Material testing of magnesium alloy AZ31B using a finite element polycrystal method based on a rate independent crystal plasticity model

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Abstract

Magnesium and its alloys are attractive structural light materials because they have a high specific strength and high specific stiffness. That is why their usage in high performance automotive and aerospace applications has been increased. However, their high anisotropy and low ductility could bring to forming failure, to avoid these a better accuracy for metal forming simulation is required. The identification of macroscopic parameters is expensive due to the experiments needed to find them, the use of multi-scale approach allows to find parameters for the model through easier experiments. A finite element polycrystal method, based on a rate independent polycrystal plasticity model, is implemented in order to perform the material testing of a cast magnesium alloy AZ31B. The parameters of the model are adjusted to better fit the experimental data through a trial and error process.

1 Introduction and Deformation texture model

Tension-compression asymmetry of mechanical properties of textured magnesium alloys is one specific phenomenon, which should be taken into account on designing the machine components. In this paper, the study of the behaviour of a cast alloy of the magnesium alloy AZ31B when undergoes simple tension and compression tests is conducted. The importance of texture in magnesium and its alloys has been proved by many researchers, the study of constitutive model that could predict the evolution of magnesium with a random texture is important in order to perform a numerical rolling to numerically calculate the evolution of the texture without conducting expensive experiments on rolled sheet to evaluate it. The active deformation systems considered are the basal, prismatic and pyramidal II slip systems and the tensile twinning. To identify the rate-independent slip/twin systems and to determine the plastic strain, a numerical scheme called successive integration method has been adopted. To evaluate the accuracy of this constitutive model in predicting the stress response in a magnesium alloy at room temperature, the numerical predictions and the literature data are compared.

The influences of microstructural parameters on macroscopic mechanical properties are investigated. In particular, expression of latent hardening, work-hardening, CRSS values are investigated, to better fit our predictions with the experimental data.
2 Finite element polycrystal model

2.1 Successive integration scheme

To simulate the deformation of the texture a rate independent crystal plasticity model (RICP) has been applied in this study, thus the stress-strain relation is described as:

$$\dot{\sigma}_{ij} = C_{ijkl}^{e} \dot{\epsilon}_{ij}^{p}$$  (1)

Where $C_{ijkl}^{e}$ is the elastic constitutive tensor, $\dot{\epsilon}_{ij}^{p}$ is the elastic strain increment that is calculated in this way:

$$\dot{\epsilon}_{ij}^{p} = \dot{\epsilon}_{ij} - \dot{\epsilon}_{ij}^{p'}$$  (2)

where $\dot{\epsilon}_{ij}$ can be transformed from the macroscopic strain increment, and plastic part $\dot{\epsilon}_{ij}^{p'}$ is calculated using the successive integration method[1], which can be expressed as following: We call $\tau^{s}$ the resolved shear stress on the $s^{th}$ slip/twin system:

$$\tau^{s} = L_{ij}^{s} \sigma_{ij}$$  (3)

where:

$$L_{ij} = (a_{i}b_{j} + a_{j}b_{j})/2$$  (4)

and $a$ and $b$ are respectively the unit vector normal on a slip/twin system and the unit vector parallel to the slip/twinning both in a deformed configuration. The conditions for judging the activity of a given slip/twinning system are as follow. When we have $\text{sign}(\tau^{s}) \dot{\gamma}^{s} > 0$ the slip system is active, when we have $\text{sign}(\tau^{s}) \dot{\gamma}^{s} < k^{s}$ it means that the slip system is inactive. Where $\dot{\gamma}^{s}$ is the shear strain increment on the $s^{th}$ deformation system, $k^{s}$ is the critical yielding stress of that slip/twinning system.

