The Effect of Precipitates on Twinning in Magnesium Alloys

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The Effect of Precipitates on Twinning in Magnesium Alloys**

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Understanding how to strengthen against twin mediated deformation is critical to controlling the mechanical properties and formability of magnesium. One route to strengthening is through precipitation of shear resistant particles. This paper presents the current understanding of how precipitate particles and $\{10\bar{1}2\}$ *twins interact in magnesium, and how this influences strength. Precipitates increase the yield stress for twin dominated deformation but none of the current models reliably predict the strengthening effect. Precipitates have never been observed to completely suppress twinning, but usually lead to an increased number of narrower twins. Precipitates are not effective in increasing the stress for twin nucleation sufficiently to preferentially activate alternative deformation modes, but the effect on the stresses for both twin propagation and growth are significant. In the propagation stage, twin tips overcome precipitates by bowing of multiple twinning dislocations. For thick twins this can probably be assisted by pile up of twinning partials behind the tip. During growth, precipitates increase the stress to propagate new twinning steps, mainly due to increasing the unrelaxed back-stress. Since nucleation, propagation, and growth of twins all*

have to occur before macroscopic yield, a complete model to predict the strengthening effect must consider all of these stages.

1. Introduction

Magnesium is the lightest structural metal and is therefore attractive for weight reduction in applications such as automotive, aerospace, and armour [1]. Magnesium is fundamentally different from the more common iron or aluminum-based alloys used in these applications since it has a hexagonal close-packed (HCP) crystal structure. An important consequence is that magnesium has a limited number of slip systems able to accommodate an imposed strain, and twinning becomes an important deformation mode. The prevalence of twinning, and in particular the $\{10\bar{1}2\}$ twinning mode, is critical in determining the macroscopic mechanical properties of magnesium alloys. For example, twinning plays a key role in strain localization and ultimately failure during loading [2]. Twinning is also responsible for the mechanical asymmetry (differences in strength in tension and compression) observed in many magnesium alloys [3]. By its nature, twinning can only accommodate a limited and geometrically defined amount of strain, and this contributes to the poor room temperature formability commonly observed in magnesium alloys. Finally, twinning results in a rapid and large reorientation of the lattice inside the twin, and this often determines the work hardening response of magnesium alloys.

Given its importance, there has been a strong focus on attempting to understand (and model) the nucleation, propagation, and growth of twins in magnesium (e.g. [4-9]). One objective of this work is to develop strategies to control deformation by twinning (e.g. to strengthen against twin mediated deformation). One of the most potent mechanisms used to strengthen against slip-mediated deformation in alloys is through the precipitation of second phase particles that act as obstacles to dislocation motion. Through a detailed understanding of this mechanism, aluminum alloys can now be readily produced that are 100 times stronger than pure aluminum. Precipitation strengthening is also used in magnesium alloys, however the maximum potency of this strengthening is limited to 20 times that of pure magnesium [10]. The lack of effective strengthening against twinning is one of several factors that contribute to the relatively poor precipitation strengthening of magnesium alloys [10].

It should be noted that deformation twinning is not only important in magnesium, but also in other industrial HCP metals (e.g. α-Ti, α-Zr). Many of these alloys also contain second phase precipitates. Therefore, understanding the interaction of precipitates and twins is also important in understanding the deformation behavior of these materials. Recently, this topic has received significant attention, with the focus of the work being on the easy ($\{10\bar{1}2\}$) twin mode in magnesium. This has been widely used as a reference system in which to understand the behavior of $\{10\bar{1}2\}$ twinning in hcp metals more generally.

This paper attempts to summarize the current understanding of precipitate/twin interactions in magnesium, which has the ultimate aim of developing a predictive model capable of use in designing magnesium alloys with increased resistance to twinning. Although this paper will focus on magnesium, many of the concepts proposed are also applicable to the most common twin mode in other HCP metals (the $\{10\bar{1}2\}$ twin) and so have implications for the mechanical behavior of α-Ti and α-Zr alloys.

2. Twinning in Magnesium

Magnesium, in common with other HCP metals, only undergoes easy slip in the basal compact direction $<\mathbf{11\bar{2}0}>$. Since slip in this direction has no c-component, it cannot accommodate any deformation along the c-axis direction. To accommodate deformation in the c-direction by slip requires formation and movement of <c+a> dislocations [11]. These dislocations require thermal activation, have a large Burgers vector, and non-planar core, all of which makes their activation at room temperature very difficult [12]. An alternative deformation mode is therefore activated, which is twinning. The easiest twinning mode to activate in magnesium (and the mode most commonly observed in other HCP metals) is the $\{\mathbf{10\bar{1}2}\}$ tensile twin [13]. This is referred to as a tensile twin in magnesium because it leads to an expansion along the c-axis direction. The remainder of this paper will focus on $\{\mathbf{10\bar{1}2}\}$ twinning, which because of its importance and prevalence has been the most intensively studied – and all discussion of twins will implicitly refer to this mode. The introduction to the $\{\mathbf{10\bar{1}2}\}$ twin in this section is necessarily brief, and a far more detailed discussion of twin nucleation and growth in HCP metals is given elsewhere ([5,6])

2.1.1. Geometry of Twinning

In geometric terms, deformation twinning is usually considered to involve a simple shear of the twinned material relative to the parent matrix along a direction η_1, and this leads to two planes that remain undistorted, the K_1 plane (in which η_1 lies) and its conjugate K_2 plane, which contains the conjugate shear direction η_2. A twinning mode is defined by K_1 and η_2 (or their conjugates), so for the $\{\mathbf{10\bar{1}2}\} < \mathbf{\bar{1}01\bar{1}} >$ twin mode in magnesium (the focus of this study) $K_1 = \{\mathbf{10\bar{1}2}\}$ and $\eta_2 = < \mathbf{\bar{1}01\bar{1}} >$ An important distinction between twinning and slip is that there is a unique and well defined amount of shear associated with each twin mode. In the case of the $\{\mathbf{10\bar{1}2}\}$ twin, the (simple) shear strain is γ=0.13. This simple shear can produce a maximum tensile strain along the c-axis of 6.5% [14]. Another important difference between twinning and slip is that twinning is unidirectional – i.e. since the $\{\mathbf{10\bar{1}2}\}$ twin always produces an expansion along the c-axis direction in magnesium, it will not be activated by c-axis compression. It is generally considered that the stress driving $\{\mathbf{10\bar{1}2}\}$ twinning is the resolved shear stress on the K_1 plane, although there remains a debate as to the significance of non-Schmid effects [15]. Twin nucleation is also stochastic in nature [9].

