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Phenomenological crystal plasticity modeling and detailed micromechanical investigations of pure magnesium

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ABSTRACT

We present a single crystal plasticity model for pure Mg incorporating slip and deformation twinning. The model uses the basic framework of Kalidindi (1998), but proposes constitutive descriptions for the slip and twin evolution and their interactions that are motivated by experimental observations. Based on compelling experimental evidences, we distinguish between the constitutive descriptions of the tension and compression twinning to better represent their roles in the overall hardening of Mg single crystals. With these improved phenomenological descriptions, we first calibrate material parameters for the different slip and twin modes by performing three-dimensional simulations mimicking the plane-strain compression experiments by Kelley and Hosford (1967, 1968) on single crystal pure Mg. In doing so, these computational responses are critically compared with their corresponding orientation-dependent microscopic (slip and twin activities) and macroscopic (stress–strain responses) experimental observations. Then, the calibrated parameters are used to predict several other experimental results on pure single- and poly-crystal Mg under different loading conditions. We also investigate the role of pre-existing heterogeneities such as initial twin population and stiff, elastic inclusions on the single crystal macroscopic and microscopic responses. Microstructural characteristics show that such heterogeneities strongly influence the local and global evolution of the slip and twin activities, and in some cases modulate the strength anisotropy that is commonly observed in monolithic single crystals. These results may provide useful indicators toward designing novel composite Mg microstructures.

1. Introduction

Magnesium (Mg) and its composites are potential candidates for structural applications ranging from energy-savvy automotive and aerospace sectors to biomedical components, due to its low mass density (~35% lighter than aluminum) and excellent biocompatibility. There has been a renewed emphasis toward developing novel micro-architectures with impressive specific strengths (strength/density) using pure Mg or its alloys by inducing barriers to plastic deformation through a variety of techniques including grain size refinement, nano-reinforcements, or combinations thereof (Gharghouri et al., 1998; Xu et al., 2007; Zhong et al., 2007).[1] For example, starting with pure Mg matrix, Zhong et al.

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[1] Although Mg alloys may be popular starting materials from a practical standpoint, pure Mg is a good model material for fundamental investigations for such novel attempts.

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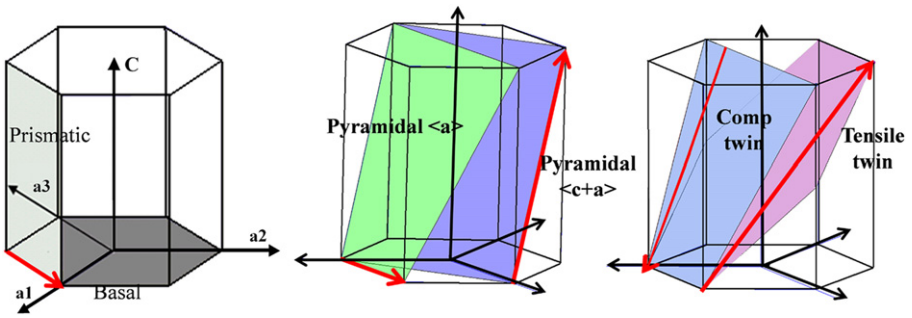

Fig. 1. Schematic diagrams of slip and twin systems in magnesium.

