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Interaction between a $Mg_{17}Al_{12}$ precipitate and $\{10\bar{1}2\}<10\bar{1}\bar{2}>$ twin boundary in magnesium alloys

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Abstract

Interactions between $Mg_{17}Al_{12}$ precipitates and $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twin boundaries (TBs) in magnesium were studied by molecular dynamics simulations. The results obtained agree well with experimental observations in which precipitates can be entirely engulfed by $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twins without being sheared. Structural analysis of the TBs in the atomic scale shows that the TBs are extremely incoherent during twin growth and highly deviate from the $\{10\bar{1}2\}$ twinning plane as previously observed in a number of experiments. The simulation studies indicate that $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning was accomplished solely by atomic shuffling that converts the parent lattice to the twin lattice without involving twinning dislocations, resulting in zero shear strain at the TBs.

Introduction

Precipitate strengthening is an important approach in alloy design. For metals with cubic structures, precipitate-dislocation interactions play a crucial role in strengthening. But for metals with hexagonal close-packed (hcp) structures such as Mg, precipitates strengthen Mg alloys in two aspects: interactions with dislocation slip and interactions with twin boundaries (TBs). It has long been recognized that precipitate strengthening in Mg alloys is much less effective than in Al alloys with a face center cubic (fcc) crystal structure. This was attributed to the facts that (1) in simple ageing of Mg alloys, the spacing between the equilibrium precipitate plates is not small enough to cause dislocations to shear the precipitates. The lack of shearing of the precipitates reduces the strengthening effect [1]; (2) the precipitate plates are parallel to the basal plane, resulting in reduced effect in blocking the basal slip that is considered the easiest slip system in Mg alloys. Accordingly, there has been effort to modify the orientations of the precipitates such that the plates are inclined with the basal plane [2]. It was anticipated that precipitate plates non-parallel to the basal plane strengthen Mg alloys more effectively.

Interactions between precipitates and twin boundaries in Mg alloys have received little attention. Twinning is generally mediated by twinning dislocations [3] at TBs. Hence, we would expect considerable interactions between precipitates and the twinning dislocations. But the most recent experimental observations [4,5], showed that the TBs of $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning interact with β-intermetallics ($Mg_{17}Al_{12}$) in an unexpected manner: the precipitates are engulfed by $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twins without being sheared. The motivation of this work is to investigate the interactions between a $Mg_{17}Al_{12}$ precipitate and $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ TBs, using molecular dynamics simulations.

Simulation method

The interatomic potentials for Mg-Al binary alloys used in this work were developed by Liu et al. [6]. The potentials are embedded atom method (EAM) type [7,8].

Figure 1 shows the cross-section view of the initial configuration in which a Mg single crystal with a β-$Mg_{17}Al_{12}$ precipitate was constructed. For simplicity of analysis of the simulation data, we neglected the effect of alloying element (Al) on the motion of a TB and just used pure Mg rather than a Mg-Al solid solution to simulate the interaction between a TB and a $Mg_{17}Al_{12}$ precipitate. We only show a thin slice (~1.5 nm thick) of the system in the middle of through thickness direction. The basal planes of the matrix are perpendicular to the figure plane, and are colored in yellow and blue to show the *ABABAB*… hcp stacking from left to right. This color scheme in 2-D view was kept unchanged throughout the simulation such that the evolution in microstructure during deformation can be recognized with clarity.

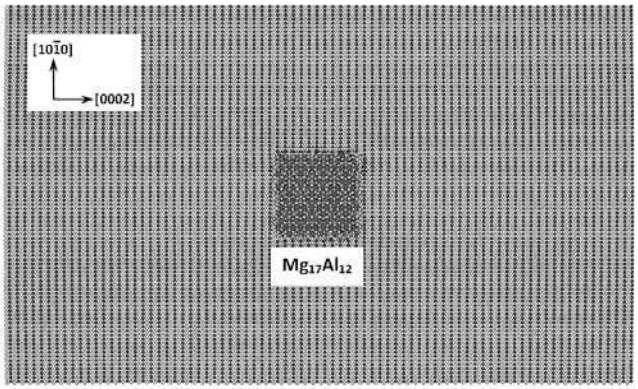


Figure 1. Cross-section view of the initial configuration of a Mg single crystal with a β-$Mg_{17}Al_{12}$ precipitate. Only a thin slice (~ 1.5 nm thick) in the middle of through thickness is shown. The basal planes of the matrix are perpendicular to the figure plane, and are colored in yellow and blue to show the *ABABAB*… stacking from left to right. The matrix and the precipitate satisfy the Burgers orientation relationship: $(0001)_M \parallel (011)_P$, and $[2\bar{1}\bar{1}0]_M \parallel [\bar{1}\bar{1}1]_P$. The system contains over one million atoms. A tensile strain was applied on the left and the right end of the box along the [0002] direction.

