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Non-classical Twinning Behavior in Dynamically Deformed Cobalt

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We performed transmission electron microscopy studies on dynamically deformed pure cobalt. The results show that the twinning plane of the most common $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning mode in hexagonal close-packed metals is non-coincident, that is, the $\{10\bar{1}2\}$ twinning plane of the parent and the twin does not coincide. Statistical measurements show that only 44% of the twins have a misorientation angle close to the theoretical value of 86.3° , and 79% of the twin boundaries (TBs) deviate from the $\{10\bar{1}2\}$ twinning plane. Thirty-two percent of the TBs deviate from the twinning plane by more than 40° . These results indicate that the $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning significantly departs from the classical twinning behavior.

Keywords: Transmission Electron Microscopy, Deformation Twinning, Cobalt

In deformation twinning, a twinning plane is the key element that is rigidly defined, connects and separates the parent from the twin lattice.[1] During twinning, the twinning plane experiences no structural changes, that is, remains invariant, and mirror symmetry can be established between the parent and the twin about the twinning plane. The parent and the twin lattice satisfy a strictly defined orientation relationship (OR).[1] Growth of deformation twins is mediated by twinning dislocations gliding on the twinning plane.[1] Consequently, a TB should coincide with the twinning plane. When strain accommodation or twin-slip interactions are involved, slight deviations between the TB and the twinning plane are permissible,[2,3] but on the atomic scale the coincidence is still well defined and the OR remains unchanged. For twinning in face-centered cubic (fcc) metals, twin nucleation and growth are mediated by the Shockley partial dislocations that glide on the close-packed $\{111\}$ planes,[4–7] and the twinning plane is always the close-packed planes. The TBs migrate as the Shockley partial dislocations propagate on the twinning plane.

For metals with low symmetry hexagonal close-packed (hcp) crystal structures, for example, magnesium (Mg), titanium (Ti), cobalt (Co), zirconium (Zr), deformation twinning plays a crucial role in accommodating

plastic strain along the direction perpendicular to the (0002) basal plane because the easy dislocation slip systems are unable to [8]. $\{10\bar{1}2\}\langle 10\bar{1}\bar{2}\rangle$ is the most commonly observed twinning mode in all the hcp metals. Crystallographically, this twinning mode should have the twinning plane $\{10\bar{1}2\}$ and a misorientation angle of 86.3° for Mg and Co. However, over the past few decades, numerous experimental observations showed that $\{10\bar{1}2\}$ TBs in hcp metals can entirely deviate from the theoretical twinning plane and the misorientation angle can also deviate from the theoretical value.[9–11] This behavior significantly differs from twinning in high-symmetry fcc metals.

In this work, we performed transmission electron microscopy (TEM) studies on $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning in dynamically deformed Co, and conducted a systematic and statistical analysis on the TB structure. Interesting twinning behavior was observed and possible mechanisms were discussed.

Co with a purity 99.9wt% was deformed by dynamic compression at room temperature with a strain rate $\sim 10^3\text{s}^{-1}$. High-resolution transmission electron microscopy (HRTEM) was then performed on an FEI Tecnai F30-G² electron microscope operating at 300kV. Detailed descriptions of our experiments can be found in Zhang et al. [12].

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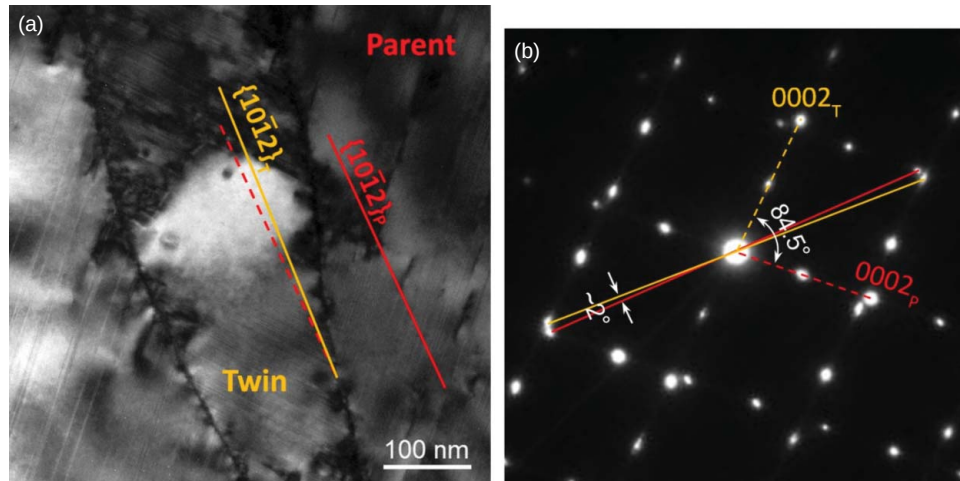