This simple geometric picture is significantly complicated by the constraints a twin will experience from surrounding parent material (leading to back-stresses [16-18]) and plastic relaxation processes (e.g. by slip or secondary twins). However, it is still useful because the geometry of the twin has many practical important consequences on the interaction with precipitates, as demonstrated later.

2.1.1. Twinning at the Atomic Scale

There are three stages to twinning, each of which is governed by distinct atomistic processes. These stages are nucleation, propagation (movement of the twin tip until blocked), and growth (or thickening), shown schematically in Figure 1(a). Nucleation is local phenomenon that usually occurs in the region of a grain boundary, where a stress concentration is present [9]. This involves reactions between grain boundary dislocations and stress-driven slip dislocations, combined with atomic shuffling. Several mechanisms for twin nucleation have been proposed on the basis of atomistic simulation [9]. Propagation involves the twin front moving across a grain until it gets blocked, either by another twin, grain boundary, or other obstacle (e.g. precipitate). The boundary between the twin (sheared) and parent (unsheared) material is considered as an array of twinning partial dislocations whose passage translates atoms from their position in the parent material to that in the twin. The twin boundary therefore consists of a stack of twinning partial dislocation loops – expansion of the loops leads to growth of the twin parallel to the twinning plane (Figure 1b). The Burgers vector for the twinning dislocation is very small (b~0.05nm [13]) much smaller than the smallest perfect Burgers vector for slip (0.32nm). This is important because many properties of a dislocation depend on the magnitude of the Burgers vector. The final stage of twinning is growth (thickening) of the twin, which requires nucleation and growth of new twinning dislocation loops [13].

It should be noted that it is usual in magnesium alloys to extract "effective yield" from the 0.1% proof stress, since the micro-yielding often leads to non-linearity in the initial portion of the stress-strain curve. For a crystal ideally oriented for twinning (Schmid factor 0.5), 0.1% plastic deformation corresponds to a twin volume fraction of 1.5% [19]. Even in a strongly textured polycrystal, this critical twin volume fraction is likely to be higher (>3%) [20]. Therefore, the "effective stress" for twinning derived from stress-strain curves will be influenced by all three stages described above. This will be demonstrated later.

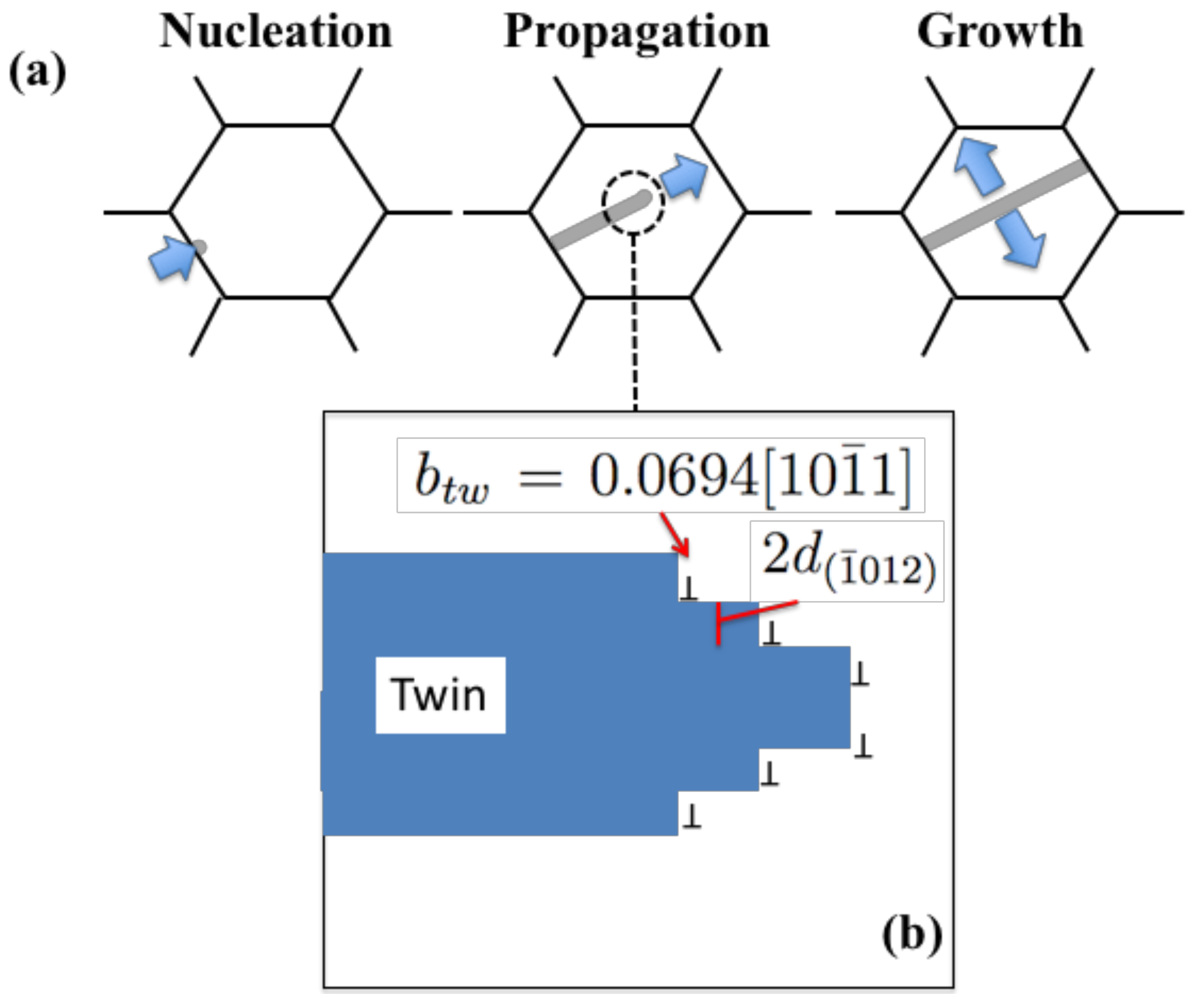

Figure 1 (a) The three stages in the formation of a twin; nucleation, propagation, and growth. (b) The dislocation model of a $\{\mathbf{10\bar{1}2}\}$ *twin tip showing the Burgers vector of the twinning partial dislocation (*$\boldsymbol{b_{tw}}$*).*

It should be noted that atomistic simulations reveal that the true growth mechanism of the $\{\mathbf{10\bar{1}2}\}$ twin in magnesium may be quite different from the simple classical picture, and involves the motion of zonal twinning dislocations (that spread over several lattice planes), with shuffling dominating the initial nucleation stages [9][21]. Nevertheless, for the remainder of this paper, it will be assumed that twinning occurs by the standard shear/shuffle method involving expansion of an array of partial dislocation loops. In understanding how precipitates influence twinning, the precise mechanism by which the twinning shear is obtained is not of critical importance.