The system contains over one million atoms, with dimensions 40×20×20 nm^3. The crystallographic orientation of the Mg matrix

is indicated in Figure 1. The $Mg_{17}Al_{12}$ precipitate has dimensions 5×5×5 nm^3, with a bcc structure and located in the center of the Mg matrix. The precipitate is colored differently from the matrix such that it can be readily identified during deformation. The matrix and the precipitate satisfy the predominant Burgers orientation relationship: $(0001)_M \parallel (011)_P$, and $[2\bar{1}\bar{1}0]_M \parallel [\bar{1}\bar{1}1]_P$. Although other orientation relationships were also reported [9-11], only the Burgers orientation relationship was considered in this work.

In our simulations, no pre-existing twin boundaries (TBs) were introduced into the system before the simulations started. The simulation scheme is such that twin nucleation and growth is initiated by an external strain. To obtain an extension twin, a tensile strain was applied by moving the atoms on the right-side end at a constant displacement rate of a/10,000 per time step (3.0 fs) along the [0002] direction, where a = 0.32094 nm is the lattice constant of Mg, corresponding to a strain rate about 8.0×10^8 s^{-1}. In this scenario, the $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ extension twinning is favored. The resolved shear stresses on the basal plane and the prismatic plane are zero, so only pyramidal slip can be activated. The simulation temperature was kept constant at 10 K. Free surfaces were applied to all three dimensions.

In addition to 2-D plots, 3-D plots were made to reveal the migration of the TB and the interaction between the TB and the precipitate. These plots are necessary to obtain unambiguous interpretation of the simulation results.

Results and discussions

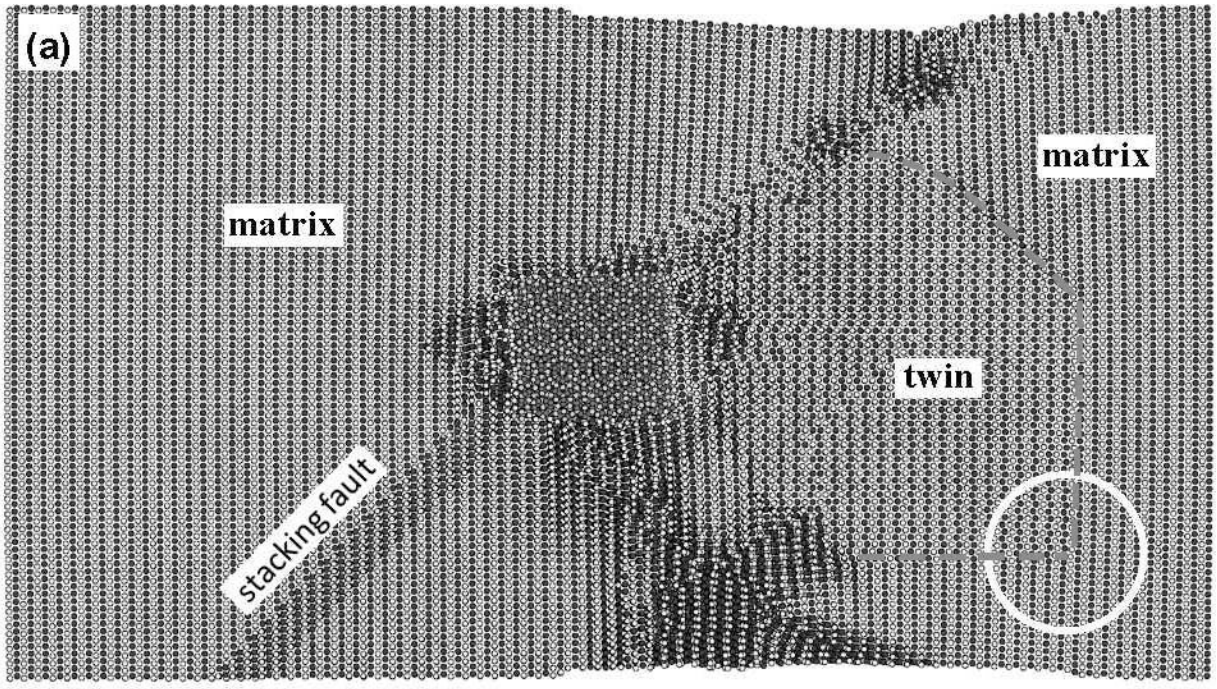
During straining along the [0002] direction, multiple pyramidal dislocations were produced. The 2-D and 3-D views of the pyramidal dislocations and the resultant stacking faults were shown in Figure 2a. These dislocations are on $\{10\bar{1}1\}$. Li and Ma [12] showed that $\{10\bar{1}1\}<10\bar{1}\bar{2}>$ pyramidal slip is energetically more favorable than $\{1\bar{1}22\}<11\bar{2}3>$ for hcp metals because its Burgers vector is smaller and the interplanar spacing is larger [13-15].

