is known, Eq. [8] can be used to compute the crystal deviatoric stress using an iterative procedure, because the resolved shear stress depends on the unknown crystal deviatoric stress through Eq. [7].

The increase in the slip and twin system resistance with continued plastic deformation is modeled using the following evolution law:

$$\dot{\tau}_0^{\alpha} = h_0 \left(1 - \frac{\tau_0^{\alpha}}{\tau_{sat}} \right)^a (\sum_{\beta} |\dot{\gamma}^{\beta}|) \quad [9]$$

and the reorientation of the crystal lattice is modeled as follows, by computing the rate of rotation based on Eq. [5]:

$$\dot{R}^* = (W_c - \sum_{\alpha} \dot{\gamma}^{\alpha} Q^{\alpha}) R^* \quad [10]$$

The inclusion of twinning was modeled following the approach described in Choi *et al.*^[17] using the predominant twin reorientation (PTR) scheme, originally developed by Tome *et al.*^[7] For each twin system in each orientation, the corresponding twin volume fraction is computed as follows:

$$f^t = \gamma^t / S^t \quad [11]$$

where S^t is the characteristic twin shear on that twin system. The accumulated twin fraction in each orientation is obtained as follows by adding the twin volume fractions over all twin systems:

$$f^{\text{acc}} = \sum_t f^t \quad [12]$$

If the accumulated twin fraction f^{acc} in any orientation exceeds a threshold twin volume fraction f^{th} , as shown in the following equation:

$$f^{\text{th}} = C_1^{\text{th}} + C_2^{\text{th}} f^{\text{acc}} \quad [13]$$

then that orientation is allowed to reorient to a new orientation given by the twin system that has the maximum volume fraction f^t . Under this scheme, the reorientation caused by twinning does not occur until the volume fraction exceeds a threshold value of C_1^{th} , and because f^{acc} increases with continued plastic deformation, the threshold value also increases with strain. Even though more than one twin system may be active in accommodating the deformation, the PTR model assumes that reorientation of the crystal is governed by the dominant twin variant. The reorientation is given by a 180 deg rotation around the twin plane normal.

The simulation procedure described earlier was used to model the deformation under asymmetric rolling conditions. The resulting deformation substructure was used as input to a MC method to simulate the static recrystallization during subsequent annealing of the deformed material. In addition to the orientations in the deformed microstructure, the MC method requires the stored energy of deformation as input. The stored energy was computed from the deformation model as follows:

$$H = 2(\sigma^2 - \sigma_0^2)/G \quad [14]$$

where σ and σ_0 are the effective stress values at the end and start of the deformation, respectively. For orientations that undergo rotation caused by twinning, the value of σ_0 was reset to the current value of σ .

The MC simulation technique involves mapping the deformation structure into a regular cubic lattice where at each lattice point the local crystallographic orientation and the stored energy of deformation are known. Because the current deformation model does not account for shape change caused by deformation, the output of the deformation simulations could be readily used for the MC simulations. In MC simulations, the total system energy is defined as follows:

$$E = \frac{1}{2} \sum_i \sum_j^{NN} J(S_i S_j) (1 - \delta_{S_i S_j}) + \sum_i H_i \quad [15]$$

where J is interface energy that depends on the orientations S_i and S_j on either side of the interface, H_i is the stored energy at site i and the energies are summed over all the sites and interfaces in the system. The nucleation model is based on a probability that depends on the stored energy of the site. In the current simulations, it is assumed that sites with the highest stored energy will have the highest probability for nucleation. All sites that are declared nuclei are re-assigned zero stored energy. The MC technique involves visiting the lattice in a random fashion and calculating the energy change resulting from an attempted non-conservative flip. The flip is then executed with a probability given by the following equation:

$$p(S_i, S_j, \Delta E, T) = \begin{cases} \exp\left(\frac{-Q}{RT}\right) \frac{\mu\gamma}{\mu_{\text{max}}\gamma_{\text{max}}} & \Delta E \leq 0 \\ \exp\left(\frac{-Q}{RT}\right) \frac{\mu\gamma}{\mu_{\text{max}}\gamma_{\text{max}}} \exp\left(\frac{-\Delta E}{RT}\right) & \Delta E > 0 \end{cases} \quad [16]$$

where μ is the boundary mobility and γ is the boundary energy that depends on the misorientation. The relative frequency of flips associated with recrystallization and grain growth is calculated based on the respective

Fig. 1—Sample geometry (left) and the position (right) of the detector banks.

driving forces. Time in MC simulations is expressed in terms of the MC step (MCS), which is the time associated with one attempted flip for each site in the domain. It can be related to real time, and the MC size can be related to a real size. However, such a correlation was not performed in this study because the main focus was on predicting the texture evolution.