Introducing a region of sheared (twinned) material into a constraining matrix (parent) will lead to the generation of internal stresses. These stresses will act against further growth of the twin (back-stress). The Eshelby inclusion method can be used to determine the magnitude and nature of the internal stress field assuming entirely elastic deformation. For a typical situation, these stresses can exceed 100 MPa in the parent, and 200 MPa in the twin [15,22]. This is sufficiently large to lead to plastic relaxation, producing zones of plastic deformation ahead of the twin tip, as demonstrated in [22]. A number of analyses of the stresses around a twin have been performed using finite element crystal plasticity methods [16-18]. These analyses show that the stress field established inside and outside the twin is quite complex, and the local stresses ahead of the twin tips (driving the propagation of the twin) can be significantly greater than the applied stress. Therefore, in making a full consideration of the effect of precipitates on twinning, it is important to consider not only the direct effect of precipitates on the twin itself, but also their effect on the plastic relaxation processes that accompany twin propagation and growth.

3. Twinning in Precipitate Containing Alloys – Observations

3.1. Mechanical Properties

A number of recent studies have focused on understanding the effects of precipitates on deformation in magnesium alloys, and on twin mediated deformation in particular. These studies broadly fall into three types: investigation of single grains, using a method such as micro-pillar compression [23], deformation of strongly textured polycrystalline material (wrought alloys) in which the loading direction can be chosen to favour the activation of twinning (e.g. [24-27]) and deformation of as-cast (weak or randomly textured material), in which only some of the grain population is well oriented for twinning [28]. Polycrystalline material is more representative of practical alloys and provides the necessary grain boundary nucleation sites for twin formation. However, even in strongly textured polycrystalline material, slip will make a significant contribution to the deformation. In this case, making a connection between the macroscopic stress-strain response and an effective stress for twinning requires either the use of a very approximate Schmid factor approach (e.g. [24]), or a full crystal plasticity model (e.g. [27]). In principle, single crystal studies should be easier to interpret, but the problem is that the environment for twin nucleation is completely different in a single crystal study and thus the applicability of the results to the practical polycrystalline case is limited. The only detailed single crystal study performed to date to investigate the effect of precipitates on twinning did not give consistent results, and this was explained by the observation that in the single crystal case twin nucleation is difficult and inherently stochastic, overwhelming any effect particles may have on the twinning process [23]. Nevertheless, the observation that no consistent difference in the stress for twin nucleation was measured when precipitates were present does suggest that the direct effect of precipitates on the stress for twin nucleation does not dominate the nucleation behaviour.

In the polycrystalline case a number of attempts have been made to determine an effective increase in the critical resolved shear stress (CRSS) for twinning due to precipitates – assuming that twinning is controlled by a CRSS. As mentioned, this requires a crystal plasticity model or use of an averaged Schmid Factor to relate the CRSS to the global measured mechanical response. Typically, the visco-plastic self-consistent (VPSC) framework developed by Lebensohn and Tomé [29] is the crystal plasticity model used for this purpose. However, neither the VPSC model nor the estimated average Schmid factor consider the true local stress state, and both methods are likely to introduce significant error. Nevertheless, the results give a useful insight into the magnitude of the strengthening effect that precipitates have against twinning. To date, these studies have focused on the most widely used classes of precipitation strengthened magnesium alloys, Mg-Al-Zn (AZ series) and Mg-Zn (Z series) [24,28,30,31]. An example of the measured increase in flow stress when precipitates are present in an AZ91 extrusion loaded to activate twinning (axial compression) is shown in Figure 2(a). It can be see that the yield stress is increased by >50 MPa, and this also strongly reduces the tension/compression asymmetry, as discussed in detail elsewhere [3].

Examples of estimated increments in the CRSS for twinning derived from such studies are summarized in Table 1. In all cases, the CRSS increment is calculated by comparing the CRSS before and after aging (to peak strength unless otherwise stated). It is assumed that the CRSS increment can be attributed fully to the effect of precipitate particles, since it was confirmed in most studies that there was negligible change in the grain structure or texture during aging. The loss of solute strengthening as precipitates form will have an effect on the CRSS increment. Following previous work, it is estimated this leads to a 10MPa reduction in strength in AZ91 [24] but has a negligible effect in Z5 [27]. The CRSS increments reported in Table 1 are corrected for this solute loss effect.

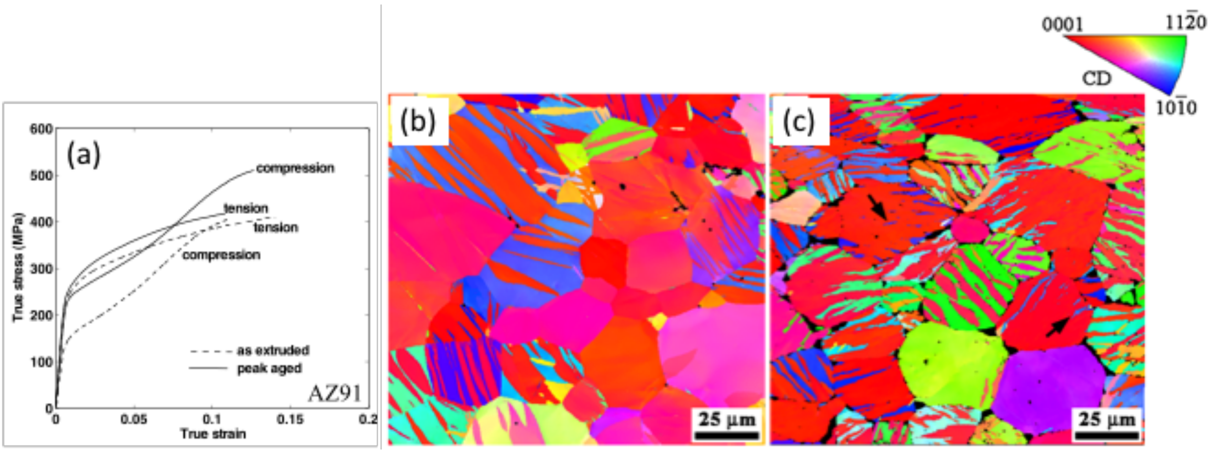

Figure 2 (a) Stress-strain response of a strongly textured AZ91 extrusion tested before and after ageing in compression and tension. Compressive yield is controlled by twinning and ageing can be seen to increase the compressive yield point by >50MPa [24]. (b,c) EBSD maps of strongly textures AZ91 compressed to active twinning (b) without precipitates (c) after precipitation. The inverse pole figure colouring is relative to the compression direction (CD) [33]. Reproduced with permission 4446450542445, 2012, Elsevier.

