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Precipitation hardening effects on extension twinning in magnesium alloys

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ABSTRACT

Precipitation is an efficient method to strengthen metallic materials. While precipitation hardening effects on dislocation slip have been studied extensively in the past, the influence of precipitates on twinning mediated plasticity and the development of corresponding hardening models that account for twin-precipitate interactions have received less attention. Here, the interaction of {10–12} extension twin boundaries (TBs) in pure magnesium with precipitates of plate-, sphere- and rod-like shapes is studied using molecular dynamics (MD) simulations. We find that TBs that engulf precipitates are absorbed by the precipitate-matrix interfaces, and the precipitates are neither twinned nor sheared but deform elastically leading to their rotation. TBs can pass small precipitates (length ≈ 20 nm) and remain intact. In contrast when TBs are interacting with large precipitates (length ≈ 50 nm), basal dislocations or stacking faults nucleate from the interfaces, causing local plastic relaxation. The stress field around a plate-like precipitate as calculated in the MD simulations suggests that a strong back-stress is imposed on the TBs. We then coarse grain these mechanisms into an analytical mean field model of precipitation hardening on twinning in magnesium alloys, which is based on the energy conservation during the TB-precipitate interaction. The model is in good agreement with the current MD simulations and published experimental observations. The hardening model shows that spherical precipitates have the strongest hardening effect on twinning, basal and prismatic plate-like precipitates have a medium effect while rod-like precipitates exert the weakest influence. We also find that most types of precipitates show a stronger hardening effect on twinning mediated plasticity than on basal dislocation slip. Finally, prismatic plate-like precipitates are predicted to have reasonable hardening effects on both twinning and basal slip. These results can help guiding the development of magnesium alloys with enhanced strength and ductility.

1. Introduction

Precipitation strengthens metallic alloys, making it a key mechanism for improving the mechanical properties of structural materials (Jiang et al., 2017). Since its discovery over a century ago (Wilm, 1911), numerous hardening mechanisms have been

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proposed for steels and aluminum alloys (Ardell, 1985; Argon, 2007; Seol et al., 2017). Although magnesium (Mg) alloys have received growing attention driven by the engineering demand for structural weight reduction in the automotive and aerospace industries (Agnew and Duygulu, 2005; Luo, 2013; Mordike and Ebert, 2001), the mechanisms involved in the precipitation hardening in Mg alloys remain a matter of debate (Nie, 2012). Generally speaking, the precipitation hardening effect in Mg alloys is typically much weaker than that observed in Al alloys. As an example, in AZ91 (Mg-9Al-1Zn) alloys with a 15% precipitate volume fraction the strength is increased by 0.067G, where G is the shear modulus, while in 7075 Al alloys with a 5% precipitate volume fraction the strength is improved by 0.3G (Hutchinson et al., 2005). This much weaker precipitation hardening effect in Mg alloys is typically attributed to the precipitate shapes and orientations, associated dislocation mechanisms, as well as the activation of deformation twinning (Nie, 2012).

The strengthening induced by second phase precipitates can be attributed to their interactions with the elementary carriers of plastic deformation, such as dislocation slip and twinning. In hexagonal close-packed (HCP) crystals like Mg, precipitate shapes are either plates that are parallel to the basal plane of the matrix as in MgAl alloys, or rods that are parallel to the c-axis as in MgZn alloys (Celotto, 2000; Nie, 2012; Polmear, 1994). In terms of plastic deformation mechanisms, dislocation slip predominantly occurs on basal planes with additional slip occurring on prismatic and pyramidal planes, depending on the ratio between the longitudinal (c) and basal (a) crystal lattice parameters. In addition, twinning is a common deformation mechanism in HCP crystals, and can be classified into extension and contraction twinning according to the strain that is carried out along c-axis (Kelley and Hosford, 1967).

The pioneering work of Nie (2003) investigated the effects of precipitate shape and orientation on strengthening and showed that the $Mg_{17}Al_{12}$ plate-like precipitates cannot effectively impede basal slip. As a result, the precipitation hardening effect in AZ91 alloys is much weaker than that in Al alloys (Clark, 1968; Hutchinson et al., 2005). It was also predicted that prismatic/pyramidal plate-like precipitates have a strong blocking effect on basal slip (Nie, 2003), but are weak in impeding prismatic slip and twinning mediated plasticity (Agnew et al., 2013). While the blocking effect of basal plate-like precipitates is weak on basal slip ($\sim$5 MPa), it is much stronger on prismatic slip and twinning, namely, on the order of $\sim$25 MPa (Stanford et al., 2012). Also, rod-like precipitates were observed to have reasonable blocking effects on prismatic slip in Mg-6Zn alloys (Jain et al., 2013) and basal slip in Mg-5Zn micropillars (Wang and Stanford, 2015), but negligible effects on twinning-induced plasticity and pyramidal slip (Wang and Stanford, 2015). For twinning deformation, a hardening model based on twinning dislocations bypassing precipitates was developed (Nie, 2012). In this model the plate-like precipitates were predicted to have a stronger blocking effect on TB motion as compared to spherical precipitates.

