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An elastic–viscoplastic crystal plasticity modeling and strain hardening for plane strain deformation of pure magnesium

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ABSTRACT

A rate-dependent elastic–viscoplastic constitutive model is proposed to simulate the plane strain deformation of pure magnesium crystal. The observed plastic deformation mechanisms of slip, twinning and their interaction are accounted for. The basal, prismatic and pyramidal slip systems in the parent grain, compressive twinning (CT) and tensile twinning (TT) are incorporated in the model. Due to the differences of generation mechanisms of twins and their effects on the deformation, the constitutive descriptions of CT and TT are distinguished to better characterize their effects on the overall hardening of magnesium single crystals. For investigating the generation of different slips and twins, the plane strain numerical schemes of seven different orientations for loading and fixed boundary are considered and their various mechanisms and characteristics of plastic deformation are discussed. The contributions of different deformation modes to the macroscopic plastic deformation of magnesium single crystals in the seven cases are presented. These computational predictions are carefully compared with their corresponding macroscopic experimental observations (stress-strain responses) and other numerical results. These results prove that it is necessary to distinguish different twinning systems and their associated hardening laws for the plastic deformation of magnesium and its alloy.

1. Introduction

Magnesium alloy, like most hexagonal close-packed (HCP) metals, is widely used in the automotive industry as well as housing 3C electronic products due to its low density, high strength and excellent performance. The basal, prismatic, pyramidal slips and pyramidal twins are the main plastic deformation mechanisms in the pure magnesium and most of magnesium alloys. The prismatic and pyramidal slips cannot be easily activated because their critical resolved shear stresses (CRSS) are much higher than that of the basal slip at room temperature. The strain perpendicular to the *c*-axis direction is provided by two independent slip systems which come from the basal plane and three close-packed directions on this plane, whereas the strain parallel to the *c*-axis direction is produced by pyramidal twinning (Christian and Mahajan, 1995).

The pioneering work of crystal plasticity theory was made by Taylor (1938). Taylor proposed a model for the analysis of polycrystalline stress–strain relationship. The grain boundary of interface was considered as a zero thickness surface and the grain orientations in the both sides of interface are different in the Taylor model. Based on this model, the geometry and kinematics of crystal plastic deformation were critically described by Hill and Rice (1972), Asaro and Rice (1977) and Peirce et al. (1982). Asaro and Needleman (1985) established a strict constitutive framework to simulate the stress–strain responds and texture evolution in the finite

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deformation. Thereafter, the extensive researches for different deformation situations were conducted: nominally homogeneous deformation mode (Rodríguez-Martínez et al., 2011), macroscopic shape change (Anand and Kalidindi, 1994; Balasubramanian and Anand, 1996), texture evolution from the entire non-uniform deformation (Kalidindi et al., 1992; Balasubramanian and Anand, 1996; Zecevic et al., 2015).

Based on the slip deformation, the introduction of deformation twinning greatly expands the crystal plastic model to simulate different polycrystalline materials and deformation mechanisms (Van Houtte, 1978; Tome et al., 1991). Interactions between twinning and slip or between twins have great influence on the macroscopic anisotropy responses for both single and polycrystalline magnesium and their alloys. Especially the relative activations of slip and deformation twinning which are closely related to the directions strongly influence hardening behavior (Caceres et al., 2008), texture evolution (Brown et al., 2005; Agnew et al., 2001), crack propagation (Potirniche et al., 2007) and toughness (Miura et al., 2005). It is a main problem to handle a large number of alignment orientations generated by twinning area for taking the deformation twinning into account in a crystal plasticity framework.