Table 1. Estimated increase in critical resolved shear stress (CRSS) for $\{10\bar{1}2\}$ *twinning due to the formation of precipitates*

Alloy	Precipitate type	Processing	Method	CRSS increment [MPa]	Reference
AZ91	Basal plates	Rolled, peak aged	Schmid Factor	31[a]	[24]
AZ91	Basal plates	Rolled, peak aged	Schmid Factor	46[a]	[31]
AZ91	Basal plates	Rolled, overaged	Schmid Factor	5	[33]
AZ91	Discontinuous Precipitates	Extruded	Schmid Factor[b]	50	[30]
Z5	c-axis rods	Extruded	VPSC	62	[25]
Z6	c-axis rods	Extruded	VPSC	29	[27]

[a] Identical processing and ageing conditions [b] Estimated Schmid Factor M=0.4 as no texture data reported

Table 1 shows that there is a considerable scatter in the results from different studies on the same alloy, but in most cases a strengthening effect of between ~30-60 MPa is recorded. The scatter is evidenced by the 15MPa discrepancy between two studies of identically processed material (AZ91, rolled and peak aged), where the CRSS difference is a result of the different methods used to determine the onset of twinning [24,31]. In one study [33], a much lower strengthening effect was recorded (5 MPa). In this case the material was over-aged at a high temperature for a long time to produce very large (>1μm) and widely spaced plates. These evidently provide poor strengthening, even when the stress was applied in a direction where twinning is expected to control yield.

Even accounting for the scatter in results, it can be seen that a large difference in strengthening effect can be obtained in the same alloy depending on the ageing treatment used to develop the precipitates. This is also seen in comparing results from the same material aged to different states. For example, in Z6 strengthening effects of 4, 29, and 11 MPa were recorded for underaged, peak-aged, and over-aged states respectively [27].

It is noteworthy that these strengthening increments are comparable (on the same order) with precipitation strengthening against slip [26,27]. This is consistent with the observation that the presence of precipitates does not usually lead to a marked change in twinning activity (twin volume fraction) as discussed below.

3.2. Microstructure

The first important point to note is that precipitates are never observed to completely suppress twinning in magnesium (Figure 2(b,c)). Indeed, twins can propagate successfully even though alloys with lamella microstructures formed by discontinuous precipitation [30]. The volume fraction of twins is generally either unaffected by precipitation or slightly reduced [28,32]. The size and number of twins is more strongly influenced, with an increased number of thinner twins formed when precipitates are present [25,28]. This has been rationalized on the basis that precipitates influence the stress required for twin growth more than that for nucleation, therefore biasing the twinning response towards more nucleation and less thickening [32]. This is perhaps not surprising, since the local events that lead to the formation of a twin nucleus take place within ~200nm of a grain boundary [9], and the grain boundary precipitate free zone widths in magnesium alloys are typically much wider than this. Therefore, the very local shear and shuffling processes that occur in the grain boundary region are unlikely to involve direct interaction with precipitates, although precipitates will influence the global (and local) stresses that drive the nucleation processes.

Partridge [34], using optical microscopy and surface oxidation performed an early study of the interaction of twins with particles. It was shown that the twin boundary deviated on approaching the oxide particles, which acted as pinning sites against twin boundary migration. Eventually, the incoherent boundary formed by deviation from the ideal twinning plane engulfed the particles, leaving them unsheared and surrounded by small regions of matrix orientation, which were classified as microtwins inside the primary twin.

The observation that the twin boundary does not produce a shearing of the particles is common to most cases studied to date (in both Mg-Al and Mg-Zn alloys) [24,25,28]. Only in the case of very thin, coherent precipitates (e.g. Mg-Gd-Zn [35]) or small metastable precipitates in the Mg-Zn system has shearing been observed [36]. Gharghouri et al. performed a detailed study of the interaction of twins and precipitates in Mg-8.5wt% Al [37]. They confirmed the precipitates are not sheared when entering the twin. In addition to becoming embedded inside a twin, precipitates have also been observed to block twin tips. This sometimes leads to the twin “pinching off” at the precipitate, which may be due to blocking and re-nucleation (discussed later). Examples of this pinching off behavior due to large impurity particles are shown in Figure 3(a). Figure 3(b) shows an example of a twin boundary undergoing deflections when engulfing rod shaped precipitates (Mg-Zn system) and

Figure 3(c) shows a twin tip being blocked at a plate shaped precipitate (AZ91 alloy). It is clear from these observations that a variety of different interactions are possible.