Figure 1. (a) A bright-field TEM micrograph of $\{10\bar{1}2\}\{10\bar{1}\bar{1}\}$ deformation twins in Co at the zone axis $[1\bar{2}10]$. The red solid line marks the trace of the $\{10\bar{1}2\}$ twinning plane in the parent, and the yellow solid line marks the traces of the $\{10\bar{1}2\}$ twinning plane in the twin. The red dashed line is parallel to the red solid line to show that the twinning planes in the parent and the twin do not coincide. (b) Selected area diffraction (SAD) pattern shows that the two twinning planes split by $\sim 2^\circ$. Note that the misorientation angle ($\sim 84.5^\circ$) deviates from 86.3° which is the theoretical misorientation angle.

Figure 1(a) shows a bright-field (BF) micrograph of a $\{10\bar{1}2\}\{10\bar{1}\bar{1}\}$ deformation twin at a relatively low magnification. Twins can be readily distinguished from general grains in deformed specimens at low magnifications. The selected area diffraction pattern (SADP) is presented in Figure 1(b) (the zone axis is $[1\bar{2}10]$). From the SADP, we can determine the traces of the basal (0002) plane and the $\{10\bar{1}2\}$ twinning plane of the parent and the twin. In Figure 1(a), the solid red line marks the trace of the $\{10\bar{1}2\}$ in the parent, and the solid yellow line marks the trace of the $\{10\bar{1}2\}$ in the twin. The dashed red line is parallel to the trace of the $\{10\bar{1}2\}$ in the parent. Clearly, the $\{10\bar{1}2\}$ twinning planes of the parent and the twin do not coincide. The split of the twinning plane is also manifested in the SADP where the $\{10\bar{1}2\}$ reflections slightly separate (marked by the solid red and the yellow lines in Figure 1(b)). The separation between the twinning planes is about 2° . The ideal misorientation angle for $\{10\bar{1}2\}\{10\bar{1}\bar{1}\}$ twinning should be 86.3° . However, the actual misorientation angle is about 84.5° . Note that the actual TBs deviate from the traces of the $\{10\bar{1}2\}$ twinning planes by a large angle, as seen in Figure 1(a).

Figure 1 shows that the misorientation angle of $\{10\bar{1}2\}\{10\bar{1}\bar{1}\}$ twinning can be less than the theoretical value 86.3° . In fact, the misorientation angle can also be larger than 86.3° and Figure 2 displays such an example in which the misorientation angle nearly equals 90° , that is, the basal planes of the parent and the twin are perpendicular to each other. The HRTEM micrograph of the twin tip and the fast Fourier transformation (FFT) of the lattice fringes (Figure 2(b)) indicate that the split between the $\{10\bar{1}2\}$ twinning plane of the parent and the twin is $\sim 4.0^\circ$. Again, we can observe that the actual TBs

deviate from the $\{10\bar{1}2\}$ twinning plane by a large angle, and the TBs are incoherent.