Due to the directionality of the twinning, to consider whether the twin occurs or not the condition that the shear stress along it must be positive ($\tau^{s} > 0$) needs to be applied. For all the systems the following differential equations are used:

$$2G (dX^{s}/d\rho) = Y^{s},$$  (5)

where $\rho(\geq 0)$ is a monotonously increasing parameter such as time, $G$ is the shear modulus and

$$X^{s} = \text{sign}(\tau^{s}) \dot{\gamma}^{s},$$  (6)

$$Y^{s} = \text{sign}(\tau^{s}) \tau^{s} - k^{s}.$$  (7)

The above equations are successively integrated under the following conditions: $X_{r} = 0$ at $\rho = 0$ and when the value of $X_{r}$ becomes negative during the integration, set $X_{r} = 0$. Continue the above integration until all $X_{r}$ remain unchanged. After obtaining $dX_{r}$ we get $\dot{\gamma}^{r}$

$$\dot{\gamma}^{r}_{\rho + d\rho} = \dot{\gamma}^{r}_{\rho} + d\dot{\gamma}^{r}.$$  (8)

Then the plastic strain in a crystal is calculated as follows:

$$\dot{\epsilon}_{ij} = (1 - \sum_{\beta=1}^{N_{\text{tw}}} s^{n_{\beta}}) \sum_{a=1}^{N^{s}} \dot{\gamma}^{a} L_{a}^{s} + \sum_{\beta=1}^{N_{\text{tw}}} s^{n_{\beta}} \dot{\gamma}^{\beta}_{\text{tw}} L_{\text{tw}}^{\beta},$$  (9)

where $\sum_{\beta=1}^{N_{\text{tw}}} s^{n_{\beta}}$ is the total volume fraction of deformation twinned region in the grain, $\dot{\gamma}^{a}$ and $\dot{\gamma}^{\beta}_{\text{tw}}$ denote the shear strain increment on slip system $a$ and twinning system $\beta$, respectively, $N^{s}$ and $N_{\text{tw}}$ represent the number of potentially active slip and twinning systems and $L$ defines the tensorial direction of the shear caused by an active deformation system.

This algorithm has been implemented where a single cubic element composed by 5 tetrahedral elements is used to simulate the single crystal of the magnesium alloy AZ31B.
2.2 Hardening model

The strain hardening can be described by the sum of the self hardening and latent hardening that is caused by the interaction among different slip/twin systems. The change of the critical resolved stress on the \( s^{th} \) slip/system is described by:

\[
\dot{\tau}_s = \sum_t h_{st} |\dot{\gamma}_t|, \tag{10}
\]

with

\[
h_{st} = h(\bar{\gamma}) q_{st}, \tag{11}
\]

where \( h_{st} \) is the hardening coefficient and \( q_{st} \) is the interaction matrix describing the self and latent hardening.

To reproduce the complex mechanical response of the single crystal magnesium, the following hardening laws are used:

- Linear hardening:
  \[
h(\bar{\gamma}) = h_0, \quad \bar{\gamma} = \sum_\alpha \int_0^t |\dot{\gamma}_\alpha| d\tau, \tag{12}
\]
  where \( h_0 \) is a constant and \( \bar{\gamma} \) is the equivalent shear strain, which is the sum of shear strains in all the slip/twin systems. The linear hardening has been used just to describe the twin hardening paired with the twin scheme.

- Voce hardening ([2],[3]):
  \[
h(\bar{\gamma}) = h_0 (1 - \frac{\tau_0}{\tau_\infty}) \exp\left(\frac{-h_0 \bar{\gamma}}{\tau_\infty}\right), \tag{13}
\]
  where \( \tau_0 \) is the initial CRSS and \( \tau_\infty \) is the saturation CRSS.

2.3 Twinning formulation

Since magnesium does not have enough independent slip systems to accumulate arbitrary deformation, twinning is an important deformation mechanism, especially at room temperature, and it should be considered in the simulations. In this study, the contribution of twinning to the grain reorientation is treated according to a modified version of the PTR scheme [4]. The procedure is summarized as follows.

