The effect of internal stresses due to precipitates on twin growth in magnesium

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ABSTRACT

Twinning is an important deformation mode in hexagonal close packed (HCP) metals, including magnesium alloys. Precipitates are used to provide strengthening in many of these alloys. The effect of precipitates in strengthening against deformation by slip is well understood, but this is not the case for twinning. Recent studies have indicated that precipitates are usually not sheared by twins, but the Orowan law for strengthening against slip by dislocation bowing does not give a good prediction when applied to twinning. It has therefore been proposed that the dominant strengthening effect inhibiting thickening of a twin arises from an additional back-stress that results from embedding a unsheared precipitate in twinned matrix. The present paper uses an Eshelby model to assess the influence of precipitate shape and habit on the internal stresses that arise from embedding a non-shearing precipitate in a (10T2) twin (the dominant twin type). It is demonstrated that the elastic stresses generated easily exceed the critical resolved shear stress for activation of slip and therefore plastic relaxation is to be expected. In all cases, the predicted plastic zone is confined to a region local to the particle. The implications of these predictions for design of precipitation strengthened HCP alloys are discussed.

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1. Introduction

Twinning is an important deformation mode in hexagonal close packed (HCP) metals, with the (10T2) twin mode being one of the easiest mechanisms to activate during room temperature loading [1]. In magnesium, the easy activation of this twinning mode combined with the strong textures generated in wrought products is responsible for mechanical asymmetry; an undesirable difference in compressive and tensile strength [2,3].

Given its importance, the (10T2) twin mode has been studied extensively in magnesium alloys and other HCP metals [1]. Many of these alloys contain second phase precipitates, either formed deliberately during an ageing treatment to provide strength, or as a result of impurities or process route. The important role such particles can have in increasing strength by inhibiting slip is well understood through relationships such as the Orowan equation and is fundamental to alloy design. However, despite the importance of twinning as a deformation mode in HCP metals, the role of precipitates on twin mediated deformation is poorly understood [1]. A number of studies have demonstrated that twin nucleation is not suppressed by the presence of precipitates. Indeed, it is commonly observed that the presence of precipitates leads to a greater number of smaller twins (when compared to the same material in a precipitate free state) [4–6]. However, non-shearing precipitates are seen to act as effective obstacles against twin growth, significantly increasing the stress required to thicken twins [2–5,7]. This effect might be exploited to increase strength and reduce anisotropy in HCP metals, overcoming two major limitations preventing their wider use. The promise of this approach has led to a number of studies focussed on understanding precipitate/twin interactions, focussing on age hardenable magnesium alloys [2,3,5,8–11]. However, there remains no model or law to predict how precipitates influence the stress required for twin growth.

An early study of precipitate/twin interactions in magnesium was performed by Ghaghouri et al. [4,12], who investigated the Mg–Al system (the basis of the most widely used commercial magnesium alloy, AZ91). They demonstrated that when twins are very small compared to the precipitate size, they can be blocked by precipitates. As the twins grow, they can attempt to avoid precipitates by local deviation of their habit (K1) plane. This requires multiple twinning dislocations to be introduced into the plane, with an associated energy cost (discussed in detail by Ghaghouri et al. [4,12]). In addition, any bulging or local thickening of the twin
boundary will be opposed by a back–stress induced by the surrounding matrix, and there is thus a strong energy penalty against the twin deviating from its ideal lenticular shape. By the time the twins have grown enough to produce measurable macroscopic yield, they were observed to have engulfed some of the precipitates and deviations in the habit plane were generally observed to be small (compared to the thickness of the twin).

Gharghouri et al. demonstrated that the precipitates, which form mainly as plates on the basal plane in Mg–Al alloys, are not themselves sheared when engulfed by a twin [4,12]. This has since been shown to also be the case for Mg–Zn alloys, where the precipitates form as rods parallel to the c–axis [5,6]. The strain incompatibility that necessarily arises from embedding an unsheared precipitate into sheared (twinned) matrix will generate a very large strain (and stress) in the matrix if accommodated elastically. No evidence for such large strains were observed, but instead Gharghouri et al. identified a concentration of dislocations in the region where high stress would be expected, indicative of a plastic relaxation process [4]. Evidence of plastic relaxation around precipitates in magnesium alloys has since been identified in other alloy systems with other precipitate types [9,11].

Attempts have been made to predict the strengthening effect of precipitates against twin growth by applying the Orowan–Ashby equation to predict the stress required to bow the twinning dislocations around the precipitates [9]. Although this approach works well to calculate the strengthening against slip, it has been demonstrated that it greatly under–predicts (e.g. by a factor of 4) the strengthening effect of precipitates against twin growth [9]. Instead, it has been argued that it is the additional back-stress expected when shear resistant particles become embedded in the twin that provides the dominant contribution to strengthening against thickening of the twin [6,8,9].