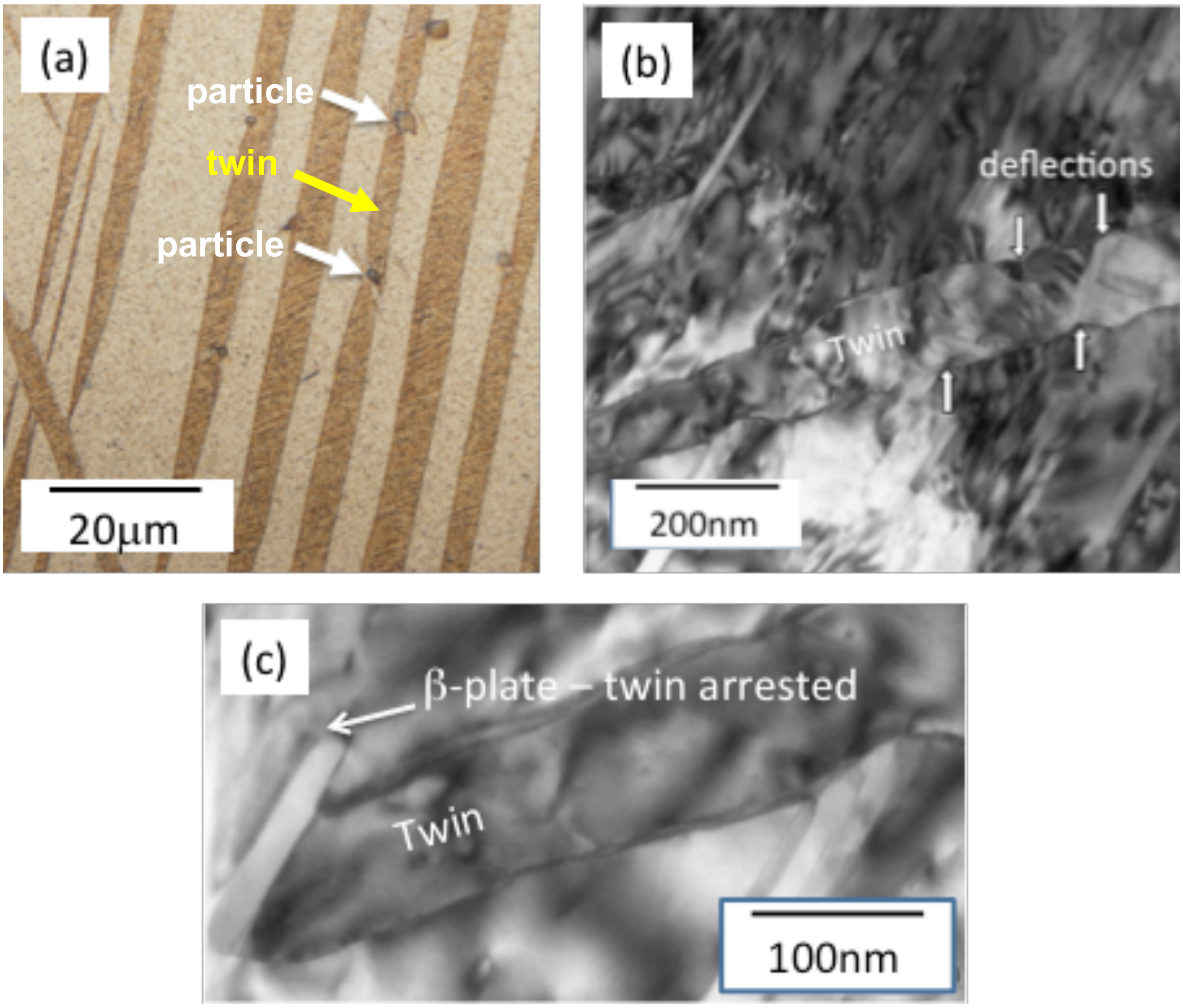

Figure 3 Example of precipitate/twin interactions observed in magnesium alloy microstructures (a) Twins "pinched off" at large intermetallic impurities in AZ91. (b) A twin boundary deflected on intersecting rod-shaped precipitates in Mg-Zn, (c) A twin tip blocked by a plate shaped β precipitate in AZ91.

When precipitates are small (nm to micron scale) and have volume fractions in the range typically achieved in age hardenable magnesium alloys (~2-10%) it is inevitable that twins will be required to engulf some of the precipitate population as they propagate and grow. If the precipitates remain unsheared, this leads to a strain incompatibility, which must be accommodated. Gharghouri et al. estimated the maximum incompatibility strain to be approximately 6.5%. Accommodation of this strain by elastic deformation would lead to large additional internal stresses. Instead, Gharghouri et al. proposed that the incompatibility is accommodated by local plastic deformation, and evidence for this was provided by intense dislocation activity observed at the regions where the highest incompatibility strains would be expected [37]. Gharghouri et al. also noted a deviation of the twin boundary from its ideal habit plane to avoid intersecting particles, and provided an explanation of how this can occur by an accumulation of twinning dislocations. Further investigation of the interaction of twins and plate shaped precipitates in a Mg-Al alloy confirmed that the precipitates are not sheared [24], but demonstrated that they do become bent (elastically) as they enter the precipitates. The bending occurs when part of the precipitate is anchored in the parent whilst part is embedded in the sheared (twinned) material. An example of this interaction for a large basal plate precipitate partially embedded in a twin in AZ91 is shown in Figure 4. Diffraction pattern analysis confirms that the precipitate is not sheared, (full details elsewhere [24]).

When the precipitate is fully engulfed, part of the simple shear associated with twinning can be accommodated by a rigid body rotation of the precipitate, whereas the pure shear component leads to the incompatibility as discussed by Gharghouri [37]. However, as the twin is partly through the engulfing process, the precipitate is not free to undergo a rigid body rotation as part of it remains anchored in the parent. In this case, the strain incompatibility will be at its greatest.