At each deformation step the increment of the twinned volume fraction in the grain \( n \) associated with each twinning system \( \beta \) is:

\[
\Delta g^{n,\beta} = \frac{\Delta \gamma^{n,\beta}}{\gamma^\beta}, \tag{14}
\]

Then the twinned fraction is accumulated after each deformation step

\[
g^{n,\beta} = \sum_{steps} \Delta g^{n,\beta}, \tag{15}
\]

here \( \Delta \gamma^{n,\beta} \) is shear strain increment contributed by the twinning system \( \beta \) in the grain \( n \), and \( \gamma^\beta \) is the characteristic shear strain associated with twinning, it is a constant and its value is \( \gamma^\beta = 0.13 \). A summation over all twinning systems gives the twinned volume fraction in the grain \( f^n \)

\[
f^n = \sum_{\beta} g^{n,\beta}, \tag{16}
\]
where $f_n$ is the volume fraction of grain $n$. A threshold value for reorientation is empirically set as

$$F_T = 0.9$$

(17)

At every deformation step the twinned fraction of each grain $f_n$ is compared with the threshold value $F_T$. If $f_n$ is greater than $F_T$, the grain is completely reoriented to the orientation of the twin and the twin system will stop its growth in the next steps.

3 Model Parameters

The simulation has been conducted on a cube sample composed of a 1000 grains (10x10x10) with random texture to simulate the cast alloy, the pole figures are shown below. The boundary condition for the uniaxial or compression in the $z$ direction all components of the displacements are prescribed at the block surfaces by the following.

$$
\begin{bmatrix}
\dot{u} \\
\dot{v} \\
\dot{z}
\end{bmatrix} =
\begin{bmatrix}
\dot{E}_x & \dot{\tau}_{xy}/2 & 0 \\
\dot{\tau}_{xy}/2 & \dot{E}_y & 0 \\
0 & 0 & \dot{E}_z
\end{bmatrix}
\begin{bmatrix}
x' \\
y' \\
z'
\end{bmatrix}
$$

$\dot{E}_z = \dot{\varepsilon}$ is prescribed as time step and we set $\dot{\varepsilon} = 0.05\%$. All the components of the macroscopic stresses except $z$ component are forced to vanish by the following.

$$
\dot{E}_x = -\nu(\dot{\varepsilon} - \dot{E}_x^p) + \dot{E}_x^p, \quad \dot{E}_y = -\nu(\dot{\varepsilon} - \dot{E}_y^p) + \dot{E}_y^p,
$$

(18)

where $\nu = 0.35$ is the poisson ratio. For evaluating the accuracy of the constitutive model in predicting the stress response in a polycrystal of magnesium AZ31B at room temperature, the numerical predictions and experimental results of simple tensile and compression tests taken from [5] are compared. The parameters used in the this model have been founded through a trial and error model to achieve a better fit of the experimental data. Here below the parameter found in this research are shown, where Table 1 contains the microscopic parameters, while Table 2 represents the self and latent hardening matrix.
Table 1 – Microscopical parameters

|       | \(\tau_0\) | \(\tau_\infty\) | \(h_0\) |
|-------|-----------|----------------|---------|
| basal | 10.52     | 36.85          | 105     |
| prismatic | 25     | 57.8           | 195.8   |
| pyramidal II | 48.7   | 87            | 334     |
| twin  | 27.43     | 76.3           | 131.3   |

Table 2 – Self and latent hardening matrix

| \(q(\alpha \backslash \beta)\) | slip | prismatic | pyramidal II | twin |
|-------------------------------|------|-----------|--------------|------|
| slip                          | 1    | 0.2       | 0.2          | 0.5  |
| prismatic                     | 0.2  | 1         | 0.25         | 0.2  |
| pyramidal II                  | 0.2  | 0.25      | 1            | 0.2  |
| twin                          | 0.5  | 0.4       | 0.4          | 1    |

4 Verification of the constitutive model

The simulation has been conducted performing both the compression and the tension test on all the three axes, but because of the isotropic nature of the sample due to the random texture, the results are almost the same on all the three axes.