Particles can also influence twin growth before the thickening stage. The initial stage of twin growth involves the twin tip propagating from the grain boundary region in which it nucleated to the opposite grain boundary. This is usually assumed to be very rapid. However, in the case where precipitates are present, it is possible that the twin tip will become blocked in this initial growth stage [7]. The blocked twin will then thicken, leading to an increase in the back-stress against further twin growth. A situation can eventually be reached where the twin thickening is stalled. To overcome this stalled growth, sufficient additional stress must be imposed to bow the thickened twin around the blocking precipitate [7]. Since multiple twinning dislocations have to be bowed simultaneously to unblock the growth of the twin tip, the required stress is much higher than for the bowing of a single dislocation during twin thickening [7].

Regardless of how the twin overcomes the particle, once an unsheared particle becomes fully embedded in a twin, it will necessarily lead to an additional back-stress as a result of the misfit between the sheared matrix and unsheared precipitate. This misfit stress is expected to be partially plastically relaxed (by dislocation slip), and this adds a considerable complication in determining the inhibition that precipitates will have against twin growth. The dislocation slip processes themselves (required to relax the back-stress) will be influenced by factors such as alloy solute content and neighbouring precipitates. Furthermore, the misfit strain consists of both $<a>$ and $<c>$ components, but the critical resolved shear stresses required to activate the required plastic relaxation processes in these directions are very different. These complex interactions are poorly understood but will be important in determining the stress required to grow twins in precipitate containing alloys.

The aim of the present work was to better understand the misfit stresses that will be generated and the likely extent of plastic relaxation that will occur around unsheared precipitates of different shapes and habits when embedded in a $\langle 10\overline{1}2 \rangle$ twin. The calculations are performed for magnesium, but have implications for strengthening against twin growth in other HCP alloys. It should also be noted that the case considered here is a specific example of the more general problem of stress induced grain boundary migration [13,14] and the analysis could also be applied to the more general case of a grain boundary passing through a distribution of unshearable precipitates, providing the correct transformation strain tensor was applied.

The present results provide an important step in attempts to better understand, and eventually model, the strengthening effect of precipitates against twinning. This could ultimately lead to a new class of HCP alloys containing precipitates specifically optimized to strengthen against deformation twinning.

2. Theory

Deformation twinning is commonly observed in HCP metals due to the limited ability of slip to accommodate an arbitrary shape change. This study focusses on magnesium alloys, and in common with HCP titanium and zirconium, there is no easy slip mode that can accommodate strains along the c–axis direction. Loading along this direction therefore usually induces yield by twin nucleation and growth, once a critical stress is reached. The most common twin in HCP metals is the $\{10\overline{1}2\}(10\overline{1}1)$ mode, which in magnesium produces an extension along the c–axis direction. Once nucleated, these twins usually grow very rapidly, since the $\{10\overline{1}2\}$ twin boundary is highly mobile in HCP metals [1]. Indeed, unlike a random high angle grain boundary, the growth of this twin type is usually not limited by boundary mobility [1], but by the back–stresses generated as it thickens [15,16].

In a precipitate containing alloy, the twin must grow through a distribution of particles with a different crystal structure to that of the matrix if it is to thicken. The material in the twin is sheared with respect to the parent, and a precipitate entering into the twin has to
accommodate this shear. Fig. 1 shows schematically (for a simplified geometry) the ways this could be achieved.

Fig. 1(a) shows the situation before the twin has formed. The twin produces a simple shear of the matrix to which the precipitate must respond. The first possible accommodation mechanism, twinning in the precipitate (b), will only be possible if the crystal structure of the precipitate is close to that of the matrix (e.g. an ordered version of the HCP structure) to provide a compatible twinning mode. In addition, the stress required to activate this twinning mode in the precipitate must be less than the stress needed to activate an alternative accommodation mode (e.g. plastic relaxation) first. In magnesium, this situation has only been observed for the case of very thin, fully coherent precipitates, such as observed in certain Mg–Zn–Gd alloys [17]. The second possibility (c), slip in the precipitate, has not been observed in magnesium, and is unlikely because the precipitate phases are usually intermetallic compounds that are much more resistant to slip than the matrix. The third possibility (d), entirely elastic accommodation, will be considered in this paper and it will be demonstrated this would lead to unsustainable stresses in the matrix and precipitate. The final possibility (e), elastic accommodation in the precipitate and slip relaxation in the matrix is that previously observed in magnesium alloys and is the most likely to occur in any alloy where the yield stress of the precipitate phase is much greater than the matrix (the usual case) [4,9,11,18].

