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Twin boundaries showing very large deviations from the twinning plane

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In deformation twinning, twin boundaries (TBs) should coincide with the twinning plane. Here we show that the TBs of the most common twinning mode in hexagonal close-packed metals, $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$, may not lie on the $\{10\bar{1}2\}$ twinning plane. Examinations using transmission electron microscopy (TEM) reveal that the TBs in Co and Mg deviate significantly from the $\{10\bar{1}2\}$ plane. High-resolution TEM confirms that the incoherent TBs entirely depart from the twinning plane with a magnitude greater than 45°.

Keywords: Twin; Twin boundary; Deformation twinning; Cobalt; Magnesium

When crystalline solids are subjected to plastic deformation, in addition to dislocation slip, deformation twinning can be activated to accommodate the microscopic strain. A deformation twin, which predated the concept of dislocation (1934), was defined as "a region of a crystalline body which has undergone a homogeneous shape deformation in such a way that the crystal structure of the resulting product is identical with that of the parent, but oriented differently" [1]. Because the two structures are identical, the boundary plane, also known as the twinning plane, must remain invariant during twinning. The parent and the twin lattices are reflected about the twinning plane.

The homogeneous shear involved in twinning carries parent atoms to the twin lattice [2]. To accomplish a homogeneous shear on a twinning plane, passage of twinning dislocations at the interface is required to complete such displacements. A twinning system comprising a twinning plane and a twinning direction along which the shear takes place can be rigorously defined in this scenario. The twin boundary (TB), i.e. the interface between parent and twin, has to coincide with the twinning plane, although microscopically local disregistry is permissible in the presence of twinning dislocation loops. In face-centered cubic (fcc) metals such as aluminum, copper, nickel, etc., the twinning plane is identical to the slip plane of dislocations, i.e. the close-packed $\{1\,1\,1\}$ planes, and the twinning dislocations are Shockley partials $\frac{1}{6}\langle 1\bar{2}1\rangle$.

In low-symmetry, hexagonal close-packed (hcp) materials such as Mg, which have attracted tremendous attention in the quest for lightweight vehicle design, twinning plays a crucial role in plastic deformation and strain-path anisotropy [3]. On one hand, the easy slip directions contained in the basal plane are incapable of accommodating strain when the unit cell is loaded normal to the basal plane. On the other hand, non-basal slip systems are harder to activate than twinning by at least a factor of 3. The most frequently observed twinning mode in all hcp metals, which is always believed to be on the $\{10\bar{1}2\}$ plane and parallel to the $\langle 10\bar{1}\bar{1}\rangle$ direction, predominates in plastic deformation among multiple twinning modes. Within the framework of classical deformation theories, numerous crystallographic models have attempted to resolve twinning dislocations on the twinning plane $\{10\bar{1}2\}$ that carry out the shear and reorient the parent to the twin [3–12]. Sources of

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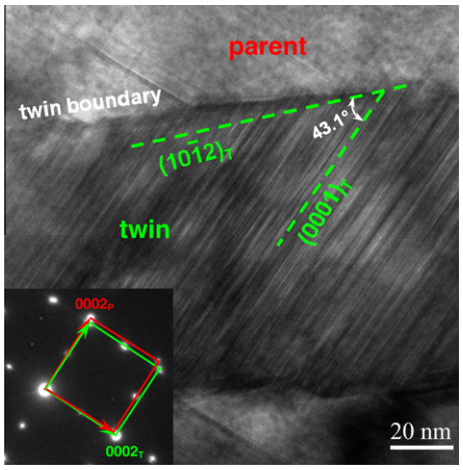

Figure 1. A bright-field TEM micrograph of deformation twins in Co with a selected-area diffraction pattern. The diffraction in the inset indicates that the crystals satisfy the $(10\bar{1}2)[10\bar{1}\bar{1}]$ twin orientation relationship (zone axis $[1\bar{2}10]$), as the [0001] axes of the parent and the twin are nearly perpendicular to each other. The basal plane and the $(10\bar{1}2)$ twinning plane are perpendicular to the plane of view, and are marked with broken lines. The trace of the twinning plane $\{10\bar{1}2\}$ makes an angle of 43.1° with the basal (0002). Apparently the trace of the $(10\bar{1}2)$ twinning plane does not match the actual twin boundary.

glissile partial twinning dislocations created from dissociation of existing dislocations in the parent have also been hypothesized [5–8]. Due to the double-layer nature of this twinning plane, Thompson and Millard [4] suggested that the twinning dislocation in this particular mode should have a double-step structure on the twinning plane, i.e. the dislocation core spreads over multiple twinning planes, each plane comprising an elementary twinning dislocation [2]. Coupled with a homogeneous shear, atomic shuffling is required to establish the correct twin orientation relationship [1,2].

