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A crystal plasticity FE model for deformation with twin nucleation in magnesium alloys

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ABSTRACT

Magnesium alloys exhibit complex deformation related mechanical behavior, viz. plastic anisotropy, tension–compression asymmetry and premature failure. Their origins are in the underlying heterogeneous deformation due to dislocation slip and micro-twin formation on different crystallographic systems. Reliable prediction of mechanical response and failure is predicated upon the ability of computational models of polycrystalline microstructures to accurately simulate such deformational heterogeneity and localization. In this paper a physically-motivated non-local crystal plasticity finite element (CPFE) model is developed for dislocation-mediated heterogeneous deformation of single and polycrystalline Mg alloys leading to micro-twin nucleation. The CPFE model uses image-based virtual polycrystalline microstructures for its simulations and is able to effectively represent stress and deformation patterns in the intra- and inter-granular regions. A micro-twin nucleation criteria is proposed from energy-partitioning following the dislocation dissociation process. The CPFE simulations of polycrystalline microstructures show satisfactory agreement with experimental observations. CPFEM studies on large grain aggregates using this criteria, reveal the critical role of crystallographic orientation and grain boundaries on micro-twin formation.

1. Introduction

The quest for low density, high strength and durable materials in high performance automotive and aerospace applications has resulted in magnesium alloys as candidate materials with high potential (Bettles and Gibson, 2005; Kainer, 2003). The density of magnesium is about 23% that of steel and 66% that of aluminum, while its weight for equivalent bending stiffness is 62% less than steel and 23% less than aluminum. Being among the lightest of structural metals with high stiffness and strength at a range of temperatures, these alloys can offer considerably increased component strength to weight ratio. These desirable properties can have the ultimate consequences of significant savings in energy consumption and reduction in CO_2 emissions. An important consideration in the processing and high performance industrial applications of Mg alloys is their deformation behavior and failure characteristics at a range of strain rates and temperatures. Of particular interest is their ductility properties, e.g. their behavior in forming processes like extrusion or rolling, or under impact loads as in crashworthiness tests. Understanding the physics of the plastic deformation and failure of magnesium alloys is therefore essential for tailoring their ductility, especially at room temperatures.

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A complicating phenomenon of magnesium and its alloys (e.g., AZ31) is their deformation induced anomalous mechanical behavior (Kaiser et al., 2003; Bohlen et al., 2007; Barnett, 2007a,b; Brown et al., 2007; Ma et al., 2011; Kadiri et al., 2013). These materials possess low-symmetry hexagonal closed packed (*hcp*) crystallographic structure, an attribute that leads to pronounced anisotropy in mechanical properties, e.g. tension–compression asymmetry of the yield strength. Low symmetry results in a variety of slip systems for the *hcp* crystalline lattice, shown in Fig. 1. At low temperatures, the critical resolved shear stress (CRSS) is much lower for basal slip $\langle 0001 \rangle \langle 11\bar{2}0 \rangle$, than it is for prismatic $\{10\bar{1}0\} \langle 11\bar{2}0 \rangle$ or pyramidal $\{11\bar{2}2\} \langle 11\bar{2}3 \rangle$ slip systems. Only the basal $\langle a \rangle$ slip can occur under low applied stresses. Any deformation involving changes in the $\langle c \rangle$ direction ensues a competition between the high CRSS $\langle c+a \rangle$ slip systems and the less understood micro-twin mechanisms (Duygulu and Agnew, 2005). The myriad of interactions among slip and twin systems lead to complex plastic behavior, involving plastic anisotropy, tension–compression asymmetry and premature failure. Local stress and dislocation concentrations at locations of microstructural heterogeneities in polycrystalline aggregates close to grain boundaries with strong texture and grain size distribution are responsible for this behavior. It is important to develop physics-based models of deformation and micro-twinning in Mg alloys with the goal of understanding the effect of microstructure on failure.