To understand the strain and stress fields associated with accommodating the misfit by either the mechanism shown in (d) or (e), it is necessary to consider the strain imposed on the precipitate by twinning, and the consequent internal stresses that will arise. The simple shear produced by twinning may be decomposed into pure shear and rotational components. Once a precipitate is embedded in a twin, the rotational component can be accommodated without a shape change in the precipitate, and therefore does not produce any misfit strain. It will however produce a rotation of the precipitate with respect to precipitates in the untwinned matrix. For the case of the {10T2} twin in magnesium, this rotation is expected to be 3.7° around [1020] as discussed by Gharghouri et al. [4]. Such a rotation has been experimentally observed in a number of magnesium alloy systems [4,5]. Note that this rotation is only able to occur freely once the precipitate is fully embedded inside the twin. Until that point, part of the precipitate remains anchored in parent material. This means that at the point the twin consumes the matrix around the precipitate, the strain incompatibility (and associated stresses) will be at a maximum. However, in determining the residual long range back–stress, it is the aggregate effect of internal stresses, dominated by precipitates inside the twin, that will be most important. Therefore, in the present work (and following Gharghouri et al. [4]) the case where a precipitate has become fully engulfed by the twin and has been free to rotate that is considered in this work.

The problem of predicting the unrelaxed back-stress in twinned material containing unsheared precipitates is a complex one. This is because it is very difficult to determine accurately the amount of plastic relaxation that occurs. Experiments show evidence of localized plastic flow in the form of dislocations, but the nature of this slip and the critical resolved shear stress required to activate it are not clear. Furthermore, the shear associated with the {10T2} twin in magnesium has a <c+a> component and thus <c+a> component dislocations (e.g. <c+a>) would be required to accommodate misfit strains in this direction. Given these dislocations are considered much harder to activate than basal dislocations, it is not clear whether misfit strain in this direction persists, or remains unrelaxed. Experimentally, it is not possible to isolate the individual dislocations in the regions of plastic relaxation because the local dislocation density is very high [4]. There is not yet a successful predictive model that can account for all of these factors.

The aim of the present work was not to produce a full model that is capable of accurately predicting the strengthening effect of precipitates against twin growth. Rather, a much simpler approach was used, where the problem was first treated as an entirely elastic one. This provides an upper bound calculation of the misfit induced stresses. By comparing these (unrealistic) “elastic only” stresses with the critical shear stress for slip, an estimate can be made of the amount of plastic relaxation that will occur, and the extent of this relaxation field. Note that such a model is a first step towards the ultimate goal of being able to calculate the strengthening effect of particles against twins.

The problem of embedding an unsheared particle into a sheared matrix, where deformation is purely elastic, can be treated by the well known method originally developed by Eshelby [19–21]. In Eshelby terminology, the precipitate is termed an “inhomogeneity”, and is a phase with different elastic properties from the matrix. A number of simplifying assumptions are required to make an analytical solution of the Eshelby equations possible. It is assumed the inhomogeneity and matrix are elastically isotropic. Unlike many other HCP metals, magnesium exhibits low elastic anisotropy, so this assumption will be reasonable. Furthermore, the inhomogeneity is assumed to be spheroidal in shape (an ellipsoid with dimensions a = b ≠ c).

To calculate the elastic misfit strain and stress field requires a knowledge of the elastic properties of the matrix and precipitate phase (stiffness and Poisson ratio) and the imposed strain (or stress). As already discussed, in the case of twinning, it is necessary to separate out the pure shear and rotational components of the imposed strain. The pure shear component must then be transformed to the precipitate axis system. The Eshelby method can then be applied to calculate the elastic misfit strains and stresses.

The common precipitate types in magnesium alloys are plates on the basal plane (basal plates), rods with their long axis parallel to the <c+a> direction (c-axis rods) and plates on prism planes (prismatic plates). Basal plates are the most commonly observed precipitates in alloys based on the Mg–Al system, which includes the most commercially important AZ class of magnesium alloys. C-axis rods are the most commonly observed precipitates in Mg–Zn alloys, which includes the commercial ZK alloy series. Prismatic plates are the most commonly observed precipitates in Mg–Y–RE (rare earth) alloys, which includes the commercial WE alloy series [22].

As already described, the Eshelby method requires the precipitate shapes to be represented by spheroids to give a simple analytical solution. These spheroids are approximations to the true shape of the precipitates. The shapes chosen for each precipitate type are shown schematically in Fig. 2 along with the coordinate system for the precipitates. The convention of Gharghouri et al. has

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2a = b = c = a = 2b = 2c = a = 2c
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Fig. 2. Shapes and orientations of the three precipitate types considered in this work (a) basal plates, (b) c-axis rods, (c) prismatic plates. a, b, c are semi axis lengths of spheroid, x axis parallel to [0001].
been used to choose the coordinate system of the strain tensor with respect to the crystal axes; $x = [0001]$, $y = [\overline{1}\overline{1}0\overline{1}]$, $z = [1\overline{1}2\overline{0}]$. The spheroid semi-axis lengths $a$, $b$, and $c$ are defined along $x$, $y$, and $z$ respectively. The aspect ratios chosen for these spheroids (Fig. 2) are chosen to be realistic compared to those observed in practice [22]. The relationship between the coordinate system and crystal directions is shown schematically in Fig. 3, along with the important planes and directions for this study.