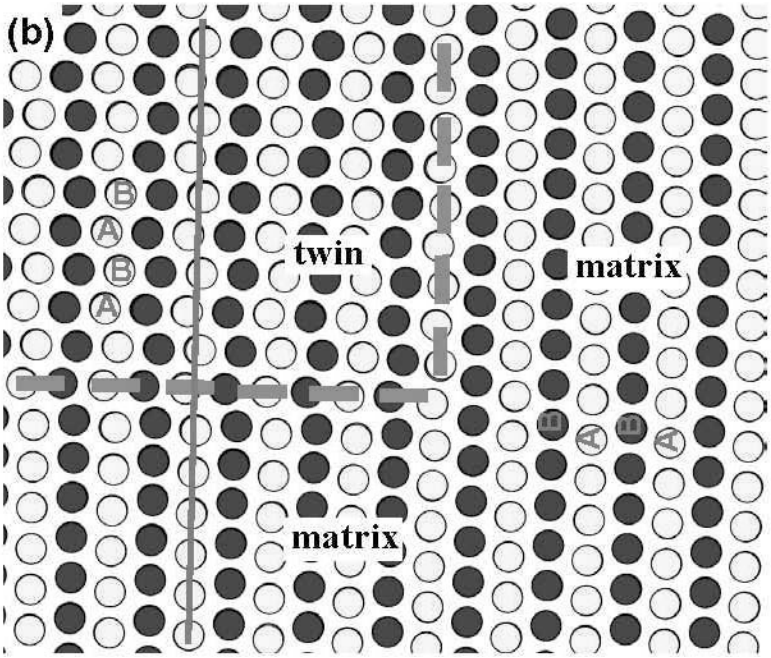
As the tensile strain increases, deformation twinning starts to take place. A $\{10\bar{1}2\}$ twin nucleated near the pyramidal dislocations. The twinned region is enclosed by the stacking faults and an incoherent TB delineated by the dashed pink line in Figure 2a can be observed. Morris et al. [16] show that pyramidal dislocations can be energetically preferred for twin nucleation because the nucleation energy barrier is reduced near the dislocation core. By incoherent, we mean that the TB does not match the $\{10\bar{1}2\}$ twinning plane. Notably it can be observed that, in the 2-D view, the TB appears hugely deviating from the $\{10\bar{1}2\}$ twinning plane. Such a deviation can be appreciated from the fact that part of the TB is nearly parallel to the basal plane of the matrix, whereas the theoretical twinning plane $\{10\bar{1}2\}$ should be at 43.1° with the basal plane. To better reveal the orientation relationship between the twin and the matrix, a circled area in Figure 2a that comprises both the matrix and the twin was magnified and shown in Figure 2b. In the twinned region (bounded by the pink dashed line), the stacking of the basal planes was marked with capital letters *ABAB*… from bottom to top, whereas the stacking of the basal planes of the matrix was also marked with *ABAB*… but from left to right. Clearly, the basal plane of the matrix was reoriented by nearly 90°, typical of $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ extension twinning. An important observation is that, after twinning, the originally flat basal planes, i.e., the blue and yellow columns of atoms, convert to the corrugated prism planes of the twin, but the atoms remain nearly in the original vertical direction. In other words, the basal plane of the matrix did not experience a shear which would otherwise deflect the direction of the columns of atoms. To reveal this interesting phenomenon, we drew a vertical red line that crosses the atoms of a basal plane in the matrix and extends into the twin. In the twinned region, the yellow atoms reside on a double-layered prism plane which is geometrically not a flat plane, but on average, the double-layered prism plane nearly parallels to the matrix basal plane. Such a pattern unequivocally demonstrates that no shear strain was produced by the $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning. 3-D view of the motion of the TB was plotted in Figure 2c. The TB is extremely incoherent in 3-D and does not coincide with a strictly defined crystallographic plane. In Figure 2c, part of the TB (indicated by the block arrow) is passing over the precipitate. As the strain increases, the TB expands, and the precipitate is being engulfed while the matrix material in the front is being twinned. Meanwhile, more stacking faults were generated in the matrix.