An even larger split of the $\{10\bar{1}2\}$ twinning plane is observed in Figure 3(a) where a twin tip was imaged in HRTEM. Figure 3(b) shows the FFT of the lattice fringes. The traces of the $\{10\bar{1}2\}$ planes in the parent (the solid red line) and in the twin (the solid yellow line) can be determined from the lattice fringes and the FFT. The split in the $\{10\bar{1}2\}$ twinning planes is as much as $\sim 10^\circ$. The actual misorientation angle equals 96.5° , which significantly deviates from 86.3° . Most of the $\{10\bar{1}2\}$ twinning planes in the deformed Co in our experiments show no coincidence. Figure 4 displays another HRTEM micrograph of a $\{10\bar{1}2\}\{10\bar{1}\bar{1}\}$ twin tip. Similar to what is shown in Figure 3, a large split ($\sim 10^\circ$) between the $\{10\bar{1}2\}$ twinning plane of the parent and the twin is revealed.

Figure 5 shows a mosaic of two TEM micrographs so that a larger area of the twins can be viewed. The basal planes of the parent and the twin are denoted by the red and the yellow lines. The misorientation angle between the parent and the twin was $\sim 95.5^\circ$. The TB observed at the top of the micrograph is almost parallel to the basal plane of the parent, indicating that the TB is incoherent. Inside the twin, basal stacking faults (SFs) that cross the whole twin can be observed. These SFs are non-equilibrium SFs that were produced by the migration of incoherent TBs, not by partial dislocations, as discussed in the following.

The non-classical twinning behavior are not only observed in dynamically deformed Co (Figures 1–5), but has also been observed in other HCP metals deformed at quasi-static strain rates.[10,11] Thus, the results (Figures 1–5) presented in this work are not isolated

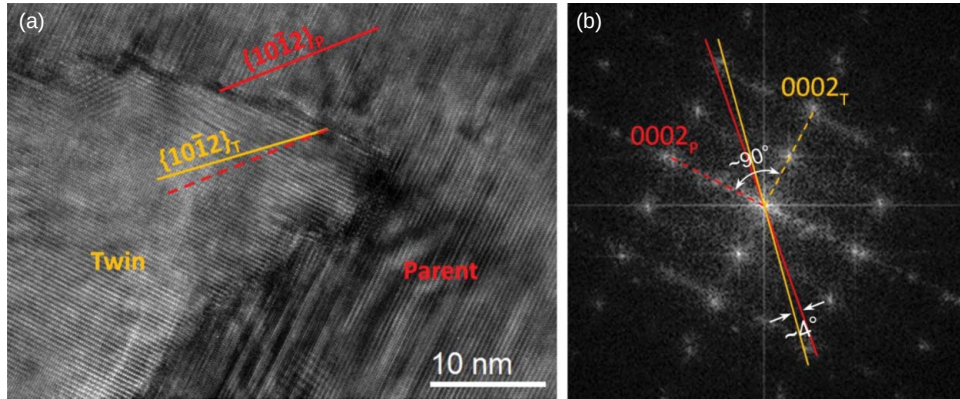


Figure 2. (a) HRTEM micrograph of a $\{10\bar{1}2\}\{10\bar{1}1\}$ twin tip. The Zone axis is $[1\bar{2}10]$. The $\{10\bar{1}2\}$ twinning planes of the parent and the twin do not coincide, and the split is $\sim 4.0^\circ$. The misorientation angle equals $\sim 90^\circ$, instead of 86.3° . The TBs are incoherent. (b) FFT of lattice fringes in (a) shows that the basal plane of the parent is parallel to the prismatic plane of the twin.