III. EXPERIMENTAL PROCEDURE

The model alloy used in the current investigations was the commercial alloy AZ31 with a nominal composition of Mg-3wt pct Al-1wt pct Zn. The as-received material was in the form of an extruded plate with a dominant basal texture ($\langle 0001 \rangle \parallel$ Normal Direction, ND). Asymmetric rolling was carried out using rolls of unequal size rotating with the same rotational speed. The roll diameters were 75 cm and 225 cm with a roll ratio of 3.0. The sample was heated to 408 K (135 °C) in a tube furnace and rolled immediately (<5 seconds) with the rolls initially at ambient temperature. The total deformation was a 20 pct reduction in height. One unique feature of the present research is the use of neutron diffraction to follow the texture changes in the sample during annealing. The *in situ* time-of-flight neutron experiment was carried out using VULCAN,^[18,19] the engineering materials diffractometer at the Spallation Neutron Source,^[20] Oak Ridge National Laboratory (Oak Ridge, TN). The measurements were made in high-resolution (HR) mode, with the chopper running at 30 Hz, with the central wavelength $\lambda = 2.4 \text{ \AA}$ and the bandwidth $\Delta\lambda = 2.88 \text{ \AA}$. The neutron incident beam of

$5 \times 10 \text{ mm}$ reaches the sample positioned with the rolling direction (RD) (or transverse direction, TD) horizontally, with the samples surface at 45° relative to the incident beam. The diffracted intensities were recorded with two scintillation detectors banks, placed at $\pm 90^\circ$ diffraction angles, respectively. Therefore, Bank 1 records the diffracted intensities for the reflecting planes perpendicular to RD (or TD), and Bank 2 records the reflecting planes perpendicular to ND. The sample mounted inside a vacuum chamber is first measured at RT, and then during the *in situ* annealing up to 623 K (350 °C), with a heating rate ranging from 30 °C to 50 °C/min. To assess the texture evolution and to determine the texture components, the samples were rotated around the vertical axis before annealing, and during annealing at maximum temperature (*i.e.*, the rotation encompassed tilting angles Ψ in the range from 0 deg to 180 deg). The positioning of the sample with respect to the neutron beam and the location of the detector banks are shown schematically in Figure 1. The tilting of the sample is shown schematically in Figure 2.

The instrument calibrations were performed with a vanadium rod and Si powder and diamond powder loaded in a vanadium can. The diffraction data were analyzed using the Generalized Structure and Analysis Software (GSAS). The single-peak fittings provided the temporal variations of the neutron peak intensities and the peak broadening during *in situ* annealing. One sample, AZ31-P3, asymmetrically rolled 20 pct at 408 K (135 °C), with dimensions of 12 mm $\times$ 8 mm $\times$ 1.43 mm, was first measured at RT for different tilting angles Ψ in 5° steps. Two samples were subjected to the following identical three-step procedure within the limits of experimental error: (1) *in situ* diffraction during heating from RT up to 623 K (350 °C), (2) the grain orientation measurement during isothermal annealing at 623 K (350 °C), and (3) the *in situ* diffraction during cooling. The on-heating and on-cooling data were recorded for the first sample for (1) $\Psi = 0^\circ$ and $\Psi = 90^\circ$ (which correspond to the RD and ND directions), and for the second sample for (2) $\Psi = 25^\circ$ and $\Psi = 115^\circ$ (which correspond to 25 deg off RD and ND, respectively). The texture measurement for the first sample encompassed a range of 0° to 45° in Ψ , whereas a range of 45° to 90° in Ψ was used for the second sample. A similar approach was used to monitor another sample mounted with the transversal direction (TD) in the horizontal plane ($\Psi = 0^\circ$). Additionally, *ex situ* X-ray diffraction was used to characterize the textures of the samples before and after annealing.

Fig. 2—Schematic showing the specimen rotation (tilt, Ψ) used in the neutron experiments.