The $(1\overline{1}0\overline{2})/(1\overline{1}0\overline{1})$ variant of the $(1\overline{0}T\overline{2}) < 1\overline{0}T\overline{1} >$ twinning system is chosen for this analysis. For this case, the transformation strain associated with the twin, rotated into the coordinate system of the precipitate, is given by Gharghouri et al. as [4]:

$$e^T = \begin{pmatrix} 0.5\gamma & -0.03\gamma & 0 \\ -0.03\gamma & -0.5\gamma & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (1)$$

Where $\gamma$ is the twinning shear ($\gamma = 0.13$). The imposition of this transformation strain on the precipitate will produce a stress in the precipitate, which will seek to relax by deforming the surrounding matrix. The Eshelby method can be applied to determine the final equilibrium state in the precipitate and matrix resulting from this relaxation process (assuming it is entirely elastic).

A MATLAB™ computer code has previously been published by Healy [23] that allows the elastic field in 3-dimensions due to a spheroidal inclusion to be calculated using the Eshelby method. This code allows either an external stress (or strain) to be applied (not the case here), or an imposed strain within the inclusion (which is the case here). The code enables prediction of the full stress and strain field in the matrix and precipitate. Full details of the code and its mathematical basis are given elsewhere [23].

This code was applied to solve the Eshelby problem for the precipitate shapes already described. The elastic properties used for the matrix and precipitate are given in Table 1. The Young’s Modulus for the precipitate corresponds to the average value measured for $\beta’$–Mg$_{17}$Al$_{12}$, which is the precipitate phase observed in Mg–Al alloys (basal plates). The elastic anisotropy of this phase is ignored [12]. The Poisson ratio for this phase is not well characterized, so was assumed to be the same as the matrix. This is only of minor importance to the calculated results. Elastic properties of the precipitate phases in other magnesium alloys (e.g. Mg–Zn system) are not reported. Since the main purpose of the present work was to isolate the effect of precipitate shape and habit, the same elastic parameters were used for all precipitate types to remove the influence of this variable. For greater quantitative accuracy, the elastic parameters of the other precipitate types would have to be measured. However, it is to be expected that all the intermetallic precipitate phases are stiffer than the magnesium matrix. Given this constraint, even large variations in the elastic parameters of the precipitate do not change the qualitative conclusions. The Eshelby code developed by Healy [23] outputs the stress and strain tensors in the inhomogeneity and in the matrix at any position (in 3-dimensions). The maximum shear stress in the matrix is also calculated and output. As will be demonstrated later, and consistent with previous estimates [4], the maximum shear stress based on this purely elastic calculation greatly exceeds the yield strength of magnesium, so plastic relaxation is expected. To estimate the likely extent of the plastic zone, the elastic stress generated need to be compared with the critical resolved shear stresses (CRSSs) for slip. This will provide an upper bound estimate of the extent of the plastic zone. It is an upper bound estimate because in practice, plastic relaxation in regions of high stress will relax the elastic stresses elsewhere, and will thus reduce the volume in which these stresses exceed the CRSS for plastic deformation.

To provide an estimate of the plastic zone size, it is necessary to use an appropriate value for the CRSS for the slip mode under consideration. As discussed in detail elsewhere [24], the CRSS values reported for magnesium have a very wide variation (over an order of magnitude), even for a single mode (e.g. basal slip). This can be explained by the different methods used to determine CRSS values. These methods include single crystal studies and fitting of crystal plasticity models to polycrystalline stress-strain curves. In the present case, CRSS values extracted from polycrystalline crystal plasticity modelling are not appropriate, since these include strengthening effects (such as grain boundary strengthening) that will not apply in the plastic zone local to particles. Instead, the most appropriate value to use is likely to be the single crystal CRSS, which excludes such strengthening effects. The solute remaining in the matrix after precipitation will provide a solute strengthening effect in the local plastic zone, and this must be accounted for by choice of appropriate single crystal values.

For basal slip, the CRSS determined from experiments on Mg–Al single crystals is on the order of 1 MPa. For prismatic slip, a CRSS value of 45 MPa was used [24]. For $\langle c+a \rangle$ slip, the appropriate CRSS value is less certain since this mode is rarely observed in single crystals deformed at room temperature [25]. In crystal plasticity modelling of polycrystalline Mg–Al alloy, a value of around 150 MPa is typically found to produce good fit to measurements [26]. A value as low as 40 MPa has been reported based on single crystal studies of pure magnesium [27], although this is inconsistent with other studies [25]. In the present work, a value of 80 MPa was estimated for the CRSS of $\langle c+a \rangle$ slip, based on the data reported in Ref. [24]. Note that the predictions are not very sensitive to the exact CRSS values chosen for any of the deformation modes.

3. Results

3.1. Elastic relaxation

The model was first applied to the case of basal plate...
precipitates in magnesium, where twin/particle interactions have been studied in most detail. The amount of misfit strain accommodated in the particle and in the matrix depends on the difference between the elastic properties of the two materials. If the precipitate is considered effectively infinitely stiff, the maximum misfit strain in the matrix is expected to be on the order of 6%, and will occur ahead of the precipitate in its habit plane [4] \( (\varepsilon_{yy}) \) with reference to the axis system defined in Fig. 3. This is the case is shown in Fig. 4(a). In this, and all subsequent plots, the stress and strain field were computed in 3–dimensions, but only a 2–dimensional section is shown (the \( x\)-\( y \) plane passing through the centre of the precipitate). This plane contains the maximum misfit strains and stresses.

