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Research paper

Temperature-dependent crystal-plasticity model for magnesium: A bottom-up approach

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ABSTRACT

A crystal-plasticity model is developed to account for temperature-dependent mechanical behaviour of magnesium in this paper. The constitutive description of plastic deformation accounts for crystalline slip and twining as well as their interactions. The temperature dependence is incorporated into the constitutive equations for both slip and twin modes based on experimental observations. A bottom-up computational modelling framework is proposed to validate the developed constitutive model. First, the crystal-plasticity model is calibrated with experimental results for plane compression at micro-scale. At meso-scale, a three-dimensional representative element volume was adopted to represent the microstructure of polycrystalline magnesium. In the combination with the proposed constitutive theory, the effects of temperature on mechanical response and evolution of twins and texture in polycrystalline magnesium were predicted. Comprehensive experimental validations at meso-scale were performed to consolidate further the developed crystal-plasticity model incorporating temperature dependence in terms of stress-strain curves, the Hall-Petch relationship and texture evolution. This work provides a useful modelling tool for understanding temperature-dependent behaviour of magnesium, which could be used to improve the formability of this family of materials.

1. Introduction

With increasing demands for improved fuel efficiency in transportation, there is a strong drive to reduce the weight of vehicles without compromising their structural resilience. Therefore, magnesium (Mg) and its alloys have attracted significant attention in recent years thanks for their high specific strength (Wei et al., 2015; Zhou et al., 2016). However, the widespread structural applications of Mg have been substantially restricted by material's poor ductility and formability. This drawback is primarily due to the underlying hexagonal close-packed (HCP) structure of Mg, which provides a limited number of slip systems for plastic deformation at room temperature (Mirzadeh, 2014). Additional slip systems may be activated at elevated temperatures; consequently, hot processing is advised to overcome the poor formability of Mg (Figueiredo et al., 2016; Mirzadeh, 2014). This needs to be performed with caution, as high temperatures may alter the material's microstructure with a concomitant change in an in-service mechanical response of a component (Yuan et al., 2016). Thus, a thorough understanding of hot deformation behaviour of Mg is necessary.

In Mg and its alloys, micro-scale deformation mechanisms include both crystalline slip and deformation twinning. In addition, a significant transition of the dominant deformation mode is observed with a temperature variation. In recent years, crystal-plasticity-based approaches that can explicitly implement different deformation modes have been widely used for fundamental investigations on deformation mechanism of various metallic materials, including Mg, further providing guidelines for design of novel materials (Zhang et al., 2016) and formability improvements (Liu et al., 2016a, c).

Based on the modelling philosophy adopted in crystal plasticity, the respective modelling technique can be categorised into top-down and bottom-up approaches (Zhang and Joshi, 2012). The top-down approach is well-suited to model polycrystalline behaviour at macro-scale, from which single-crystal parameters are inferred. The commonly used top-down approaches can be classified into isostrain (Taylor, 1938), isostress (Sachs, 1928) and self-consistent (Eshelby, 1957) schemes. There are some successful examples for these different top-down approaches, for instance, the isotrain-type (Ardeljan et al., 2016; Knezevic et al., 2009), isostress-type (Toth et al., 1990) and visco-plastic self-consistent (VPSC) models

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(Beyerlein and Tomé, 2008; Kabirian et al., 2015). The top-down approach is relatively easy to implement numerically and can reduce computational cost by incorporating a coarse finite-element (FE) mesh. However, this approach suffers from a high computational time cost at element-level simulation, which impedes parallel computation in FE analysis. Thus, the top-down approach may essentially decrease computational efficiency. Its another drawback is the fact that the choice of a homogenization scheme affects significantly the estimation of single-crystal parameters (Ardeljan et al., 2016). By contrast, the bottom-up approach involves the use of a calibrated (based on experiments) small-scale single-crystal-plasticity (SCP) model, incorporating typical deformation modes such as slip, twinning or both. To predict a response of polycrystalline component, individual crystal grains and orientations are represented via the SCP model, which is then employed to assess a stress-strain response and texture evolution during the deformation process. Here, the intra-grain interaction is modelled in a physically representative manner (in contrast to the use of homogenization). Successful implementations of the bottom-up approach were developed for a variety of crystalline materials, FCC (Cyr et al., 2015), BCC (Lim et al., 2015) and HCP metals (Abdolvand and Daymond, 2013; Cheng and Ghosh, 2015) and references there in. Compared to the top-down approach, the bottom-up approach has a higher demand on computational resources, but such an approach is amenable for parallelisation in an FE solver.

In Mg and its alloys, much of the modelling effort involves the use of top-down approach. For example, VPSC models were employed to provide an insightful understanding activity of slip and twin mode at different temperatures in AZ31 alloy (Kabirian et al., 2015; Zhang et al., 2016). In the works, the so-called predominant twin reorientation (PTR) scheme proposed by Tomé et al. (1991) was widely adopted to determine the twin-phase formation. In the PTR scheme, only one twin phase with a highest contribution to total volume fraction was activated in a grain. In these VPSC-based approaches, a critical resolved shear stress (CRSS) needs to be calibrated at different temperatures, which is their primary drawback. Recently, Ardeljan et al. (2016) proposed a Taylor-type modelling scheme, in which the temperature dependence was incorporated into constitutive laws, thus addressing its effect with introduction of appropriate parameters.

For bottom-up approaches, several SCP-based models were developed recently, with their parameters identified through single-crystal experiments (Becker and Lloyd, 2016; Gan et al., 2016; Zhang and Joshi, 2012). Additionally, these models were also employed to characterise polycrystals at meso-scale (Chang and Kochmann, 2015; Zhang and Joshi, 2012). However, these studies were limited to investigations at room temperature. To date, only some limited attempts were made to capture temperature dependence with different sets of model parameters were used for different temperature conditions (Hidalgo-Manrique et al., 2015). Thus, it is imperative to incorporate temperature dependence into constitutive laws for bottom-up approaches, which will allow for modelling across a wider temperature range exploiting a broader design space.