![Fig. 2 – Evaluation of the fitted curves.](image)

As it can be noticed the compression curve is better approximated that the tension one, but we can state that our model can represent the trend of the cast AZ31B under tension and compression. In Fig. 3 and Fig.4 the relative activities of each slip system during the deformation are shown, as it can be foreseen the activities are very similar, this because having the random distribution of the texture gives the sample an almost isotropic nature, the basal slip and the twinning occur first due to the lower CRSSs, as expected, once the twinning reach the saturation and they stop the other two slips take over the deformation, specially the pyramidal II, that it is indeed only left deformation that occurs along c-axes of the grains.
The value of the threshold $F_T = 0.9$ has been set empirically to have the best fit with the experimental data. Here above the Fig.5 shows the effects of the twin's parameter, as it could be expected, the higher it is the later the twin reaches its saturation and at this point corresponds the increase of steepness of the curves.
Increasing the threshold value means that the twins will stop their growth later on during the deformation, when this happens we can notice that the stress required to keep the plastic deformation occurring is higher, this because normally the twin would occur because of its lower CRSS, but blocking it implies that the system has less deformation systems available and this will make the material stiffer. Before the strain reaches 0.75% the lower the FT curve the higher the stress needed, after that point the trend is the opposite, this happens because the effect of the latent hardening of the twin has an important role and a larger deformation along twin strain would result in a stiffer matrix.

5 Conclusion

As written before, this model can represent the deformation of the cast AZ31b with good precision, a better fitting could be reached, but it would not be worth it to be found in the case of the cast sample, because of two reasons: the first one is that is difficult to isolate the contribution of each parameter to the curve if every slip system is active at the same time with almost the same magnitude, as illustrated in Fig.3 and Fig.4, in the case of an extruded tube or a rolled sheet the anisotropy in various direction would make easier to evaluate the parameters giving that for each angles there are different slip systems activated. The second one is that the magnesium and its alloys are usually used when in the form of extruded tubes or rolled sheet, so a deeper investigation of those it would be preferred. In the future this constitutive model will be applied to the numerical testing of a rolled sheet of AZ31B.

References

[1] H. Takahashi, H. Motohashi, M. Tokuda and T. Abe. (1994) Elastic-Plastic Finite Element Polycrystal Model International Journal of Plasticity 10 63.

[2] S.B. Yi, C.H.J. Davies, H.-G. Brokmeier, R.E. Bolmaro, K.-U. Kainer and J. Homeyer. (2006) Deformation and texture evolution in AZ31 magnesium alloy during uniaxial loading. Acta Materialia 54, 549–562.

[3] S.R. Agnew, M.H. Yoo and C.N Tome’. (2001) Application of texture simulation to understanding mechanical behavior of Mg and solid solution alloys containing Li or Y. Acta Materialia 49, 4277–4289.

[4] Jalili, M., Soltani, B., (2019) Investigation the micromechanisms of strain localization formation in AZ31 Mg alloy: A mesoscale 3D full-field crystal plasticity computational homogenization study, European Journal of Mechanics / A Solids, doi: https://doi.org/10.1016/j.euromechsol.2019.103903.

[5] Shimizu I. (2018), Biaxial Compressive Behavior and Tension-Compression Asymmetry on Plastic Deformation of Cast and Extruded AZ31 magnesium Alloys Advanced Experimental Mechanics, Vol.3, 141-146

[6] Paramatmuni, C., Kanjarla, A.K, A crystal plasticity FFT based study of deformation twinning, anisotropy and micromechanics in HCP materials: Application to AZ31 alloy, International Journal of Plasticity, https://doi.org/10.1016/j.ijplas.2018.10.007