As shown in Table 1, the precipitate phase is not effectively infinitely stiff; indeed, the stiffness of the \( \beta\text{-Mg}_17\text{Al}_{12} \) is less than twice that of the matrix. This has an important effect on the results, because the precipitate can also deform significantly to accommodate some of the misfit. When the correct stiffness is used for the precipitate, the misfit strains generated in the matrix are predicted to be greatly reduced, as shown in Fig. 4(b).

The maximum shear strain will lead to both normal and shear stresses. The maximum shear stress is an important parameter in governing when plastic yield will occur. The maximum shear stress predicted for the case plotted in Fig. 4(a) (an infinitely stiff precipitate) is shown in (c). The greatest value of the maximum shear stress, which occurs just ahead of the plate tip, is approximately 1600 MPa. This is clearly far in excess of the shear stress required to activate plastic relaxation (recall the CRSS for basal slip is around 1 MPa). Even when elastic deformation of the precipitate is accounted for (Fig. 4(d)), the maximum predicted shear stress is still in excess of 200 MPa.

The same calculation was repeated for the case of c-axis rod shaped precipitates. Again, the calculation was performed assuming both that the precipitate is effectively infinitely stiff and also allowing the precipitate to elastically deform (with its stiffness the same as that for the basal plate case). The maximum misfit strain generated around a c-axis rod shaped precipitate is considerably less than that around a basal plate and occurs along the c-axis direction \( (\varepsilon_{xx}) \), with a maximum magnitude of 4% (Fig. 5(a)). When elastic relaxation of the precipitate is accounted for, this reduces to a maximum of 0.13% (Fig. 5(b)). The maximum shear stress arising from this misfit strain is approximately 900 MPa when the precipitate is considered infinitely stiff, which is reduced to 50 MPa when elastic deformation of the precipitate is accounted for. Although these stresses are much less than for basal plates (approximately 1/4 of the value when elastic deformation of the precipitate is accounted for) they are still in excess of the expected stress required to activate plastic deformation.

An important feature of these predictions is that the region of very high misfit strain (and stress) is localized close to the particles. For example, within one plate diameter of the plate tips, the maximum predicted shear stress falls from over 200 MPa to less than 10 MPa. At distances further than two plate diameters from the precipitate, the maximum shear stress drops to less than 1 MPa. Finally, the case of prismatic plate precipitates will be considered. In this case, there are three unique orientations of precipitate, so the geometry of the problem is more complex. The analysis here will focus on the case where the prismatic plate is most

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**Fig. 4.** Elastic misfit strains and stresses calculated around a basal plate (a) maximum normal strain in \( y \) direction assuming an infinitely stiff precipitate (b) as (a) but using a realistic stiffness for precipitate (80 GPa), (c) maximum shear stress (infinitely stiff precipitate), (d) maximum shear stress (realistic precipitate stiffness). Note the different colour scaling necessary in each case. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
unfavourably oriented to accommodate the twinning shear (habit plane perpendicular to the twinning shear). This will lead to the greatest misfit strains and stresses. On average, \(\frac{1}{3}\) of the plates will be in this orientation. The case considered is for a prismatic plate on the \(\{1\overline{1}00\}\) plane. As in the other cases, the calculations were performed for both the case of an infinitely stiff and an elastically deforming precipitate. The results for the plane of maximum shear (\(x-y\) plane) are shown. In this plane, the prismatic plates are viewed edge-on. The misfit strains and stresses calculated for this prismatic plate orientation are the greatest of any precipitate type (Fig. 6). As can be seen from Fig. 6(b–c) it is predicted that the maximum shear stress arising from the misfit exceeds 100 MPa in a region extending approximately twice the particle length into the matrix along the \(x\) and \(y\) axes. This is the case even when elastic deformation of the precipitate is allowed.

3.2. Plastic relaxation

The calculations of the preceding section demonstrate that shear resistant precipitates entering twinned material will general a large misfit strain, which in turn will lead to a misfit stress that is expected to activate plastic relaxation. This plastic relaxation will occur by dislocations, and it is useful to consider what type of dislocations will be needed to provide the necessary accommodation.

As discussed by Charghouri et al. [4], and immediately apparent on inspection of the misfit strain tensor (shown in Equation (1)) there will be a misfit to be accommodated along both the \(<c+a>\) and \(<c>\) directions. Prismatic and basal slip can potentially accommodate misfit in the basal plane, but non-basal slip is required to accommodate the \(<c>\) component of the misfit.