Table I. Materials Parameters Used for the Deformation Model

Mode	System	τ_0^z (MPa)	h_0 (MPa)	τ_{sat} (MPa)	a
Basal $\langle a \rangle$	$\{0001\}\langle 2\text{-}1\text{-}10 \rangle$	25	100	70	1.1
Prism $\langle a \rangle$	$\{10\text{-}10\}\langle \text{-}12\text{-}10 \rangle$	68	130	210	0.8
Pyramidal $\langle a \rangle$	$\{\text{-}10\text{-}11\}\langle \text{-}12\text{-}10 \rangle$	68	130	210	0.8
Pyramidal $\langle c + a \rangle$	$\{11\text{-}22\}\langle \text{-}1\text{-}123 \rangle$	68	130	210	0.8
Tension twin	$\{10\text{-}12\}\langle \text{-}1011 \rangle$	80	50	100	1.1
Compression twin	$\{10\text{-}11\}\langle 10\text{-}1\text{-}2 \rangle$	240	50	300	1.1

Fig. 3—Variation of integral intensity with heating time (temperature) for tilt angles of $\Psi = 0$ deg and $\Psi = 25$ deg (relative to RD) and $\Psi = 90$ deg and $\Psi = 115$ deg (relative to ND). The heating profile is superimposed (green line).

Fig. 4—Diffracted intensity profiles vs tilting angles for various (hkl) reflections: (a) black lines—at RT (before heating) and (b) red lines—at the peak temperature of 623 K (350 °C). Note: The scan at 623 K (350 °C) started after 35 min from the beginning of heating.

IV. COMPUTATIONS

The coupled crystal plasticity–MC code was used to model the evolution of microstructure and texture during static recrystallization after deformation typical of shear rolling. The through-thickness gradients in the actual shear rolling process were neglected, and the deformation process step was simplified as a plane strain compression + shear deformation path with a total reduction in thickness of 20 pct. The initial microstructure and texture used in the simulations were closely matched to the grain morphology and texture in the experimental sample using a microstructural mapping technique. Table I lists the material parameters used for the simulation of shear rolling, where the values for the slip systems and the tension twin systems were taken from Reference 17, whereas the slip system strength values for the compression twin systems were taken to be proportionately higher than the corresponding values for the tension twins. The values of C_1^{th} and C_2^{th} were taken to be 0.25 and 0.5, respectively,^[17] and the shear modulus for magnesium was assumed to be 17 GPa.

V. RESULTS

The integral intensity of three diffraction peaks, (0002), (11 $\bar{2}$ 0), and (10 $\bar{1}$ 1), during continuous heating and cooling are shown in Figures 3(a) and (b). Both plots include the thermal history of the *in situ* measurement (green) that shows a central gap corresponding to the period of time during which the texture measurements were made. For comparison, the integral intensity was normalized to the initial value for each type of diffraction peak. As the initial texture shows a preferential orientation of basal poles along ND, the intensity variation of the (0002) peak comes from grains close to ND direction ($\Psi = 90$ deg, Figure 3(a)) or 25 deg off ($\Psi = 115$ deg, Figure 3(b)), whereas the other two

peaks belongs to grains aligned close to RD direction ($\Psi = 0$ deg, Figure 3(a)) or 25 deg off ($\Psi = 25$ deg, Figure 3(b)). The intensity changes observed in Figure 3(a) are reversible, as they are mainly induced by the variation of the Debye–Waller factor with temperature. This behavior was confirmed by the measurements on the sample aligned with the TD direction in the horizontal plane. Figure 3(a) shows that only a minor redistribution of the diffracted intensities occurs resulting from annealing. However, a careful examination of Figure 3(b) shows that a significant reduction of the (0002) peak occurs at this tilt angle. Figures 4(a) through (d) show a comparison of the diffracted intensity as a function of the specimen tilt in the as-deformed condition and the annealed condition after reaching a peak temperature of 623 K (350 °C). Because no significant change is noted in the peak intensities during the time taken for texture measurements shown in Figure 3, it can be assumed that the data shown in Figure 4 is essentially isochronal. Four diffraction peaks were selected for these plots, including those presented in Figure 3. A significant asymmetry can be observed in the initial texture, which is presumably caused by shearing. The asymmetry in the (00.2) intensity continues to exist after recrystallization with a slight shift to the left, although the peak intensity reduces slightly. A similar shift is also observed for (10.1) and (11.0) peaks.