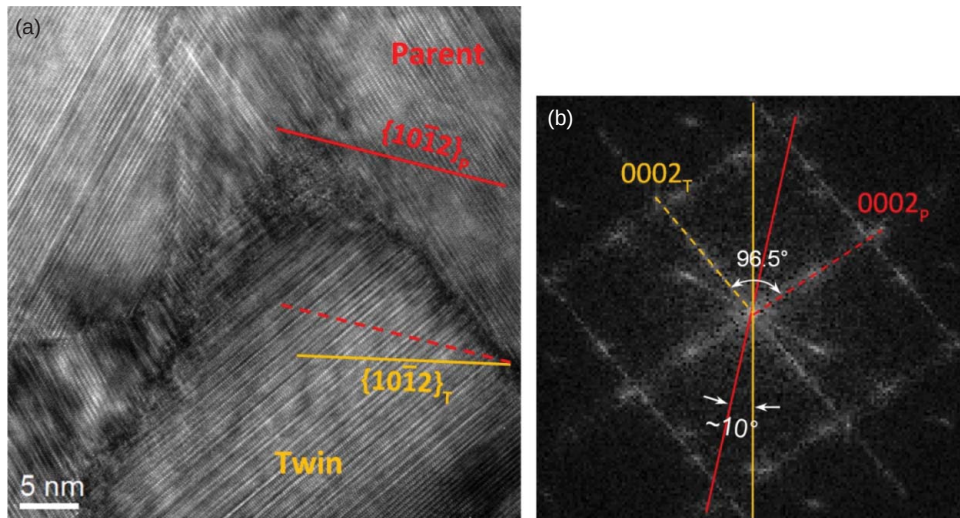


Figure 3. (a) HRTEM micrograph near a $\{10\bar{1}2\}\{10\bar{1}1\}$ twin tip in deformed Co. With a similar color scheme to that in Figure 1, a large split between the $\{10\bar{1}2\}$ twinning planes in the parent and the twin can be observed. (b) SAD pattern shows that the two twinning planes split by as much as $\sim 10^\circ$. Note that the misorientation angle equals $\sim 96.5^\circ$.

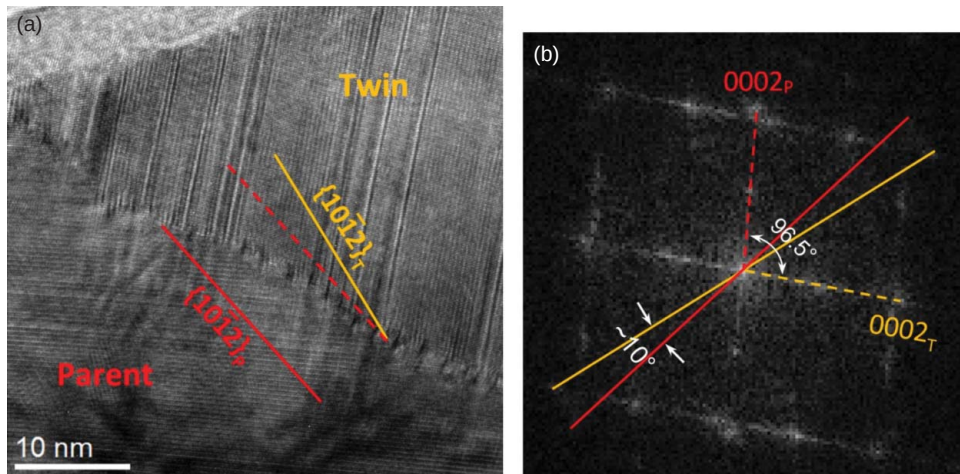


Figure 4. Another HRTEM micrograph near the tip of a $\{10\bar{1}2\}\{10\bar{1}1\}$ twin in Co. (a) The twinning planes in the parent and the twin do not coincide. (b) SAD pattern shows that the misorientation angle largely deviates from 86.3° , and the two twinning planes split by $\sim 10^\circ$.