The resolved shear stress resulting from the elastic misfit stress on the basal, prismatic and \(<c+a>\) slip systems with the highest Schmid factor can be determined by appropriate rotation of the stress tensor. The relevant planes, directions, and angles are shown in Fig. 3. To determine the resolved shear stress for basal and prismatic slip, it is necessary to rotate \(30^\circ\) clockwise around the \(x\) axis; the new \(y\) axis will then be antiparallel to the slip direction along which the resolved shear stress is a maximum. To determine the maximum resolved shear stress for \(<c+a>\) slip, this rotation must be followed by a rotation of \(31.6^\circ\) around the new \(z\) axis. The new \(x\) axis will then be parallel to the slip direction along which the resolved shear stress is a maximum. The rotation matrices to perform the necessary coordinate system transformation are then straightforward to determine using the standard method and apply in MATLAB\textsuperscript{TM} to determine the resultant shear stresses. For simplicity, this analysis is limited to consideration of the single slip system for each mode that will develop the maximum shear stress.

Focussing on the case of basal plate precipitates, where the misfit is greatest, the maximum resolved shear stresses on a basal, prismatic, and \(<c+a>\) slip system are as shown in Fig. 7. The potential size of the plastic zone was calculated by determining the region in which the resolved elastic misfit shear stress exceeds the critical resolved shear stress for the slip system in question. As discussed, this represents a likely upper bound estimate of the plastic zone size, since in reality plastic relaxation in high stress areas will reduce the surrounding elastic stresses. Furthermore, this analysis considers each slip mode in isolation, whereas in practice the activation of easy slip modes will reduce the stress available to activate more difficult modes. Nevertheless, the calculation is
Fig. 6. Elastic misfit strains and stresses calculated around a prismatic plate precipitate (a) maximum normal strain in \( y \) direction assuming an infinitely stiff precipitate (b) as (a) but using realistic stiffness for precipitate (80 GPa), (c) maximum shear stress (infinitely stiff precipitate), (d) maximum shear stress (realistic precipitate stiffness). Note the different colour scaling and minimum contour value necessary in each case. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 7. Maximum elastic misfit stresses for a basal plate precipitate resolved for (a) basal slip (b) prismatic slip (c) \(<c+a>\) slip.
useful in assessing whether a particular slip mode is likely to occur, and over what maximum distance it will operate.

For basal plates and c-axis rods, the regions in which the resolved shear stress exceeds the CRSS for basal and prismatic slip are shown in Fig. 8. For \( <c+a> \) slip, only a very small region, below than the minimum dimension of the precipitate, is predicted where the CRSS is exceeded. This is not shown, since as already argued, these calculations represent an upper bound estimate of the plastic zone. Therefore, it is highly probable that for the assumed CRSS value used here, relaxation by a more easily activated mode will mean that in practice there will be insufficient unrelaxed stress to activate \( <c+a> \) slip.

For prismatic plates oriented most favourably to block twin growth, the predicted maximum elastic shear stress, region of potential basal slip, region of potential prismatic slip, and region of potential \( <c+a> \) slip are shown in Fig. 9. The large misfit stresses generated in this case (as shown in Fig. 6) translates into predicted plastic zone sizes that are larger for prismatic plates than either of the other precipitate types. Furthermore, it is predicted that for this case, the stress levels reached could be sufficient to activate \( <c+a> \) slip in a significant region (extending up to approximately one plate diameter into the matrix).

4. Discussion

This paper presents a simple analysis of the elastic misfit stress and strain predicted around an unsheared precipitate when it becomes engulfed by a \( \{10\overline{1}2\} \) twin in magnesium, assuming no plastic relaxation occurs. This calculation has been used as a basis of estimating the region in which plastic relaxation is possible around the precipitate. This approach decouples the elastic and plastic accommodation processes, so is necessarily approximate, since in practice both operate together. Nevertheless, such a calculation is useful in providing an upper bound estimate of the plastic zone size around the precipitates.

The first observation is that if accommodation was purely elastic, the misfit strains and associated stresses would be very large, regardless of whether the precipitates are basal plates, prismatic plates, or c-axis rods. This is consistent with the predictions of Gharghouri et al. [4] and is a result of the relatively large shear associated with twinning. Such large strains are not measured around precipitates engulfed by twins [4], and thus it is to be expected that a plastic relaxation process occurs. Evidence for this plastic relaxation in the form of dislocation loops at the tips of c-axis rod or plate shape precipitates has been directly observed in several magnesium alloy systems [4,5,9]. It is also predicted that elastic deformation of the precipitate (in the case of \( \beta-Mg_17Al_{12} \)) plays a significant role in reducing the misfit strain, and it is thus not sufficient to assume the precipitate to be fully rigid. One reason for this is that the stiffness of the \( \beta-Mg_17Al_{12} \) phase is low for an intermetallic compound; less than twice that of the magnesium matrix. The stiffness of the precipitate phase is thus likely to be an important parameter in determining the resistance offered to precipitate growth, with a stiffer precipitate producing higher misfit stresses.