From the aforementioned studies, it can be summarized that different types of precipitates contribute differently to the hardening effects on the different deformation modes in Mg alloys. No single precipitate type is capable of inducing a strong hardening effect on all the deformation modes in Mg alloys. Given so many variants and combinations of precipitate shapes, orientations and deformation modes, it is necessary to develop a systemic understanding of precipitation hardening effects in Mg alloys, since precipitation is a key strategy for adjusting their tension–compression asymmetry and improving their overall strength and ductility (Hidalgo-Manrique et al., 2017; Jain et al., 2010; Robson et al., 2011).

The precipitation hardening effects on twinning deformation were reported to be much stronger than those on basal dislocation slip (Stanford et al., 2012), and thus can be utilized to improve the material strength. Hence, a physics-based model capable of predicting the precipitation hardening effects exerted by different types of second phase precipitates on twinning is of high interests. However, disagreements still exist in the literature regarding the basic nature of the interaction between twin boundaries (TBs) and precipitates, yet, understanding these effects is a precondition for including them in a physics-based model. As early as 1965, Clark reported that rod-shaped precipitates are re-orientated in {10–12} twins of Mg-5Zn alloys and concluded that this is a result of the precipitates being sheared by the twins (Clark, 1965). Later, Gharghouri et al. reported that precipitates in a Mg-7.7Al alloy are engulfed by the TB but not twinned, leading only to a rigid body rotation (Gharghouri et al., 1998), as also observed in recent experiments of Mg-6Zn (Jain et al., 2015), AZ91 (Stanford et al., 2012), Mg-5Zn (Robson et al., 2011) and Mg-5Zn micro-pillars (Wang and Stanford, 2015). However, Stanford et al. observed that precipitates are neither twinned nor rotated in twinned Mg-Zn alloys, whereas many basal stacking faults appear within the twins (Stanford and Barnett, 2009).

Most theoretical studies on precipitation hardening in the literature focused on the interaction between dislocations and precipitates, such as the Orowan mechanism (Liao et al., 2014; Nie, 2003; Orowan, 1948). However, the interactions between TBs and precipitates have received much less attention. Unlike dislocations which are line defects, TBs are interfaces and thus involve different types of mechanisms leading to strain hardening (Christian and Mahajan, 1995). Nevertheless, the classical Orowan model was still utilized to explain the precipitation hardening effects on twinning (Hidalgo-Manrique et al., 2017; Nie, 2012). This was rationalized by the fact that twinning deformation is mediated by the glide of twinning dislocations on the twin planes. However, the Orowan model is not capable of adequately reflecting the difference between dislocations and TBs, and was shown to substantially underestimate the precipitation hardening effects on twinning by up to 75% (Hidalgo-Manrique et al., 2017; Robson et al., 2011; Stanford et al., 2012). This is because in addition to the obstacle effects of precipitates on TBs, a long-range interaction acting as a local back-stress exists between the precipitates and twinning dislocations (Brown and Stobbs, 1971; Jain et al., 2015; Robson, 2016). Then based on the back-stress calculations, Robson et al. showed that the critical resolved shear stress (CRSS) on twinning deformation is proportional to the precipitate volume fraction (Bate et al., 1981; Robson et al., 2011). Yet, this prediction is in poor agreement with experimental observations, in which the CRSS was shown to saturate with increasing precipitate volume fraction (Stanford et al., 2012). Robson et al. attributed this overestimation to the lack of a plastic relaxation around the precipitates in the back-stress model (Robson et al., 2011), as is typically observed in Mg-Al and Mg-Zn alloys (Gharghouri et al., 1998; Stanford and Barnett, 2009). Therefore, a physical model capable of accurately predicting the precipitation hardening effects on twinning is still unavailable. In Mg alloys, twinning deformation is very common. The lack of the precipitation hardening model on twinning would