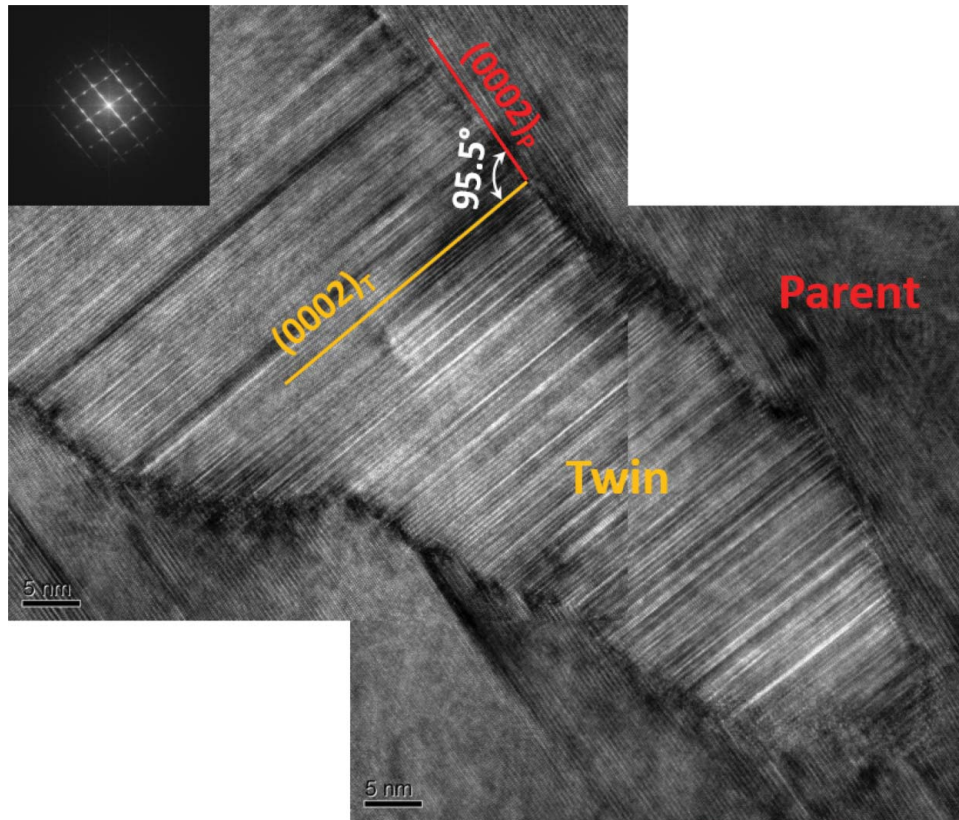


Figure 5. A mosaic of two TEM micrographs of $\{10\bar{1}2\}\{10\bar{1}\bar{1}\}$ twins. The misorientation angle between the parent and the twin is $\sim 95.5^\circ$. Note that the top TB is nearly parallel to the basal plane of the parent, indicating that the TBs are incoherent.

observations. To ascertain this, we performed statistical measurements of the misorientation angle between the $\{10\bar{1}2\}\{10\bar{1}\bar{1}\}$ twins and the angle between the actual TBs and the theoretical $\{10\bar{1}2\}$ twinning plane in our TEM observations of the twins. The results are shown in Figure 6(a) and 6(b). The distribution of the deviation between the actual TBs and the $\{10\bar{1}2\}$ twinning plane is shown in Figure 6(a). Among the 34 measurements, only 7 TBs coincide with the twinning plane. This indicates that 79% of the TBs deviate from the twinning plane. Seventy-six percent of the TBs deviate from the twinning plane by more than 10° , and 32% by more than 40° . Notably, when the deviation is 45° , the parent and the twin on both sides of the TB satisfy a special relationship: either the basal plane of the parent is parallel to the prismatic plane of the twin, or the prismatic plane of the parent is parallel to the basal plane of the twin, that is, $\{0002\}_P || \{10\bar{1}0\}_T$ or $\{10\bar{1}0\}_P || \{0002\}_T$ (these two scenarios are structurally equivalent). Hence, nearly one-third of the TBs are these two types of interface. The distribution of the misorientation angle of the $\{10\bar{1}2\}\{10\bar{1}\bar{1}\}$ twins is shown in Figure 6(b). Only 44% of the measured misorientation angles are nearly equal to the theoretical value of 86.3° , indicating that more than half of the twins do not have a misorientation angle of 86.3° . Nearly 20% of the twins have a misorientation angle deviating

from 86.3° by $\sim 10^\circ$. These measurements suggest that the mechanism of $\{10\bar{1}2\}\{10\bar{1}\bar{1}\}$ twinning should be very different from the classical twinning, because the extent and magnitude of the deviations in terms of the misorientation angle and the non-coincidence between TBs and the twinning plane in the deformation twins were not observed in any other twinning mode in metals, under any loading conditions.