The misfit strain has both \( <a> \) and \( <c> \) axis components. It is predicted that the elastic stress that arises from the misfit strain is unlikely to be sufficiently large to activate \( <c+a> \) slip for basal plates and c-axis rods, so the \( <c> \) component of the misfit will not be relaxed. However, both prismatic and basal slip will be activated and will relax the misfit in the basal plane. It is predicted that the plastic zone will be restricted to a region local to the precipitate, extending to less than one particle diameter in any direction. This means that providing the space between the precipitates exceeds

![Fig. 8. Potential zone of plastic relaxation for (a) basal plates, basal slip (b) basal plates, prismatic slip (c) c–axis rods, basal slip, (d) c–axis rods, prismatic slip.](image-url)
approximately two particle diameters, the plastic zone around one precipitate can be considered independent of the zone around a neighbouring precipitate. In this case, the interaction between the plastic zones will occur only through the long-range back-stresses that are generated inside the twin. The prediction that plastic relaxation occurs in a region that is localized to approximately one particle diameter is consistent with the limited experimental observations available [4,12].

A key question that remains to be addressed is to predict how precipitates influence the stress required to grow a twin. This is important if precipitation is to be successfully included into models for strengthening and work-hardening of HCP alloys. Experiments show that precipitation can have a very strong effect on the stress required for twin growth [9], which in turn can strongly influence important mechanical property characteristics such as yield asymmetry [8].

Several attempts have been made to measure directly the influence of precipitation on the increase in critical resolved shear stress required to grow twins (Δτ_{twin}). This is usually achieved by producing a strongly textured material, which is then loaded in a direction to activate twinning. Correlation of the measured stress-strain curves with fitted CRSS values (e.g., using crystal plasticity models) are used to infer a value of Δτ_{twin}. More recently, attempts have been made to use micro-pillar compression to directly measure Δτ_{twin}, but so far with limited success [11]. Often, the derived Δτ_{twin} value is compared with the Orowan stress calculated for bowing of the twinning dislocation in an attempt to predict the strengthening effect. Such data from some recent studies are summarised in Table 2. The accuracy of the derived Δτ_{twin} is poor, because the fitting process is prone to large errors, and is influenced by factors apart from precipitation. This is evidenced by the large differences reported in Δτ_{twin} values derived in different studies on the same alloy. Nevertheless, the data do clearly indicate that there can be a strong strengthening effect of precipitates against twin growth (more than doubling of the CRSS [9,6]) and this greatly exceeds the predicted increase based on calculating the stress required to bow the twinning dislocation (Orowan).

The Orowan calculations reported in the literature are made on the basis of looping single twinning dislocations around the precipitate. This is likely to apply once the twin has already grown fully across a grain and is at the thickening stage. As proposed by Kada et al. [7], the initial step in a twin tip overcoming the blockage by a precipitate is likely to require the bowing of multiple twinning dislocations simultaneously, the estimated stress for which is expected to be reduced by dislocation...
dissociation [7]).

In predicting the effect that these increases in $\Delta T_{\text{twin}}$ will have on the mechanical response of the material, it is important to consider also the effect of precipitates on other deformation modes. For example, it has been demonstrated that the relative strengthening effect of precipitates against twinning compared to slip is greater in AZ91 than Mg–5Zn, even though the absolute value may be less. This is because c–axis rods in Mg–5Zn are far more effective in blocking slip dislocations than the basal plates in AZ91 [8,22].

There are no reliable data for the case of prismatic plates. One of the main reasons for this is that the commercial alloys in which such precipitates occur (Mg–Y–RE, e.g. WE43) also have weak texture, a large direct influence of solute RE on twinning, and smaller relative difference between CRSS values for slip modes [28]. It is not possible to load such materials to produce twin dominated yield; in all cases, a significant contribution from basal and other slip modes is also expected [28]. It has been shown in such alloys that precipitation does not strongly influence the twin volume fraction and that crystal plasticity modelling can reproduce the observed stress–strain behaviour after precipitation without increasing the CRSS for twinning [28]. This, however, is not proof that the precipitates do not increase the stress for twin growth because of the dominant influence of texture spread and other deformation modes. Furthermore, it is not yet known whether twins shear the precipitates in this class of alloy.

As demonstrated in the present study, non–shearing prismatic plates would certainly be expected to have a strong effect in increasing the stress required for twin growth due to the large misfit stresses they will necessarily generate. Plastic relaxation of this misfit should also be difficult since these precipitates are well oriented to block slip [22]. The reason this does not seem to be the case in WE43 requires further study [28]. One complicating factor is the effect that solute will have on twin boundary mobility. It has been demonstrated that RE solute atoms can segregate strongly to twin boundaries in magnesium [29]. These atoms are known to have a large size misfit and low mobility in magnesium. They might be expected to therefore provide a potent drag effect against twin boundary growth. In the case of RE containing alloys, it is possible that solute drag is of similar (or more) importance than precipitation in determining the effective CRSS for twin growth. This would explain why a large increase in the apparent CRSS for twin growth is not observed on ageing.