Major computational approaches have been developed for continuum-scale simulation of polycrystal aggregates of Mg alloys. The elasto-visco-plastic self-consistent or EVPSC method started in (Hutchinson, 1976), evolved in (Molinari et al., 1987) and was further developed in (Lebensohn and Tome, 1993, 1994) to account for large anisotropic viscoplastic deformation. Features like dislocation slip inside a twin band, detwinning, effect of solid solution and dislocation transmutation caused twin hardening have been included for *hcp* crystals in recent developments (Proust et al., 2009; Wang et al., 2012; Raeisinia and Agnew, 2010; Kadiri and Oppedal, 2010; Oppedal et al., 2012). In the EVPSC scheme, each grain is treated as an ellipsoidal inclusion embedded in a homogeneous medium representing the averaged behavior of all other grains, while preserving equilibrium and compatibility. It is an efficient method for modeling the behavior and texture evolution of large grain aggregates. Grains however are not in direct interaction with their neighbors, and the effect of grain boundary, grain shape and stress heterogeneity inside each grain are not explicitly represented. Crystal plasticity finite element models or CPFEM have been implemented to model deformation in Mg alloys in (Staroselsky and Anand, 2003; Graff et al., 2007; Izadbakhsh et al., 2011, 2012; Zhang and Joshi, 2012; Abdolvand and Daymond, 2013). A non-local constitutive model has been developed by (Ma et al., 2006) for CPFEM with the emphasis on accumulation of geometrically necessary dislocations (GNDs).

Modeling deformation twinning is a key to effective failure prediction for Mg alloys. The formation of micro-twins is facilitated by the low number of easy slip systems in *hcp* metals. However, a number of important fundamental questions remain, e.g. how does a micro-twin nucleate, how the twin boundary migrate or when does a grain saturate with accommodating twins. The formation of micro-twins by the nucleation and glide of twinning dislocations are not on close packing planes as discussed in (Serra et al., 1991). The glide of twin dislocations not only provides shear deformation but also requires a collaborative shuffling of atoms over more than one crystallographic plane (Hirth and Lothe, 1982). This non-planar atomic shuffling, together with twin shear, reorients the initial crystallographic lattice in a mirror-symmetry and thickens the twin. Two types of twin nucleation theories, refereed to as homogeneous and heterogeneous theories, have been proposed for *hcp* metals. The homogeneous theory (Koehler et al., 1954) assumes nucleation from a perfect crystal lattice, while the heterogeneous theory (Mendelson, 1970; Capolungo and Beyerlein, 2008; Beyerlein and Tome, 2010; Ghazisaeidi and Curtin, 2013) considers the effect of existing defects and microstructure on twinning. The homogeneous models require very high stress levels, close to material's theoretical strength, which can only happen in extreme loading conditions. The heterogeneous models are more suited for micro-twinning under lower-strain rate and quasi-static loading conditions. Beyerlein and Tome (2010) considered the twin nucleation from defects at low angle grain boundaries.

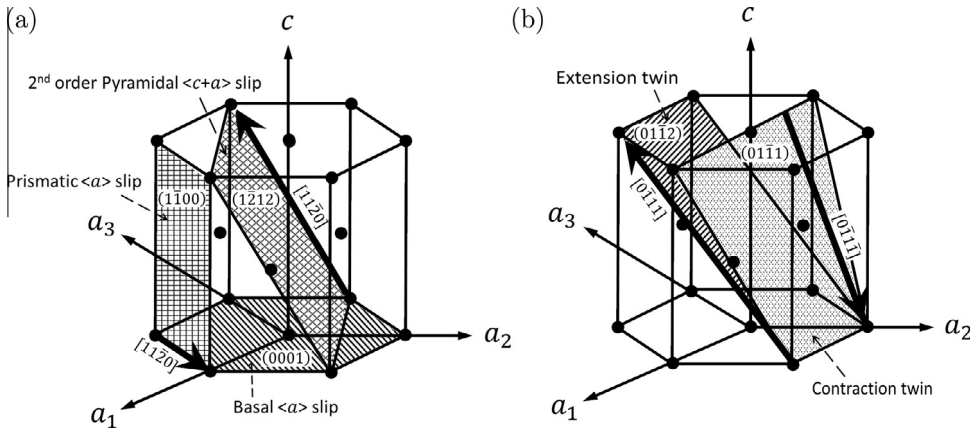

Fig. 1. Schematic showing: (a) active slip systems and (b) twin systems in *hcp* magnesium alloys.