The TEM observations and the statistics shown in this work indicate that (i) for the most commonly observed $\{10\bar{1}2\}\{10\bar{1}\bar{1}\}$ twinning, the twinning plane of the parent and the twin does not coincide, and the actual TBs deviate from the theoretical twinning plane by a large angle; (ii) the misorientation angle deviates from 86.3° . Hence, this twinning mode significantly departs from the twinning models proposed previously.[1,13–15] In the following, we discuss possible mechanisms for the non-classical twinning behavior observed in this work and others.

Non-coincident twinning planes were also observed in Ti,[10] and the mechanism was ascribed to the presence of the sessile Frank partial dislocations at the TBs as a result of dissociation of glissile dislocations in the parent. However, if sessile partial dislocations are present on the TBs, reverse twinning that has extensively been observed in experiments would not be

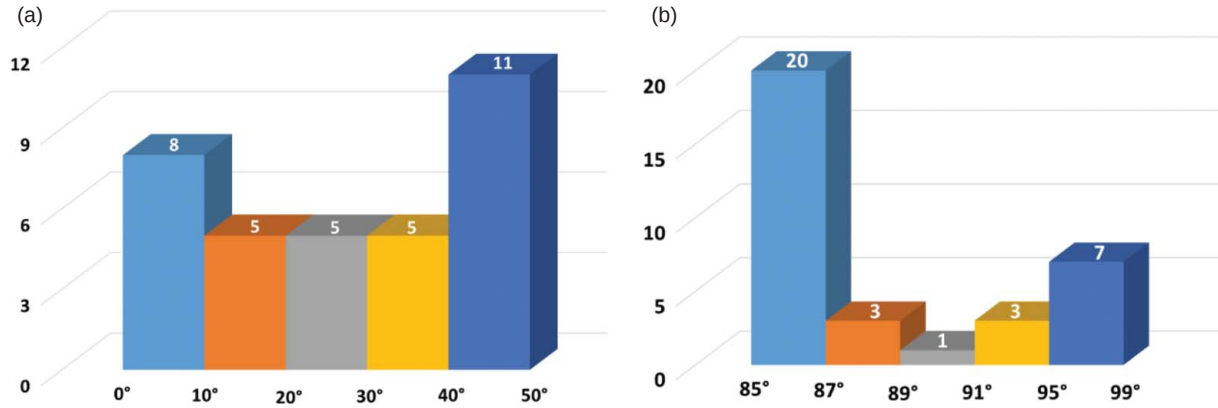


Figure 6. (a) Distribution of the angle between the actual TBs and the theoretical $\{10\bar{1}2\}$ twinning plane. Only 7 out of 34 measured TBs coincide with the twinning plane, that is, 79% of the TBs deviate from the twinning plane. Seventy-six percent of the TBs deviate from the twinning plane by more than 10° , and 32% by more than 40° . (b) Distribution of the misorientation angle of $\{10\bar{1}2\}$ twins in deformed Co. Only 44% of the measured misorientation angles are close to the theoretical value of 86.3° .

possible.[16,17] Microscopically, twin-slip interactions and strain accommodations may cause the actual TBs to slightly deviate from the twinning plane,[1,9] but these interactions are unable to change the misorientation by a large angle because the misorientation is uniquely defined for each twinning mode under the invariant plane strain condition, that is, the twinning plane should remain structurally unchanged during twinning. In Figures 1–5, SFs on the basal planes in the twin and the parent are observed. These SFs run across the whole twinned regions and are one to two orders magnitude wider than the equilibrium width of the basal SFs. Recent atomistic simulations [18] show that these non-equilibrium basal SFs, which are observed in almost all deformed hcp metals,[19–22] result from the migration of incoherent TBs. During twin growth, parent atoms shuffle to the faulted sites of the twin and no partial dislocation slip is involved in the formation of these wide SFs. This indicates that the incoherent TBs in Figures 1–5 are not caused by dislocation slip inside the twins.