As the tensile strain further increases, the twinned region continues to expand and reaches the surfaces, as shown in Figure 3, which is the final stage when the precipitate was engulfed by the twin. In the 2-D view, at the top and the bottom interfaces between the precipitate and the matrix, a thin layer of retaining matrix material can be seen, although the precipitate is entirely embedded inside the twin. In 3-D, the TB has swept over the precipitate without causing shear deformation to it. Some of the defects generated during deformation in the matrix prior to twinning were "cleaned" up by twinning.

Our simulation results confirm that a $Mg_{17}Al_{12}$ precipitate can indeed be engulfed by $\{10\bar{1}2\}$ deformation twins without being sheared while the TB is passing the precipitate. Our simulations also reveal that the TBs are extremely incoherent and can hugely deviate from the $\{10\bar{1}2\}$ twinning plane. In other words, the twinning plane of this predominant twinning mode for hcp metals is far from strictly defined. This phenomenon vastly differs from other twinning modes in hcp, fcc and bcc metals in which a twin boundary has to match the twinning plane at least in the atomic scale, although microscopically small deviations no more than a few degrees are allowed due to the presence of twinning dislocation loops at the TB and strain accommodation. It is required that a TB match the twinning plane because a twinning plane has to be an "invariant plane" during straining [3] and the glide of twinning dislocations is strictly confined in the twinning plane. If $\{10\bar{1}2\}<10\bar{1}\bar{2}>$ twinning were mediated by twinning dislocations, as suggested previously [17-18], we would expect a strong interaction between the precipitate and the twinning dislocations. The twinning dislocations would either shear the precipitate if $Mg_{17}Al_{12}$ is deformable, or be impeded at the precipitate/matrix interface if $Mg_{17}Al_{12}$ is non-deformable. Either of these two cases would result in strengthening to the material, especially if the intermetallic precipitate is non-deformable. But these interactions did not occur in experiments [4-5] and in our atomistic simulations.

Partridge and Roberts [19] first reported extremely incoherent TBs in Zn and Mg in their interesting experiments. Large deviations between TBs and the $\{10\bar{1}2\}$ twinning plane were also observed by Zhang et al. [20] in their transmission electron microscopy (TEM) analysis on deformed pure Co and


(a)
matrix
matrix
twin
stacking fault


(b)
B
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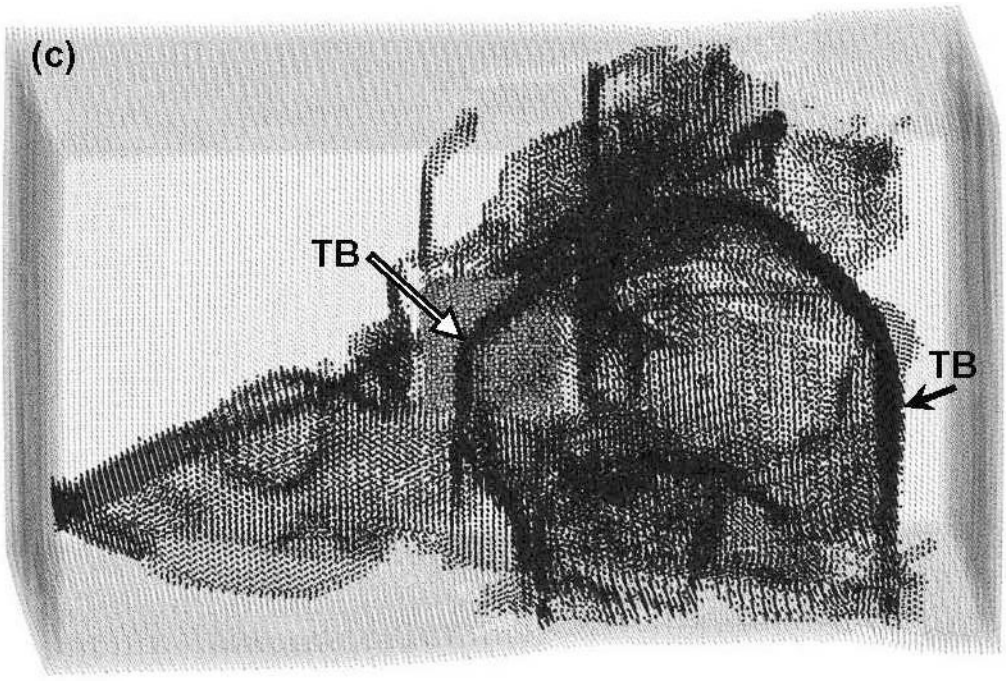