In general, the effect of precipitates on twinning is poorly understood [1], but the prediction made here that large misfit stresses will arise when a non–shearing precipitate becomes embedded in a twin is generally applicable to other HCP alloys. The extent to which these misfit stresses can be plastically relaxed will vary between alloys. The extent of plastic relaxation will determine the residual long range back–stress due to the misfit, which will act globally against twin growth. This is complicated by the fact that the plastic relaxation processes themselves will depend on long range internal stresses in the matrix caused by the interaction of both twinning and slip dislocations with the particles. It has been argued that one of the reasons that the basal plates in AZ91 provide a large increase for the stress to grow twins (relative to their effect on slip mode) is that they are better oriented to block plastic relaxation by basal slip in the twin compared to their limited effect on basal slip in the parent [8]. Local to the particles, stress concentration and dislocation debris associated with plastic relaxation processes will provide further obstacles to the passage of twinning dislocations, in addition to the long range back-stress effect. A complete model to predict the effect of precipitates on the strength and work hardening behaviour during twin mediated deformation would have to account for these factors.

It is important to note however that the prediction that precipitates will increase the stress for twin growth does not imply that precipitates will lead to a lower twin volume fraction. This is because precipitates will also strengthen other deformation modes (e.g. slip) and, for a given loading direction, twinning may remain the easiest way for the crystal to respond. It is commonly observed in magnesium that precipitation does not reduce the twin volume fraction, despite the fact that precipitates increase the stress required for twin growth. This is because the CRSS for $\{10\overline{1}2\}$ twinning, the easiest mode that can accommodate deformation in the $<c\bar{a}>$ direction, is approximately 30 MPa less than that for $<c\bar{a}>$ slip [25]. To promote $<c\bar{a}>$ slip over twinning would therefore require twinning to be strengthened by approximately 30 MPa more than $<c\bar{a}>$ slip, and it is hard to envisage how this could be achieved using precipitation alone.

Based on this analysis, suggestions can be made about designing an alloy microstructure to be resistant to deformation by twinning. To do this, it is necessary to maximize the unrelaxed back–stress provided by the precipitates against twin growth. This requires first choosing a system that will generate a high level of misfit, and secondly ensuring maximum resistance to plastic relaxation of the misfit. A high back–stress will be generated by choosing a precipitate morphology, such as non–shearing prismatic plates, that provide maximum misfit and by maximizing the volume fraction of this precipitate. Plastic relaxation of this back–stress will be suppressed by a distribution of precipitates that provide maximum strengthening against slip in the twin (basal or prismatic plates are both effective [8]). A mixture of small finely and large precipitates may be advantageous to maximize strength against both slip and twinning. Large precipitates can block the early stages of twin growth. Fine, closely distributed precipitates are needed to maximize the Orowan stress against both slip and twinning dislocation motion.

Maximizing strength in HCP metals requires suppression of both slip and twinning. To do this requires a new approach to the design of precipitation strengthened HCP alloys, which correctly accounts for the different ways in which precipitates interact with slip dislocations and growing twins.

5. Conclusion

Precipitates can have a strong effect in suppressing twin growth, as proven for magnesium alloys. The dominant factor that contributes to this effect is the additional back-stress that is introduced when non-shearing precipitates become embedded in a twinned matrix. This back-stress arises from the misfit that develops as a result of the strain incompatibility between the sheared (twinned) matrix and unsheared precipitate.

A model based on the Eshelby approach has been used to calculate the misfit strains and stresses around unheated precipitates of different morphologies and habits, embodied in a $\{10\overline{1}2\}$ twin in magnesium, assuming deformation to be entirely elastic. These calculations have been used to explore the role of plastic relaxation when a twin passes through a microstructure containing non-shearing precipitates, and the implication for designing alloys that strengthen against twinning.

- Accommodation of the misfit strain involves deformation of both the matrix and precipitate, leading to large internal stresses. For precipitates typical of those encountered in magnesium, elastic deformation of the precipitate is important in reducing the misfit stresses.
- The elastic misfit stresses generated are greatest around prismatic plates, then basal plates, with c–axis rods generating the lowest misfit stresses.
The stresses generated by purely elastic accommodation easily exceed the critical resolved shear stress for basal and prismatic slip. However, the critical resolved shear stress for $<c+a>$ slip is only exceeded in a significant volume of matrix for the case of prismatic plates.

Both basal and prismatic slip are expected to be activated to relax the misfit stress for all precipitate types. For prismatic plate precipitates, $<c+a>$ slip may also be activated.

The zone within the matrix in which plastic relaxation is active is predicted to remain localized to the particle (within one particle diameter) and thus in most cases the plastic zones around neighbouring precipitates are unlikely to overlap.

Non-shearing prismatic plates with a habit perpendicular to the twinning direction are predicted to lead to particularly large misfit stresses, and thus are expected to be highly effective obstacles against twin growth.

Exploiting precipitation to maximize the strength of HCP alloys requires a consideration of their effect on both slip and twinning. The precipitate characteristics that will strengthen most against twin growth are different from those that provide maximum resistance to slip dislocations, and an optimized microstructure should contain precipitates of both types.

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