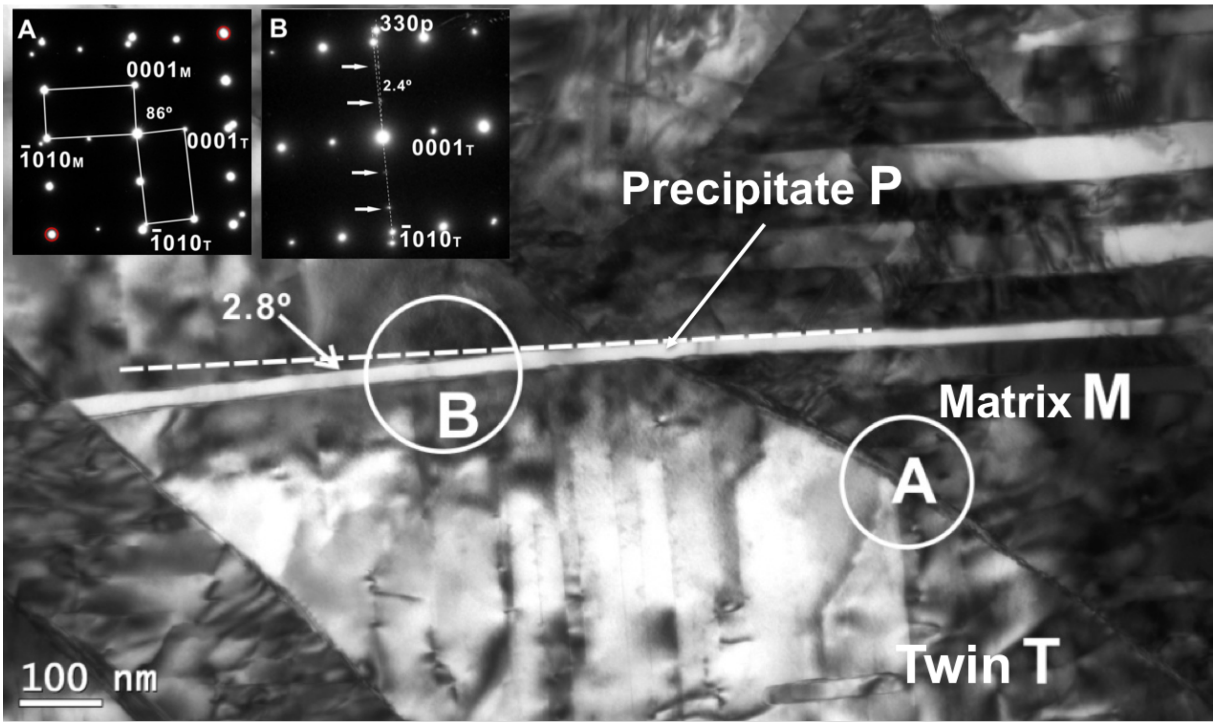

Figure 4 Example of large basal plate precipitate partially embedded in a twin in AZ91. Diffraction pattern A at the twin interface shows the expected orientation relationship between matrix (M) and twin (T). Diffraction pattern B demonstrates the precipitate (P) does not adopt the full twinning shear (details in [24]). Reproduced with permission 4446450542445, 2012, Elsevier.

If the local plastic relaxation processes around the precipitate occur before the precipitate is fully embedded in the twin, then the full theoretical rigid body rotation may not be observed since all (or part) of the strain incompatibility will already have been removed. Measurements of the rotation of precipitates suggest that in most cases all or part of expected rigid body rotation occurs [25,37].

The misfit that will be created when an unsheared particle is embedded inside a twin will depend on the particle shape and orientation. Robson [38] performed an analysis of this effect using the Eshelby method. Of the common precipitate types observed in magnesium alloys, plates on the prismatic plane (as observed in Mg-rare earth alloys) were predicted to lead to a greater misfit than plates on the basal plane (as in Mg-Al alloys), which in turn led to a greater misfit than rods aligned in the c-axis direction (as in Mg-Zn alloys). However, since this approach is purely elastic, the critical role of plastic relaxation is not included.

It is nevertheless reasonable to expect that precipitates leading to a greater level of misfit will provide a greater strengthening effect, suggesting prismatic plates to be most effective. This is consistent with the observation that such precipitates provide the maximum age hardening response in magnesium alloys [39]. However, there are additional complications since the solute rare-earth in alloys that form prismatic plate precipitates also has a profound effect on the texture and directly inhibit twin growth [40,41]. A direct determination of the strengthening effect of prismatic plates against twin growth remains an outstanding challenge.

3.3. Predicting Strengthening Effect

The Orowan equation provides a useful physical understanding of the effect precipitates have against slip dislocations. This equation can predict to reasonable accuracy the strengthening effect of non-shearing precipitates against slip and has proved a vital tool in alloy design when slip dominates deformation. There are various variations of the basic Orowan equation, with that given by Bacon et al. [42] being appropriate for screw dislocations:

$$\Delta\tau = \frac{Gb}{2\pi(1-\nu)l}\ln\frac{\bar{D}}{r_0} \tag{1}$$

Where G is the shear modulus, b is the Burgers vector of the dislocation, ν is the Poission's ratio, l is the gap between particles, $\bar{D}$ is harmonic mean of the particle spacing and particle diameter, and r_0 is the inner cut off radius (usually set equal to b).

It would be very useful to have an equivalent simple equation to predict the strengthening effect of precipitates against twin-mediated deformation, but it remains unclear what the physical basis for such an equation should be.

Several methods have been proposed to calculate the precipitate strengthening against twin growth. The most obvious is to directly apply the Orowan equation (i.e. a variant of Equation 1), treating the twinning partial dislocation in the same way as a slip dislocation. However, as Equation 1 shows, the Orowan strengthening is directly proportional to the Burgers vector (b) of the dislocation undergoing bowing, and since b for the twinning partial is approximately 5 times smaller than that for slip, the calculated strengthening effect is also around 5 times smaller, which is inconsistent with measurements (Table 2).

An alternative method is to assume that it is the additional long range back-stress arising from the strain incompatibility that dominates strengthening. It is difficult to calculate this accurately because local plastic relaxation effects will reduce this back-stress. Nevertheless, in some cases, the back-stress under a fully elastic assumption does give a reasonable approximation to the measured strengthening effect [27]. However, generally such a simple back-stress calculation greatly overestimates the strengthening effect [43]. Usually, the approximate methods used to calculate the back-stress assume the precipitates to be completely rigid, but as discussed by Robson [38], the intermetallics that form precipitates in magnesium are not very stiff, and their elastic deformation has a marked effect in reducing back-stress. Plastic relaxation will further reduce the back-stress. A rigorous calculation of plastic relaxation effects is difficult and requires a precise definition of the microstructure included in a crystal plasticity finite element framework.

An important distinction between Orowan and back-stress based calculations (for particles of the same shape and orientation) is that the critical microstructural parameter in the Orowan equation is the interparticle spacing, whereas in the back-stress calculation the critical parameter is the volume fraction. It is clear from published strengthening data that elastic back-stress based calculation alone cannot explain the observations, since the strengthening effect is seen to vary greatly between (for example) peak aged and overaged conditions, even when the volume fraction, shape, and orientation of precipitates are similar.

Recently, Barnett has proposed an alternative method for calculating the strengthening effect. This recognizes that the twin tip during the propagation stage is not a single twinning partial dislocation, but is a super-dislocation wall, consisting of a stack of partial dislocations. The stress required to bow a twin front that consists of n twinning dislocations is given by Hirth as [44]:

$$\tau_s = \frac{nGb}{4\pi(1-\nu)\lambda} \ln \frac{\lambda}{(n-1)h} \qquad (2)$$

Where n is the number of dislocations in the wall and λ is the distance over which the bow is occurring (equivalent to l in equation 1 for the case of bowing between precipitates).