Figure 2. (a) A $\{10\bar{1}2\}$ twin nucleated near the pyramidal dislocations. The twin boundary (TB) is delineated by the dashed pink line. The TB hugely deviates from the $\{10\bar{1}2\}$ twinning plane. (b) The circled area in (a) that comprises both the matrix and the twin was magnified. In the twin (bounded by the dashed line), the stacking of the basal planes is marked with capital letters ABAB… from bottom to top, distinctive from the stacking of the basal planes of the matrix (also marked with ABAB… but from left to right). The change in the stacking sequence indicates that twinning reoriented the matrix lattice by about 90° and the $\{10\bar{1}2\}$ twinning indeed took place. After twinning, the initially flat basal planes convert to the corrugated prism planes of the twin, but the atoms remain nearly in the same vertical direction. A vertical straight line demonstrates that zero shear strain was produced by the $\{10\bar{1}2\}$ twinning. (c) 3-D view of the TB. The TB is extremely incoherent. Part of the TB is passing over the precipitate, as indicated by the block arrow.

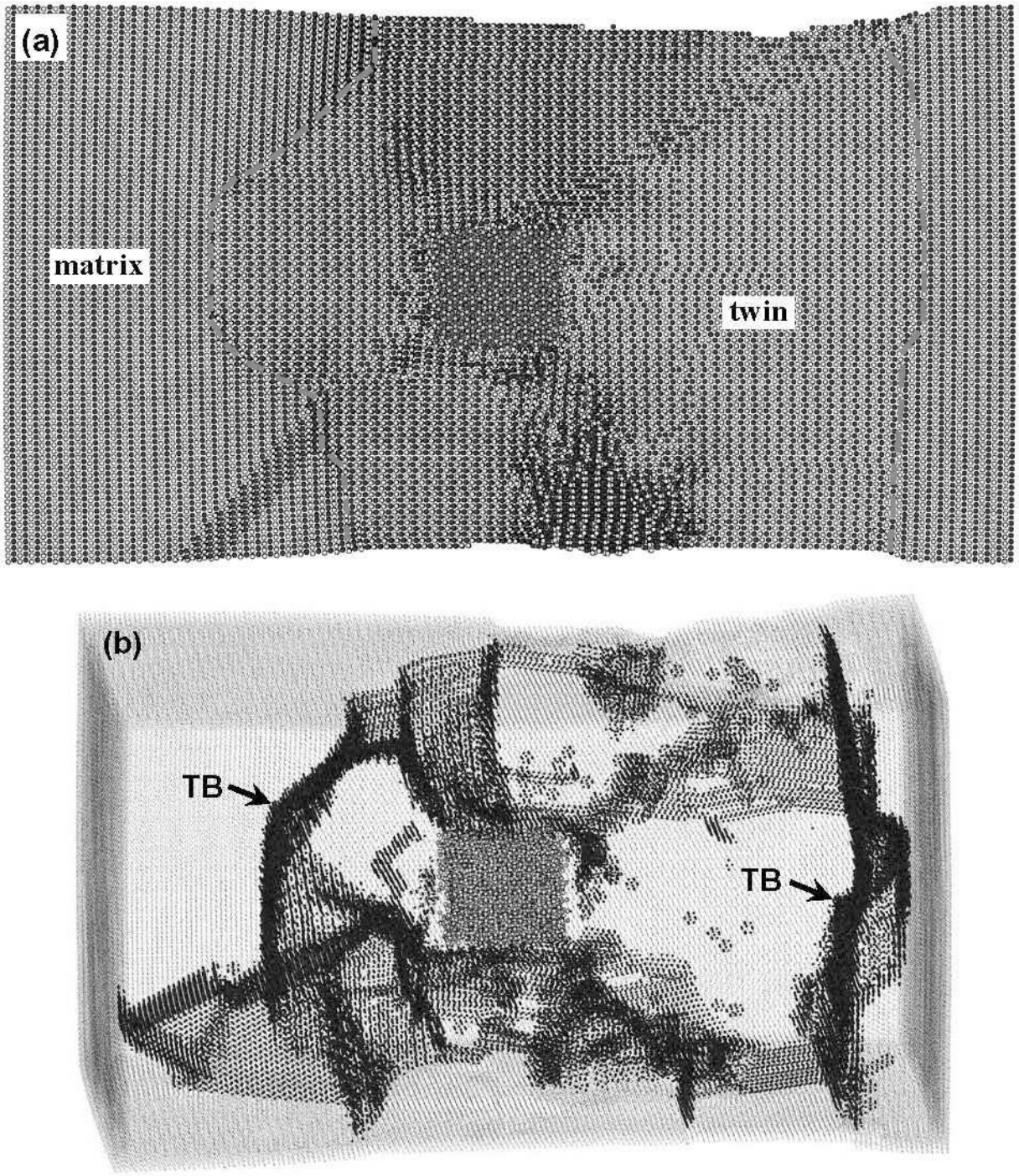

Figure 3. (a) The precipitate is entirely engulfed by the twin without being sheared. The TBs are extremely incoherent. (b) 3-D view. The twinned region expands, digesting the defects generated in the matrix during deformation.

Mg samples. The TBs were observed to deviate from the $\{10\bar{1}2\}$ twinning plane with a magnitude greater than 45°, similar to the deviations observed in our atomistic simulations. Most recently, Liu et al. [21] reported *in-situ* TEM observations of tensile tests on single crystal pure Mg and found that in both twinning and detwinning no shear strain was produced on the specimen.

The experimental observations and our simulations strongly suggest that $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning in hcp metals is not mediated by twinning dislocations. In fact, if $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning were controlled by twinning dislocations, the extensively observed reversible twinning in Mg [22-24] should not happen because dislocation-dominated plastic deformation in crystalline materials is irreversible.

Bilby and Crocker [25] calculated the Burgers vectors and the required atomic shuffling for the twinning modes in hcp lattices. Christian and Mahajan [3] described in detail shear and shuffling of individual twinning modes in various lattices. Shuffling is necessary for most of the twinning modes in hcp metals because a homogeneous shear cannot carry the parent lattice to the twin lattice. Local adjustments are needed to accomplish twinning with a correct lattice structure and orientation relationship.