A twinning plane is the key element in defining a twinning system in crystalline solids. Using conventional and high-resolution (HR) transmission electron microscopy (TEM), we measured the traces of the twinning plane $\{10\bar{1}2\}$ and the actual TBs in hcp metals Co and Mg. An abnormally large deviation was uncovered.

Pure, polycrystalline Co samples were deformed dynamically at room temperature [13], and the microstructure of the tested samples was examined by TEM and HRTEM. Figure 1 shows a bright-field TEM micrograph at a relatively low magnification. The lattice fringes are barely resolved. The diffraction spots in the inset reveal two sets of diffraction patterns from disoriented crystals. The electron beam parallels to the zone axis $[1\bar{2}10]$, indicating that the crystals indeed satisfy the $\{10\bar{1}2\}\langle10\bar{1}\bar{1}\rangle$ twinning relationship, as the *c* axes, i.e. [0002], of the parent and the twin are nearly perpendicular to each other. From the orientation relationship, traces of the basal planes of the twin and the parent, as well as traces of the $\{10\bar{1}2\}$ twinning planes, can be precisely determined. Two broken lines in Figure 1 mark the traces of the basal of the twin (0001) and the $\{10\bar{1}2\}$ twinning plane, and the two traces meet at an angle of 43.1°. We can immediately see that the trace of the $\{10\bar{1}2\}$ twinning plane does not match the actual TB.

Even greater deviation was revealed in other twins and HRTEM micrographs of the $\{10\bar{1}2\}\langle10\bar{1}\bar{1}\rangle$ TBs, and traces of the twinning planes are shown in Figure 2. Lattice fringes from the basal planes can be seen as well. In the inset of Figure 2a, the diffraction pattern indicates that the grains satisfy the $\{10\bar{1}2\}\langle10\bar{1}\bar{1}\rangle$ twin relationship. The zone axis runs parallel to $[1\bar{2}10]$, and the TBs, twinning planes, and the basal planes of the twin and the parent are all parallel to the zone axis. In this orientation, there are only two possible twinning planes, and their traces are marked with two broken lines. It can be seen that the actual TBs deviate strikingly from the

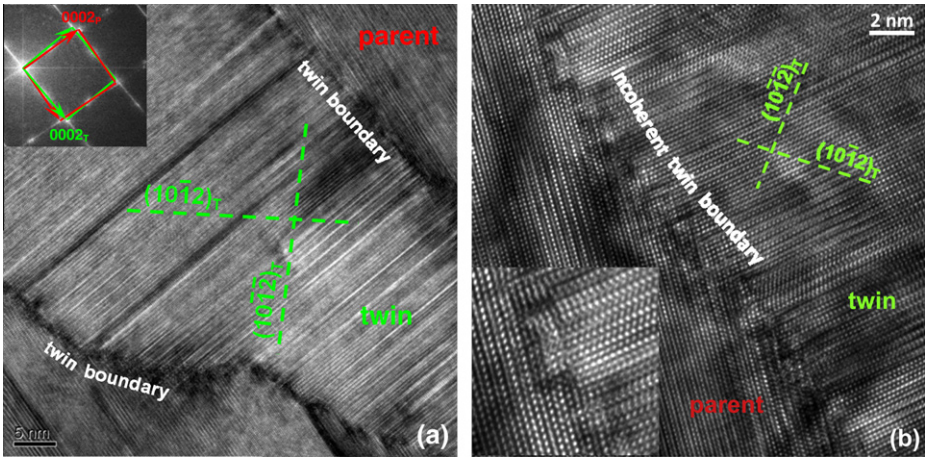

Figure 2. High-resolution TEM micrographs showing that the twin boundaries in Co conspicuously deviate from the twinning planes. (a) Twin boundaries near the twin tip are shown. The diffraction pattern in the inset indicates that the twin and the parent indeed satisfy the $\{10\bar{1}2\}\langle10\bar{1}\bar{1}\rangle$ twin relationship (zone axis $[1\bar{2}10]$). In this orientation, the two possible twinning planes $\{10\bar{1}2\}$ are marked with broken lines. We can see that the actual twin boundaries largely deviate from the twinning planes. The deviation can also be appreciated by noticing that the top twin boundary is nearly parallel to the basal plane of the parent. (b) A higher magnification showing the lattice fringes near the twin boundary evidencing a very rough interface as can be better seen in the higher-magnified inset. The twin boundary is actually incoherent.