The aim of this paper is to develop a SCP model to account for the temperature dependence of Mg, henceforth, referred to as T-SCP (temperature-dependent single-crystal plasticity) model. This model was incorporated into a bottom-up modelling framework to investigate the effects of temperature on the mechanical response and texture evolution of single-crystal and polycrystalline Mg. This paper is organized as follows: in Section 2, a self-contained description of the governing relations of the proposed T-SCP model was presented. Section 3 presents a modelling strategy of the bottom-up approach based on a commercial FE software package ABAQUS. In Sections 4 and 5, simulation results and experimental validations are presented and discussed for single-crystal and polycrystalline case at meso-scale, respectively. We end with some concluding remarks in Section 6.

2. Constitutive formulas

In this section, a phenomenological T-SCP model is presented to account for the temperature-dependence of single Mg crystals (or grains). In the T-SCP model, four slip and two twin systems were considered for the Mg crystal as listed in Table 1. Here, four slip planes are considered: basal, prismatic, pyramidal ⟨a⟩ and pyramidal ⟨c+a⟩ and two twin planes: tensile twin (TT) and compressive twin (CT) (see Fig. 1). Standard notation is adopted here: scalars are in italics, vectors and tensors are indicated with lower-case and upper-case bold letters.

2.1. Kinematics

Following a classical crystal plasticity (CP) theory, the deformation gradient $\mathbf{F}$ can be decomposed into the elastic and plastic parts, as,

$$\mathbf{F} = \mathbf{F_e}\mathbf{F_p}, \tag{1}$$

where the subscripts 'e' and 'p' denote the elastic and plastic parameters, respectively. The velocity gradient $\mathbf{L}$ is introduced following its definition $\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1}$, as,

$$\mathbf{L} = \dot{\mathbf{F}}_\mathbf{e}\mathbf{F}_\mathbf{e}^{-1} + \mathbf{F_e}(\dot{\mathbf{F}}_\mathbf{p}\mathbf{F}_\mathbf{p}^{-1})\mathbf{F}_\mathbf{e}^{-1} = \mathbf{L_e} + \mathbf{L_p}. \tag{2}$$

For Mg crystal, the plastic deformation is assumed to arise from both crystalline slip and twinning due to its HCP structure with a large aspect ratio. Consequently, the plastic velocity gradient, $\mathbf{L_p}$, incorporates contributions from the slip and twin modes as

$$\mathbf{L_p} = \mathbf{L_p^{sl}} + \mathbf{L_p^{tw}} + \mathbf{L_p^{sl-tw}}. \tag{3}$$

Here $\mathbf{L_p^{sl}}$, $\mathbf{L_p^{tw}}$ and $\mathbf{L_p^{sl-tw}}$ represent the plastic velocity gradient induced by the slip in the untwined region (or parent phase), deformation twinning in the untwinned region and secondary slip in the twinned region (or child phases), respectively (Kalidindi, 1998). In this paper, the assumption of pseudo slip is adopted for twinning, and its effectiveness has been demonstrated in prior work (Ardeljan et al., 2016; Gan et al., 2016; Kalidindi, 1998). For the sake of clarity, the superscript α is used to represent the slip system in the parent phase, β for the twin system in the parent phase and $\tilde{\alpha}$ for the secondary slip system in the child phase. The three terms in Eq. (3) can be further expressed as

$$\begin{aligned}
\mathbf{L_p^{sl}} &= \left(1 - \sum_{\beta}^{N_{tw}} f^\beta\right) \sum_{\alpha=1}^{N_s} \dot{\gamma}^{(\alpha)} \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \\
\mathbf{L_p^{tw}} &= \sum_{\beta=1}^{N_{tw}} \dot{\gamma}^\beta \mathbf{s}^\beta \otimes \mathbf{m}^\beta \\
\mathbf{L_p^{sl-tw}} &= \sum_{\beta=1}^{N_{tw}} f^\beta \sum_{\tilde{\alpha}=1}^{N_s} \dot{\gamma}^{\tilde{\alpha}} \mathbf{s}^{\tilde{\alpha}} \otimes \mathbf{m}^{\tilde{\alpha}}
\end{aligned} \tag{4}$$

where $\dot{\gamma}^\alpha$ is the shear slip rate on the slip system α, f^β is the volume fraction of child phase β, and $\dot{\gamma}^\beta$ is the shear strain rate arising from deformation twinning. N_s and N_{tw} are the total numbers of slip and twin systems, respectively. The unit vector $\mathbf{s}$ represents the direction of slip/twin and $\mathbf{m}$ is the unit vector normal to the corresponding slip/twin plane. Furthermore, the velocity gradient can be expressed in terms of a symmetric rate of stretching $\mathbf{D}$ and an antisymmetric rate of spin $\mathbf{W}$:

$$\mathbf{L} = \mathbf{D} + \mathbf{W} = (\mathbf{D_e} + \mathbf{W_e}) + (\mathbf{D_p} + \mathbf{W_p}). \tag{5}$$

From Eqs. (2)∼(5), we obtain

$$\mathbf{D_e} + \mathbf{W_e} = \dot{\mathbf{F}}_\mathbf{e}\mathbf{F}_\mathbf{e}^{-1}, \ \mathbf{D_p} + \mathbf{W_p} = \mathbf{L_p^{sl}} + \mathbf{L_p^{tw}} + \mathbf{L_p^{sl-tw}}. \tag{6}$$