This equation implies the bowing stress increases in proportion to the number of dislocations in the wall and for a twin tip that exceeds the minimum thickness for growth (n~100 [45]), the bowing stress may be orders of magnitude greater than that for a single bowing partial [45]. Such a calculation will over-estimate the strengthening effect (by about a factor of 5 for a realistic twin thickness). However, a further complexity arises because as pointed out by Barnett and Wang [46], it is not necessary for the entire twin tip to bow the obstacle simultaneously. Instead, bowing with a lower stress will be possible if only the leading partials are initially involved. As demonstrated by dislocation dynamics simulations [46], in this case the trailing partials may actually lower the bowing stress by pushing the leading partials due to the interaction force between dislocations. Thus, a rather complex situation can arise where the bowing stress is predicted to initially increase with twin thickness (due to the need to bow multiple partials) before decreasing (due to the interaction between the leading and trailing partials). In this model, the stress for bowing therefore also becomes a function of the twin width during propagation.

Table 2 gives a summary of the calculated strengthening against twinning using the various methods discussed above, compared with experimental measurements. Barnett and Wang's dislocation dynamics based strengthening calculations are not included since the aim is to compare only predictions based on simple analytical models [46]. As Table 2 suggests, the current methods proposed for calculating the strengthening effect of precipitates against deformation by twinning give answers that vary by a factor of more than 20. None of the models give good agreement with all the experimental data. Not only are the models inaccurate, they are also qualitatively incorrect; for example, they do not correctly predict the rank order of strengthening effects.

Each of these modelling approaches identifies different precipitate parameters as being most important to maximize strengthening against twinning. Therefore, the current methods are not useful tools for alloy design. A key issue is the lack of fundamental understanding of how precipitates influence twinning, and which stage of the twinning process is most strongly influenced (nucleation, propagation, or growth). This will be addressed next.

Table 2. Calculated increases in effective CRSS for twinning based on currently proposed methodologies compared for precipitates of effective diameter d, length l (or thickness t), and volume fraction V_f. Experimentally derived values shown for comparison (see Table 1). All values in MPa, rounded to nearest whole MPa.

Ppts	d [nm]	t or l [nm]	V_f	Twin single	Twin super	Back-stress	Basal in twin	Exp. [MPa]	Ref
Basal plates	313	45	13%	7	219	247	189	31,46[a]	[24,31]
Basal plates	2800	400	4%	1	8	81	4	5	[33]
c-axis rods	14	250	1.8%	8	264	16	10	29	[27]
c-axis rods	20	120	2.3%	7	225	21	16	62	[25]

[a] Identical processing and ageing conditions

4. Proposed Mechanism for Precipitate Effect on Twinning

There is now a sufficient understanding of $\{\mathbf{10\bar{1}2}\}$ twin formation in magnesium to draw some initial conclusions about the likely processes by which precipitates influence strength when twinning is activated. In what follows, it is reasonably assumed that macroscopic yield is determined by the initial twins to nucleate, propagate, and grow leading to the relaxation of stress in the grain undergoing twinning.

Nucleation has already been discussed, and the evidence suggests that the typical precipitate distributions obtained in magnesium alloys do not lead to a strong suppression of nucleation. It is possible that elimination or narrowing of the precipitate free zone may directly influence twin nucleation, but it is difficult to achieve this in a practical magnesium alloy.

The next stage of twinning is propagation. Propagation is driven by the system seeking to relax the elastic strain energy that has accumulated in the grain in which the twin forms. It is generally accepted that the stress required for nucleation is significantly higher that that required for propagation [45], so there is an excess stress available to drive the propagation of the twin. This is analogous to the nucleation and then sudden growth of a crack. Whether precipitates provide effective obstacles to twin propagation will depend on whether they can exert an inhibiting effect on the twin front that exceeds the excess stress driving twin propagation. Finite element (FE) simulations show that stress acting on the twinning dislocations at the twin tip is strongly dependent on the amount of plastic relaxation that takes place in the surrounding matrix [16,17]. For typical values of grain size and twin aspect ratio, the forward stress at the twin tip may be two to three times the applied resolved shear stress. This means that in a typical case, the forward stress exceeds 100MPa [16].

In the propagation stage, there are a number of different mechanisms by which the twin tip could negotiate a particle, and these are shown schematically in Figure 5. Experimental evidence exists for each of these mechanisms. One important factor that is likely to govern which mechanism operates is the ratio between the twin thickness and the blocking particle size, resolved in the twin thickness direction (indicated as l in Figure 5). When the twin thickness is larger than l, (Figure 5(a)) part of the twin tip will not be blocked and will be able to continue growing. Alternatively, if l is small or the twin tip approaches to the end of the precipitate, then a small deflection from the ideal habit plane will be sufficient to enable the tip to continue propagation (b). This mechanism was proposed by Gharghouri et al. based on their observations and they provide an explanation for the interaction that leads to the deflection of the twin tip [37]. For this mechanism to operate, the forward force on the twinning partials must be sufficient to provide new steps in the twin boundary and overcome the additional back-stress that will result in deviation from ideal twin shape.

Finally, if l is large relative to the twin thickness, then there will be a large energy penalty associated with either thickening the twin sufficiently to overtop the precipitate or deflect sufficiently to avoid it. In this case, bowing is likely to be inevitable, but the details of the bowing process involve the interaction of multiple partials at the twin tip as already discussed (Figure 5(c)). In this case, the most accurate prediction of the bowing stress requires treating the twin front as a super-dislocation in which multiple twinning partials bow together. This bowing is substantially assisted by the leading partial dislocations at the twin tip being pushed by those from behind, so is likely to be easier for a thick twin [46].

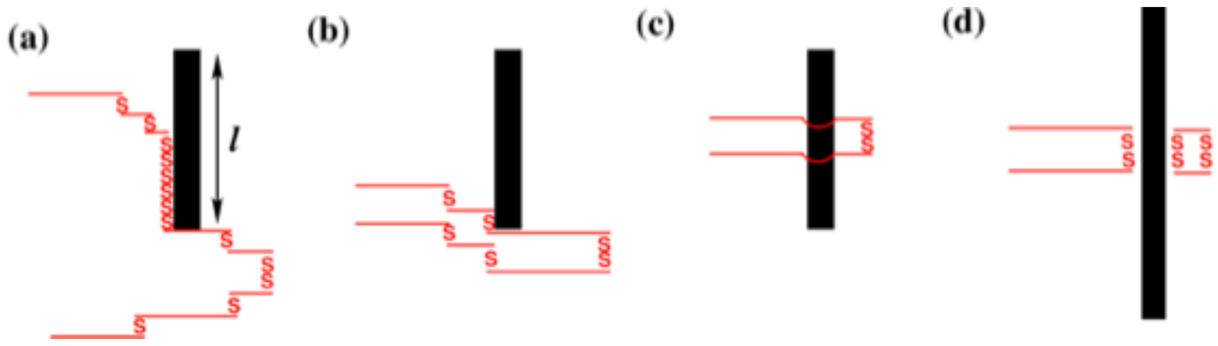

Figure 5 Mechanisms by which a twin tip can overcome a precipitate during the propagation stage. (a) a thick twin for which part of the twin tip is not blocked (b) a twin tip near the edge of a precipitate can deviate slightly from its habit plane to avoid intersection (c) bowing of the twinning partials around the precipitate (d) a very large precipitate which cannot be bowed; nucleation of a new twin is activated on the far side of the precipitate. The number of twinning dislocations ("S") shown is greatly reduced compared to that expected in practice (>100) for clarity.