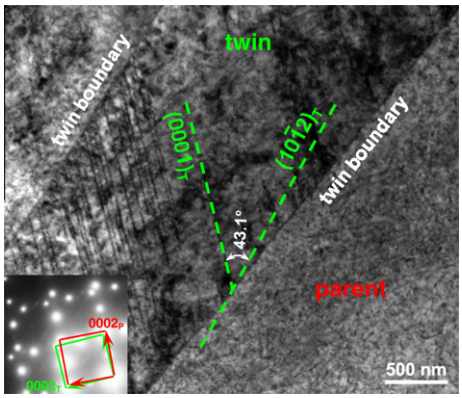

Figure 3. TEM micrograph of deformed Mg shows that the actual twin boundary deviates (~10°) from the trace of the twinning plane $\{10\bar{1}2\}$. The diffraction pattern in the inset identifies the twinning mode as $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ since the [0002] axes of the parent and the twin are nearly perpendicular to each other (zone axis $B = [1\bar{2}10]$). The straight dark lines inside the twin are the traces of the stacking faults and coincide with the trace of the basal plane (0002).

twinning plane $\{10\bar{1}2\}$, with a deviation greater than 45°. In fact, the TB near the top is almost parallel to the basal plane of the parent. To view the structure of the TBs, we show lattice fringes at a higher magnification in Figure 2b. The TB appears very coarse and incoherent in this two dimensional (2-D) view. In 3-D, the TB is a rough interface that does not coincide with a crystallographic plane. A section of the TB is magnified in the inset to highlight the incoherency.

Regardless of the *c*/*a* ratio, the $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning takes place predominantly in hcp metals. Hence it is likely that such deviation of TBs from the $\{10\bar{1}2\}$ twinning plane observed in Co may be universal to all hcp metals. Indeed, such deviation was also uncovered in commercially pure, polycrystalline Mg. The sample was compressed to 4% plastic strain at room temperature. Before compression, the sample was annealed for 3 h at 550 °C, so that the starting microstructure had a low dislocation density. We then performed TEM analysis on the TBs. Figure 3 shows a TEM micrograph in which edge-on TBs were recorded. The actual TB deviates significantly (~10°) from the trace of the twinning plane $\{10\bar{1}2\}$ (marked with a broken line). In the inset, two sets of diffraction patterns can be identified, which satisfy the $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twin orientation relationship, as the [0001] axes of the parent and the twin are nearly perpendicular to each other (zone axis $B = [1\bar{2}10]$). The diffraction patterns also indicate that the TBs are parallel to the electron beam, and the basal planes in the parent and the twin are perpendicular to the plane of view. The straight, dark lines inside the twin, representing the traces of stacking faults, coincide perfectly with the trace of the basal plane (0001). With these dark lines as a reference, the trace of the twinning plane $\{10\bar{1}2\}$, which also makes an angle of 43.1° with the traces of the basal (0001) (marked with broken lines), can be precisely determined. The TEM observation confirms that the $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ TBs in pure Mg can also deviate from the $\{10\bar{1}2\}$ twinning plane.

Macroscopically, twins assume lenticular morphologies, allowing the TBs to depart from the coherent twinning plane by no more than a few degrees. Strain accommodation, twin–slip interaction, twin–twin interaction, and intersection between a TB and an anti-phase boundary may also locally disrupt the registry of a TB [2,14]. In Figures. 1–3, high-density stacking faults with traces parallel to the basal plane can be observed (the nature of these stacking faults was not characterized in this work), and these planar defects intersect the TBs. This twin–slip interaction is able to generate steps in the TBs such that a small deviation can be produced to the overall TB. Zheng and Ma [14] observed asymmetric TB in BaNb0.3Ti0.7O3 thin film. At the intersections of a TB and anti-phase boundaries, steps are produced in the TB, and the overall TB departs from the {111} twinning plane by about 8°; between the steps, however, no deviation can be seen.

The large deviations of the actual TBs from the $\{10\bar{1}2\}$ twinning plane in Co and Mg seem at odds with the classical twinning theory. For other twinning modes [15–18] in hcp and fcc metals where twinning dislocations are well defined, the TBs are coherent and match well the twinning plane on the atomic scale. Hence, it is conceivable that the most common twinning mode in hcp crystals may be controlled by a mechanism other than the widely accepted twinning dislocations. If the $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning were mediated by twinning dislocations, as presumed previously [3–12], such a large deviation (Fig. 2) should not exist on the atomic scale because the twinning dislocations are strictly bounded in the twinning plane. Thus, the $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning mode should embrace characteristics unique to other twinning modes.