The following presents a more likely mechanism for the non-classical twinning behavior from the perspective of lattice correspondence required in deformation twinning. In classical twinning, there exists a lattice correspondence between the parent and the twin, that is, planes/directions of the parent are linearly mapped to planes/directions of the twin.[1,15,23] For twinning modes in hcp metals, twinning is accomplished via a homogeneous shear and atomic shuffling, because a homogeneous shear is unable to carry all the parent atoms to the twin lattice. Particularly, for $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning, the $(0002)_P$ basal plane of the parent is mapped/transformed to the $\{10\bar{1}0\}_T$ prismatic plane of the twin, and the prismatic plane of the parent is mapped/transformed to the basal plane of the twin.[23] The theoretical misorientation angle equals 86.3° for Co and Mg. However, structurally, the prismatic plane is

a corrugated, double-layered plane, whereas the basal plane is a single-layered, flat plane. Hence, to achieve the required lattice correspondence, large shuffles must be involved because a homogeneous shear cannot transform a flat basal plane to a corrugated prismatic plane or vice versa. If we closely examine the particular case shown in Figure 2 where the misorientation angle is nearly 90° , it can be seen that the basal plane of the parent is parallel to the prismatic plane of the twin. Immediately, this implies that no homogeneous shear should be involved, and the Burgers vector of the elementary twinning dislocation must be zero anywhere on the TB, because any non-zero Burgers vector would destroy the parallelism of $\{0002\}_P||\{10\bar{1}0\}_T$ or $\{10\bar{1}0\}_P||\{0002\}_T$. In this special case only shuffling is needed to accomplish twinning. In fact, it can be analytically and computationally proven that the Burgers vector of the twinning dislocation of the $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning mode should be zero. The external strain is accommodated by the misfit strains between the parent and the twin lattice.[24] The most recent *in situ* TEM observations [25,26] of twinning and detwinning in single-crystal Mg validate this conclusion: during $\{10\bar{1}2\}$ twinning and detwinning, no measurable shear strain was produced on the specimen. The specimen uniformly narrows during twinning and uniformly widens during detwinning. Xu et al. reported [27] that a special interface that satisfies $(0001)_P||\{10\bar{1}0\}_T$ has a high mobility and plays an important role in $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning. It is worth noting that this is exactly the scenario described in the shuffling-dominated twinning mechanism [28] in which the lattice transformation between the basal plane of the parent and the prismatic plane of the twin and vice versa is solely accomplished by atomic shuffling. Xu et al. [27] claimed that the motion of this type of TB is mediated by the misfit dislocation. However, a twinning mode should only have a unique value and direction of the twinning

shear.[1] It is unlikely that two completely different dislocations on the same TB mediate the TB migration simultaneously, because different twinning dislocations would produce different lattice correspondences.

In cases that the misorientation angle does not equal 90° , that is, the basal plane of the parent is not parallel to the prismatic plane of the twin, for example, Figures 1, 3–5, the atomic shuffling can be adjusted to accommodate such deviations without introducing any homogeneous shear. The absence of the shear explains well why $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning is reversible.[16,17] Experimentally, it was widely observed that in cyclic loading or upon removal of the external load, $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twins shrink and the TBs move backward.[16,17] This is because the zero-shear lattice transformation between the parent and the twin is reversible.[24] It was also observed that a migrating TB engulfs precipitate without shearing them or leaving dislocation loops around them in Mg alloys.[29,30] Therefore, the zero-shear in $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning naturally explains well these experimental observations.

To conclude, we performed TEM observations and statistical measurements on the structure of $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ TBs in dynamically deformed Co. The results show that the actual TBs can deviate from the theoretical $\{10\bar{1}2\}$ twinning plane by a large angle, and the TBs are incoherent. The misorientation angle also largely deviate from the theoretical value 86.3° , and the $\{10\bar{1}2\}$ twinning plane of the parent and the twin does not coincide. These observations indicate that the invariant plane strain condition, which is required for deformation twinning, breaks down, and the mechanism of $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning should be very different from the twinning dislocation theories proposed before.

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