Even when the precipitate presents an apparently impenetrable obstacle to twin propagation, such as the large plates formed by discontinuous precipitation in Mg-Al alloys [30], the stress at the twin tip may often be high enough to enable nucleation of a new twin on the far side of such an obstacle (Figure 5(d)). In this case, it is likely that the precipitate will behave similarly to a grain boundary, except that the lattice on both sides of the precipitate is originally in the same orientation, favoring the nucleation of a new twin of the same variant and giving the appearance that a single twin has apparently propagated through the microstructure unimpeded by the precipitates.

Although in some cases, strengthening against propagation of the twin may dominate the overall strengthening effect that precipitates provide against twinning, this is likely only to be true where the precipitate spacing is small enough to provide an Orowan stress sufficient to overcome the concentrated stress at the twin tip driving its forward motion. It is noteworthy that to date no magnesium alloy has been observed in which all the twins are preventing from propagating to the opposite grain boundary.

As FE simulations demonstrate, the stress concentration driving twin propagation is determined largely by the extent of plastic relaxation that occurs. Again, the comparison between a twin and a crack growing to relax a local concentration of stress is a useful one. In this interpretation of the observations, an important effect of precipitates on the stress required for twinning is determined by the effect of precipitates on plastic relaxation processes. Less plastic relaxation will lead to higher local stresses at the twin tip during propagation but also higher back-stress inhibiting thickening [17]). This will tend to bias the system towards thinner twins when precipitates inhibit plastic relaxation, consistent with observations.

Finally, we consider the effect of precipitates on twin thickening. This is important because macroscopic yield (from which measured CRSS values are derived) does not correspond only to these first stages of twinning, but also requires extensive twin growth and/or nucleation of additional twins after the initial burst. For example, consider a fine-grained magnesium alloys (grain size 5μm), in which 1 twin forms per grain [47]. If it is assumed this twin nucleated and propagated with the minimum possible thickness (a reasonable assumption), an estimate can be made of the volume fraction of twined material after the propagation stage. Taking the minimum thickness as ~40nm [45], and assuming a lamella twin that crosses the grain at its widest point, this gives an estimated volume fraction at the end of propagation of approximately 1%. As discussed previously, this is significantly less than the twin volume fraction at the point where CRSS values are usually extracted (0.1% proof stress). Therefore, CRSS values that are commonly derived from such tests are influenced not only by nucleation and propagation but also by growth.

Twin growth (thickening) involves the nucleation and propagation of additional twinning dislocations, which must overcome the back-stress in the matrix that opposes the twinning shear, in addition to the Orowan stress to bow non-shearing precipitates. In this case, each increment of thickening theoretically requires bowing of only individual twinning partials rather than a super-dislocation wall as in propagation. As demonstrated, the Orowan stress in this case is very small, and an order of magnitude less than a typical back-stress. Therefore, the inhibition of twin thickening is likely to be back-stress dominated.

Precipitates will increase the magnitude of the back-stress by inhibiting the plastic relaxation processes that serve to reduce it. They will also induce an additional back-stress if they remain unsheared inside the twin as already discussed. Unfortunately, it is not trivial to calculate the back-stress since it is strongly influenced by the geometry of the twin and (precipitate influenced) plastic relaxation processes. In general, only a full crystal plasticity model is able to consider all of the relevant factors. Recently, there has been progress in this direction using a combined crystal plasticity/phase field approach [48] and this shows promise as a framework in which precipitate effects can be incorporated. However, such an approach requires sophisticated computation and a simple (if approximate) equivalent to the Orowan equation for slip would still have great utility in guiding alloy design.

To date, the existing simple models are not adequate to predict the strengthening effect of precipitates against twin thickening in all cases. It is suggested that since back-stress (and plastic relaxation) dominates the stresses against twin growth, the search for a simple model should focus on estimating the extent to which plastic relaxation is inhibited by precipitates.

Conclusions

Precipitates provide strengthening against twin mediated deformation in magnesium alloys. Understanding the origins of this strengthening effect and developing methodologies to predict it are critical to efforts to improve the mechanical performance of magnesium. This understanding must consider all three stages in forming a twin; nucleation, propagation, and growth. Current evidence suggests that precipitates do not directly strongly suppress nucleation of the $\{10\bar{1}2\}$ twin in magnesium, and their main effect is therefore on the propagation and growth processes. During the propagation stage, there are several mechanisms by which twin tips can overcome a precipitate dispersion. These include deflection of the twin, Orowan looping (where the interaction of individual twinning dislocations must be considered), and re-nucleation (in cases where the obstacle size is sufficient to completely block the twin). To date, no magnesium alloy has been observed in which a precipitate dispersion is able to completely suppress propagation. Twin growth (thickening) is clearly influenced by precipitates, as evidenced by the observation that thinner twins form when precipitates are present. It is proposed that for the thickening process, it is the effect of precipitates on the back-stress that is of most importance. Although none of the current models can accurately predict the strengthening effect, they do point towards the factors that must be considered. In the propagation stage, the stress required to loop the twinning super-dislocation will probably dominate. Increasing this stress requires reducing the inter-particle spacing on the K_1 plane. In the growth (thickening) stage, maximum inhibition will come from maximizing the back-stress through using a precipitate that induces a high level of elastic misfit when inside the twin and also inhibit plastic relaxation (by slip or twinning). Shear resistant prismatic plate precipitates with a small interparticle spacing are expected to be most effective of the common precipitate types observed in magnesium alloys in both regards, but this remains to be clearly proven.

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