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Effects of reinforcement morphology on the mechanical behavior of magnesium metal matrix composites based on crystal plasticity modeling

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ABSTRACT

In this work, we investigate the role of elastic inclusions in a plastically anisotropic matrix using crystal plasticity modeling and simulation. Magnesium (Mg) is taken as a model matrix material, which exhibits large plastic anisotropy that originates from slip and twinning mechanisms with dramatically different activation stresses. Using an idealized setup of a periodic unit cell comprising single crystal Mg matrix with an embedded elastic inclusion, we investigate the role of inclusion shape and alignment in the evolution of composite flow responses under compressive and tensile loads. This idealization serves as a model setup for highly textured microstructures that result from extrusion or rolling processes. Detailed analysis reveals how slip and twinning mechanisms evolve with strain and how they depend on the reinforcement morphology. Results indicate that under the loading condition that preferentially activate $\{10\bar{1}2\}$ extension twinning, the inclusion morphology and alignment significantly influence the amount of flow hardening at a given strain and its evolution as a function of increasing strain. This twinning induced hardening effect exists in addition to the classical hydrostatic constraint effect induced by the presence of elastically stiff inclusions. We propose a simple empirical expression, which quantifies this coupling. On the other hand, when extension twinning is not an active deformation mechanism, the flow hardening characteristics are similar to the classical MMCs that deform by dislocation slip. We also investigate the effects of reinforcement aspect ratio and volume fraction on the composite responses. Finally, we briefly discuss how these observations on single crystal MMC models can be extended to textured polycrystalline Mg MMCs.

1. Introduction

Magnesium (Mg) and Mg-alloys are potential candidates for structural applications ranging from fuel-intensive automotive sector to biomedical components due to attractive properties such as low mass density, high damping capacity and excellent biocompatibility. The Achilles' heel of Mg alloys as preferred structural materials is their lower stiffness and strength relative to their nearest competitor, aluminum (Al) and Al-alloys. Moreover, the hexagonal close-packed crystal structure of Mg is plastically highly anisotropic, due to which its yield strength (σ_y), flow stress (σ_f) and ductility are strongly influenced by underlying texture. For single crystal Mg, the ratio of critical activation stresses for the plastically hardest mode and the plastically softest mode can be ∼ 100 together with dramatically different flow behaviors as well as ductility (Kelley and Hosford, 1968), which can cause issues

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in processing and manufacturing. There is a growing interest in designing Mg-alloy microstructures with mechanical properties that are tunable based on the expected functionalities. Strategies to mitigate some of these issues include: (i) grain refinement (Yoshida et al., 2003; Yuan et al., 2011), (ii) alloying, (iii) synthesizing composite architectures (Kainer, 1991; Ye and Liu, 2004; Poddar et al., 2007; Habibi et al., 2010; Deng et al., 2012; Shanthi et al., 2012; Shen et al., 2013b) and (iv) texture modification (Young et al., 2007). While each of these approaches can be exploited independently, they are not mutually exclusive (Li and Lavender, 2015). Indeed, it may be beneficial to consider combinations of these strategies in order to design microstructures that provide desired properties. Examples of designed MMC microstructures can be found in the literature (e.g. Clyne and Withers, 1995; Rabinovitch et al., 1983; Wang et al., 2006; Li and Lavender, 2015). For instance, it is possible to design Mg matrix nano-composites with desired texture, which result in concurrent enhancement of strength and ductility (Habibi et al., 2010, 2012). Further, by choosing appropriate alloying elements, such architectures can exploit different strengthening (and sometimes, softening) mechanisms in mitigating the tension–compression strength differential.