The overall texture of the sample in the as-deformed condition and after the recrystallization anneal at 623 K (350 °C) was measured using X-ray diffraction, and the results are shown in Figure 5. The X-ray results also show that the (00.2) texture intensity decreases at the center and shows a wider spread in the annealed condition compared with the deformed condition. A similar trend is also observed in the other pole figures. The neutron diffraction measurements shown in Figure 4 roughly correspond to a subset of the intensities from the X-ray pole figures given in Figure 5, along a vertical line through the center of the pole figures that

Fig. 5—Deformation and annealing textures for AZ31-P3 obtained using X-ray diffraction.

corresponds to a 0 deg to 180 deg rotation about the TD, and therefore, they do not show the significant reductions in the intensities along the RD observed in the X-ray pole figures. However, an overall consistency exists in the variation of the texture components as measured by X-ray diffraction and by neutron diffraction along the RD.

Figure 6 shows the texture in the experimental sample prior to deformation and the texture in the computational domain obtained by mapping the experimental texture. The mapping procedure provides a reasonable agreement between the texture in the experimental sample prior to asymmetric rolling and the input texture used for the deformation simulations. Orientation imaging microscopy of the experimental sample shows fairly equiaxed grains, and such morphology was also used in the mapped grain structure. Because the friction conditions between the roll and the AZ31 sheet were not known, the deformation simulations using the crystal plasticity model were carried out using increasing levels of shear. However, as the shear to compression ratio was increased beyond 1.0, the deformation texture

showed a spread along TD in agreement with other experimental observations.^[21] Based on the fact that the measured deformation texture shown in Figure 5 indicates a largely RD spread, it was assumed that the maximum operating shear in the rolling experiments did not exceed a shear ratio of 1.0. Figure 7 shows the deformation and recrystallization textures obtained from simulations. Figure 8 shows the computed (0002) intensity at a tilt angle of $\Psi = 25$ deg as a function of the simulation time. The simulations match the trend in the (0002) intensity measured in the *in situ* annealing experiments shown in Figure 3(b).

VI. DISCUSSION

By comparing experimental textures with simulated textures shown in Figures 5 and 7 respectively, we observe a good qualitative agreement between the two. The recrystallization simulations capture the general weakening of the deformation texture components during static recrystallization. The weakening is particularly noticeable for the (0002) intensity that may be beneficial for RT ductility. Comparing Figures 3(b) and 8, shows that the simulations capture the weakening of the (0002) component as a function of simulation time, qualitatively consistent with the *in situ* annealing data. However, some significant differences are noted between the experimental and modeling data. The computed deformation textures are stronger than the experimental textures, especially for the (0002) pole figures, because we have neglected the gradient in the compression:shear ratio that exists in asymmetric rolling as a function of the specimen depth. The choice of material parameters, with higher critical resolved shear stresses for the twin systems compared with the slip systems, meant that the deformation was accommodated predominantly by slip. This was verified by examining the overall activity of the

Fig. 6—(0002) pole figures showing the comparison between the (a) experimentally measured texture in the sample before rolling and (b) the texture obtained from mapping to the computational domain used in the mesoscale modeling.

Fig. 7—Deformation and recrystallization textures obtained by the mesoscale model, for compression to shear ratio of 1.0.

Fig. 8—Variation of (0002) intensity at $\Psi = 25$ deg as function of simulation time during recrystallization.

different types of slip and twin systems, and it was found that deformation occurred mainly by slip on the basal $\langle a \rangle$ and pyramidal $\langle c + a \rangle$ systems. Future work is needed to investigate the effect of changing the relative activity of the pyramidal $\langle c + a \rangle$ and the compression twin systems on the deformation and recrystallization textures. The present model is also a simplification of the intragranular nature of twinning that occurs in real microstructures. Detailed microscopy investigations of twinning and the role that twins play in the nucleation of the recrystallized grains suggest that the twins essentially act as linear features that block dislocation activity in the direction perpendicular to the twin thickness. As a result, high stored energies and localized matrix rotations occur in the vicinity of the twins or twin intersections that act as potential nucleation sites for the recrystallized grains. However, in the current simulations, the relative growth kinetics associated with twin growth and twin thickening are not captured accurately. Therefore, the twin morphology that develops is not realistic. However, the twin volumes do provide heterogeneous nucleation sites through the formation of the twin-matrix interfaces. Also, the partitioning of the strain between the matrix and a hard twin region is not captured accurately in the neighborhood compliance model. Nevertheless, the model reasonably captures the evolution of the recrystallization texture. Future work will focus on the use of large-scale finite element calculations based on the crystal plasticity approach that can handle the strain partitioning more accurately. Also, the probabilistic twin nucleation and growth models developed recently^[9] will be used to realistically evolve the twin nucleation and growth morphology during deformation.

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