(2007) and Habibi et al. (2010) have recently shown that its mechanical performance including the yield strength, hardening and ductility of pure Mg can be dramatically improved by adding dilute amounts of nano-scaled reinforcements. These significant improvements are intimately tied to the manner in which the underlying deformation mechanisms are modulated by the small-scaled heterogeneities and in order to optimally design such microstructures it is important to develop prognostic tools that enable their detailed understanding. A cleaner understanding of the inelastic deformation mechanisms in Mg is also vital to successful applications. However, modeling such intricate holistic responses is a challenging task because of the myriad interactions between the different deformation mechanisms (Fig. 1) that prevail in this hexagonal close-packed (HCP) crystal structure (Christian and Mahajan, 1995). In Mg, the basal slip (i.e. $(0001)\langle 11\bar{2}0\rangle$)[2] and two non-basal slip modes—the prismatic $\{10\bar{1}0\}\langle 11\bar{2}0\rangle$ and the pyramidal $\langle a\rangle(\{10\bar{1}1\}\langle 11\bar{2}0\rangle)$ provide deformation parallel to the basal plane only. Thus, even when these slip systems are activated simultaneously they cannot accommodate arbitrary plastic deformation. Furthermore, the secondary pyramidal $\langle c+a\rangle$ slip, $(\{11\bar{2}2\}\langle 11\bar{2}3\rangle)$ which provides another non-basal (out-of-basal-plane Burgers vector) deformation is relatively difficult to activate at room temperature due to its high critical resolved shear stress (CRSS). Therefore in Mg, like in most HCP metals, deformation twinning (DT) provides an additional mechanism to accommodate *c*-axis deformation, which is intimately tied to the lattice parameter, *c*/*a* ratio (Yoo, 1981). In Mg, the most commonly observed DT mode is the $\{10\bar{1}2\}\langle 10\bar{1}1\rangle$ extension (tensile) twinning when the *c*-axis experiences tension, whereas the less common, $\{10\bar{1}1\}$ and $\{30\bar{3}4\}$ contraction (compressive) twinning modes may sometimes occur under *c*-axis compression (Reed-Hill and Robertson, 1957a, 1957b; Yoshinaga et al., 1973).[3] $\{10\bar{1}3\}$ tensile twinning, is also reported in experiments as a double twin mode (Ma et al., 2011). The interactions between aforementioned deformation mechanisms result in a significant anisotropy in the macroscopic response for both, single and textured polycrystalline Mg and their composites. Especially, the relative activities of the slip and DT modes are strongly orientation-dependent and influence the hardening behavior (Caceres and Lukac, 2008), texture evolution (Agnew et al., 2001; Brown et al., 2005), crack propagation (Ando et al., 2006) and ductility (Miura et al., 2005). Kelley and Hosford (1968, 1967) (also referred to as K–H in this paper) and Wonsiewicz (1966) performed comprehensive investigations on pure Mg single crystals at both room and higher temperatures. Their plane-strain compression experiments have led to a detailed account of the orientation-dependent macroscopic and microscopic response of pure Mg single- and poly-crystals. Recently, Chapuis and Driver (2010) also performed experiments on single crystal pure Mg for a limited types of orientations, but also explored the temperature effects.

A variety of modeling approaches have been developed at the continuum scale to describe the rich mechanics for a broad class of HCP metals including Mg (Brown et al., 2005; Graff et al., 2007; Kalidindi, 1998; Proust et al., 2007; Roters et al., 2010; Salem et al., 2005; Staroselsky and Anand, 2003; Tomé et al., 1991; Wang et al., 2010). Among them, sophisticated self-consistent polycrystal plasticity models (e.g. Brown et al., 2005; Tomé et al., 1991; Wang et al., 2010) incorporating dislocation slip and DT have been developed to study the macroscopic behaviors including strain hardening, texture evolution and internal stress variation. These *top–down* approaches are elegant in that they are well-suited to model polycrystalline behaviors and in the process, obtain estimates of single crystal parameters. On the other hand, it is also useful to develop a *bottom–up* approach relying on single crystal plasticity (SCP) whose constitutive parameters for the individual slip and twin modes are identified by critically comparing them with single crystal experiments at the macroscopic and microscopic levels. Once identified, they may be employed in predicting several features in single as well as polycrystalline Mg such as the orientation-dependent stress–strain responses, hardening behaviors, texture evolution, fracture, and so on. Compared to the homogenized approaches, the bottom–up approach serves as a model length-scale to admit newer features that are discovered in sub-scale experiments and simulations (e.g. molecular/dislocation dynamics) For example, they may prove valuable in distinguishing between the mechanics of Mg at conventional length-scales and the emerging field of the mechanics at small length-scales (Byer et al., 2010; Lilleodden, 2010). It is also naturally

[2] Throughout the paper (*hkil*) indicates a specific slip/twin plane, [*uvwx*] specific slip/twin direction, {*hkil*} indicates family of a particular slip/twin plane and $\langle uvwx\rangle$ indicates family of particular slip/twin directions.

[3] The $\{10\bar{1}1\}\langle 10\bar{1}\bar{2}\rangle$ compression twins have been widely reported. It is believed that the $\{30\bar{3}4\}$ twin is a sequence of $\{10\bar{1}1\}$ twins (Reed-Hill, 1960).