The broader focus of this paper is on the mechanics of Mg metal matrix composites (MMCs). Several experimental reports indicate the effects of reinforcement size and volume fraction on the mechanical behavior of Mg MMCs (Chowdhury et al., 2010a, 2010b; Deng et al., 2010; Hu et al., 2010; Lelito et al., 2012; Wang et al., 2012; Meixner et al., 2011). Often, adding second phase particles to Mg matrix strengthens either the tensile or the compressive responses, but seldom both. Even if both the strengths are enhanced, they usually do not address the issue of strength differential. Furthermore, strength enhancement is usually concomitant with a reduction in the strain to failure, barring few exceptions (Habibi et al., 2010, 2012). The strong plastic anisotropy of the basal, non-basal (pyramidal $\langle a\rangle$, prismatic $\langle a\rangle$ and pyramidal $\langle c+a\rangle$) slip modes and the presence of twinning ($\left\{10\bar{1}2\right\}$ extension twinning (ET) and $\left\{10\bar{1}1\right\}$ contraction twin (CT)) results in highly asymmetric stress–strain characteristics. The presence of hard, elastic reinforcements further complicates the situation by introducing complex stress states (Inem and Pollard, 1993; Szaraz et al., 2007; Deng et al., 2012). Chua et al. (1999) observed that the 0.2% yield strength (YS), ultimate tensile strength (UTS) and ductility for Mg alloy with 10 volume percent SiC reinforcement (size from 15 to 50 μm) were all lower than their un-reinforced Mg-alloy counterparts. On the other hand, Rauber et al. (2011) showed improvement in the YS and UTS with SiC volume fraction increasing from 5% to 30%. For extruded Mg MMCs, Garcés et al. (2005) reported decrease in the tension–compression asymmetry ratio with increasing volume fraction of $\mathrm{SiC_p}$ from 5% to 13%. They indicated that the matrix texture dominated the response in comparison to the strengthening effects due to grain size and load transfer from the matrix to the reinforcement. They also reported weakening of the basal texture with increasing reinforcement volume fraction. More recently, Garcés et al. (2012) also reported systematic reduction in ET activity with increasing reinforcement volume fraction for similar Mg MMCs.

These complex and at times seemingly paradoxical experimental observations are attributed to the interactions between the deformation mechanisms in Mg, which depend on texture and reinforcement details. However, a clear understanding of how reinforcement morphology affects the deformation micromechanics in Mg matrix is missing, which calls for systematic investigations. To this end, computational investigations that adopt accurate description of HCP plasticity can provide fundamental insights into the micromechanics of Mg MMCs. Motivated by these objectives, we performed computational investigations of idealized Mg MMC microstructures using a crystal plasticity model (Zhang and Joshi, 2012). In this paper, we present the results of that investigation. In particular, we elaborate on the effects of the reinforcement shape and alignment on: (i) the macroscopic flow response, (ii) the micromechanics of flow hardening and (iii) the tension–compression flow stress asymmetry.

In the next section, we discuss the details of finite element modeling, simulation set up and material model that was adopted in our investigation.

2. Details of Mg MMC models

The microstructural design variables that influence the mechanical behavior of an MMC are: (i) matrix texture; (ii) matrix grain size, (iii) reinforcement size, (iv) reinforcement volume fraction, (vi) reinforcement shape, (v) reinforcement alignment, and (vi) reinforcement distribution. Obviously, considering all these design variables in a single analysis is a formidable task. In order to keep the problem tractable, we made the following assumptions in setting up the simulation models. First, we considered two relatively dilute reinforcement volume fractions, $f_r = 0.05$ and 0.10. Second, we ignored the effects of the matrix grain size and reinforcement size. Finally, we considered only regular arrangement of reinforcements thereby avoiding complicating effects of reinforcement clustering. In the following, we briefly discuss considerations pertaining to matrix texture, reinforcement shape and its alignment with respect to crystallographic orientation.

2.1. Matrix texture

Given the strong orientation dependence of Mg stress–strain characteristics, it is expected that any strengthening due to reinforcement addition will be influenced by the underlying texture. While it will be useful to consider representative volume elements (RVE) comprising textured polycrystalline matrix with embedded inclusions, such an exposition is computationally prohibitive at this stage, especially from the viewpoint of capturing both the micromechanics and its macroscopic effects. We considered a computationally simple alternative, which is a unit cell comprising a single crystal with an embedded inclusion, subjected to periodic boundary conditions (b.c.s). In addition, we only considered situations where these unit cells were loaded perpendicular to the c-axis in tension or in compression. This invariably places some constraints: it