Bilby and Crocker [1] and Christian and Mahajan [2] demonstrated that atomic shuffling must be involved in principal twinning modes in hcp crystals, except for the $\{11\bar{2}1\}\langle 11\bar{2}\bar{6}\rangle$ mode. The magnitude of the crystallographically defined Burgers vector of the elementary twinning dislocation on the $\{10\bar{1}2\}$ equals $(3-\gamma^2)\cdot a/(2\sqrt{3+\gamma^2})$, where a is the lattice parameter, 0.321 nm for Mg and 0.251 nm for Co, and γ is the *c*/*a* ratio, 1.624 for Mg and 1.623 for Co [4]. Calculations show this magnitude equals 0.024 nm for Mg and 0.019 nm for Co. For a double-step zonal dislocation [2], the Burgers vector would be 0.05 nm for Mg and 0.04 nm for Co. These Burgers vectors are only a tiny fraction of any dislocations identified in experiments and substantially shorter than the magnitude of atomic shuffling required to complete the twinning. Such a small Burgers vector of a twinning dislocation cannot be reconciled with the large shuffling when "twinning dislocations" are strenuously defined because atoms at the TB move even in opposite directions and off the $\{10\bar{1}2\}$ twinning plane. Crystallographically, the exceptionally small "twinning dislocation" implies that, for the most common $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning mode in hcp metals, the twin lattice almost exists in the parent lattice already before any twinning shear is applied. Only local atomic shuffling is needed to accomplish the $\{10\bar{1}2\}$ twinning. In other words, this particular twinning mode is controlled by atomic shuffling.

Li and Ma illustrated how atomic shuffling accomplishes the $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning [19]. In their model, the lattice conversion between the twin and the parent is accomplished by atomic shuffling that converts the parent basal planes to the twin prism planes, and the parent prism planes to the twin basal planes. No well-defined dislocations are involved in the lattice conversion. This conversion between the parent and the twin lattices creates $(\sqrt{3}-\gamma)/\gamma$ misfit strain along the [0001] axis of the parent lattice (6.7% for Mg and Co), rendering this twinning mode highly efficient in accommodating the tensile strain along the [0001] axis [9]. This shuffling-dominated twining mechanism has been validated by extensive experimental observations. It explains well the structural origin of the reversible twinning or pseudo-elasticity that was repeatedly observed in hcp metals [20–23], and the non-Schmid effect [24], In addition, the shuffling-dominated twinning allows a twin variant to penetrate a grain boundary or another variant [25].

The large deviation of the actual TBs from the twinning plane $\{10\bar{1}2\}$ can be understood with the shuffling mechanism. Because shuffling does not have to be confined in the $\{10\bar{1}2\}$ twinning plane, it is permissible for the actual TBs to migrate far off the $\{10\bar{1}2\}$ plane during twin growth. As shown in Figure 2, the TBs do not have to be flat to match the twinning plane, even in the atomic scale. In fact, Partridge and Roberts [26] observed abnormal TB migration in Mg. They found that the $\{10\bar{1}2\}$ TB can evolve into extreme incoherency under small stresses.

Finally, although our TEM observations are seemingly at odds with the classical twinning theory, the shuffling-dominated twinning can actually be considered an extreme case that still falls inside the framework of the classical theory. The relative magnitude of homogeneous shear and shuffling plays a critical role in determining the configurations of twinning dislocations; as pointed out by Christian and Mahajan [2], shuffling can be as important as the magnitude of shear. In the case of $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning, shuffling dominates shear; in other twinning modes, i.e. $\{10\bar{1}1\}\langle 10\bar{1}\bar{2}\rangle$ and $\{11\bar{2}1\}\langle 11\bar{2}\bar{6}\rangle$, shear dominates shuffling. In these latter cases zonal twinning dislocations can be well defined on the twinning plane and perfect coincidence between TBs and the twinning plane can be observed [15].

To conclude, we have presented TEM and HRTEM examinations of the $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning in Mg and Co, and reveal that in this most commonly observed twinning mode in hcp metals the actual TBs can deviate significantly from the $\{10\bar{1}2\}$ plane. These deviations can be explained by atomic shuffling, which plays a dominant role in the $\{10\bar{1}2\}$ twinning.

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