For the predominant twinning mode in hcp metals, i.e., $\{10\bar{1}1\}<10\bar{1}\bar{2}>$, the magnitude of the theoretical Burgers vector of an elementary twinning dislocation [26] equals 0.024 nm, which is less than one tenth of the Burgers vector of the basal dislocations. Thompson and Millard [26] first suggested that this twinning dislocation comprises two twinning planes in the same time, i.e., a two-layer zonal dislocation. Even so, the overall Burgers vector would still equal 0.05 nm, much smaller than any known Burgers vectors of matrix dislocations. Such an unusually tiny Burgers vector of the twinning dislocation strongly suggests that the controlling mechanism of this particular twinning mode vastly differs from other modes. In fact, this small Burgers vector implicitly conveys important structural information: the twin lattice almost exists in the parent lattice already, before an external load is applied or any twinning shear is initiated.

Li and Ma [27] demonstrated how atomic shuffling can accomplish the $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning, without involving well-defined twinning dislocations. In their model, the lattice conversion between the twin and the parent is achieved by atomic shuffling that converts the parent basal planes to the twin prism planes, and the parent prism planes to the twin basal planes. This direct lattice conversion requires atomic shuffling to create correct hcp lattice and twin orientation relationship. No twinning shear is involved at all. Because of the shuffling dominated twinning, the twin boundaries can pass precipitates, but leaving the precipitates unsheared. Also, because no twinning dislocations are involved, the actual twin boundaries do not have to match the $\{10\bar{1}2\}$ twinning plane and can be extremely incoherent, as seen in our simulations.

Conclusions

We simulated interactions between a $Mg_{17}Al_{12}$ intermetallic precipitate and a $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ deformation twin in Mg, using molecular dynamics. The results reveal that the precipitate can be entirely engulfed by the twin, consistent with experimental observations. The TB sweeps over the precipitate without shearing it. The TBs in the atomistic simulations were observed extremely incoherent and hugely deviate from the $\{10\bar{1}2\}$ twinning plane, also consistent with experimental observations. These observations suggest that $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning is not mediated by twinning dislocations.

A mechanism that is able to account for the zero shear strain and other properties of $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twinning was discussed. In this mechanism, atomic shuffling dominates the twinning and no twinning dislocations are needed at TB. Zero shear strain is produced by atomic shuffling.

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