Based on Taylor's approach, Van Houtte (1978) proposed predominant twin reorientation (PTR) model in which the twins were introduced. The Monte Carlo method consisting of random samples was adopted and the whole grains were reoriented by the twinning in their model. PTR model gave a good explanation for the grain reorientation caused by the twinning. The volume fraction of twinning of each grain was carefully tracked in PTR model, so the lattice can be rotated instantaneously when the accumulated value of the volume fraction of twinning reaches a certain value. The orientation of whole grain would be changed into a dominant twinning orientation after the rotation. Namely, the position of grain in global coordinate system will be changed according to the plane and direction of twinning. There is no change for the orientation of twinning region at the end of each simulation step. The primary, second slips and primary twinning were considered as the major plastic deformation in this model. Lebensohn and Tome (1993) successfully introduced the PTR model into a viscoplastic self-consistent (VPSC) model to simulate the evolution of polycrystalline texture and plastic deformation.

Tome et al. (1991) investigated the reorientation of the crystal lattice caused by twinning based on the volume fraction transfer (VFT) scheme. Compared to the traditional schemes, their model predictions are better in agreement with the experiment results especially in the prediction of texture evolution for the mode of twinning predominate deformation. Based on the PTR model, Tome et al. (1991) proposed a weighted method to manage a large number of new orientations produced by twins. The VFT method divided the Euler space into different cells, so the volume fraction was assigned to each cell and evolved with the change of deformation. Consequently the influence of each twin system on the texture can be considered. A drawback of VFT scheme is the absence of equivalence property of grain and a realistic hardening solution cannot be obtained.

Kalidindi et al. (1992) presented a finite element program and a fully implicit time integration scheme to predict the texture evolution of face centered cubic metals during bulk deformation processing, and only slip was considered in their paper. Kalidindi (1998, 2001) improved this model in which the twinning was incorporated to investigate the deformation and texture evolution of face-centered cubic (FCC) metals with low stacking fault energy. The defect that the twin region was considered as a new untwined grain in which more slips and twins can be generated in the PTR and VFT schemes was handled in the improved model. Some original dimensionless equations for the hardening and volume fraction of twinning were presented in the above model. Salem et al. (2005) adopted this model to simulate the deformation of α-titanium with different hardening functions for primary slip and twinning. The advantage of their approach is the ability to track the changes of volume fraction for each grain twinning and their orientations are same to the initial direction of the grain. So the Cauchy stress in the grain can be achieved through the volume average of matrix and twin region. However, there is a shortcoming that the reorientations of grains only come from the shear of the matrix in their approach. Lévesque et al. (2010) employed a constitutive framework based on the model presented by Kalidindi (1998) to simulate three various stress states of magnesium alloy. But they believed that the assumption of a uniform deformation gradient over the twinned and un-twinned regions is physically unsound. The slip-twin interactions and differences between CT and TT have not been included in their model. Zecevic et al. (2015) incorporated statistical stress fluctuations, twin boundary hardening and de-twinning into the activations of thermally activated slip and twinning. They found that the internal residual stresses have significant influence on the flow stress drop, twin activation, de-twinning and the formation of additional twin variants.

Crystal plasticity method can predict the yield surface of face-centered cubic polycrystalline, including the texture, polycrystalline homogenization method and the influence of anisotropy of slip on the stress-space contours (Kalidindi and Schoenfeld, 2000). Van Houtte et al. (2002) found that the finite element model can get better results than the thin plate model in the polycrystalline plasticity deformation and texture evolution. Although the thin plate model performed more lightly, this problem can be solved by using more complex mesh structure. There are more details in describing microstructure in the finite element model. Phan et al. (2015) implemented a crystal plasticity finite element model to study the influence of intrinsic features and grain size on the deformation behavior of ultrafine-grained materials. This model coupling with a modified Hall–Petch relation can predict the Hall–Petch and true stress–strain curves at the grain level. Saai et al. (2010) proposed a dislocation-based model for the finite element simulation of FCC single crystal behavior. In their simulations, they made a comparison between the mechanical dissipated powers estimated from temperature fields and the ones computed from local mechanical variables.

El-Danaf et al. (1999) investigated the influence of the stacking fault energy of face-centered cubic polycrystalline on the stress of deformation twinning. They found that the dislocation density and similar slip length play a