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On the $\{10\bar{1}2\}$ "twinning shear" measured from line deflection

X.Y. Zhang [a,*], B. Li [b,d,**], Q. Sun [c]

[a] School of Materials Science and Engineering, Chongqing University, China
[b] Department of Chemical and Materials Engineering, University of Nevada, Reno, NV 89557, United States of America
[c] School of Material Science and Engineering, Southwest Jiaotong University, Chengdu, China
[d] Nevada Institute for Sustainability, University of Nevada, Reno, NV 89557, United States of America

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ABSTRACT

A recent experimental measurement of the "twinning shear" of $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ mode in magnesium reported a value of 12.6%, which is close to the theoretical value. The measurement was based on observation of line deflection across a twin boundary. Here we demonstrate that line deflection is solely a result of lattice transformation in deformation twinning, and can happen even when no homogeneous simple shear occurs on the twinning plane, which is exactly the case for $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ mode. Lattice correspondence analysis and high resolution transmission electron microscopy observations of incoherent twin boundaries with different misorientation angles are presented to validate our conclusion.

Deformation twinning plays a crucial role in mechanical behavior of metals with hexagonal close-packed (hcp) crystal structures [1]. Among all the reported twinning modes, $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ is the most commonly observed in experiments and accordingly the most important one. The mechanism of this twinning mode has been studied extensively over the past decades, especially in recent years when hcp magnesium (Mg) and its alloys have attracted tremendous attention as potential lightweight engineering materials [2–8]. Historically, this twinning mode has been treated classically just like any other twinning modes in metals, that is, a twinning mode must be associated with a finite twinning shear which is responsible for a "homogeneous shape deformation" during twinning [9]. This requires: (1) the twinning plane be invariant because the parent and the twin lattices remain in contact during twin boundary (TB) migration; and (2) the shear be a simple shear because there is no volume change. In the classical theory, the defect that mediates TB migration was predicted to be a two-layer zonal twinning dislocation [1,10].

However, early experimental observations showed that an actual TB was able to migrate into extreme incoherency which completely departed from the $\{10\bar{1}2\}$ twinning plane, aka the first invariant plane K_1 [11]. Numerous transmission electron microscopy (TEM) observations revealed similar behavior [12–16]. Serra et al. [17] simulated TB migration of all four major twinning modes with molecular dynamics. Their results showed that a TB became incoherent during migration instead of staying on the $\{10\bar{1}2\}$ plane; in stark contrast, TBs in other twinning modes remained coherent or nearly coherent [18,19]. The anomalous behavior in $\{10\bar{1}2\}$ mode prompted Serra et al. to propose "disconnections" [17,20] over "zonal twinning dislocations" to describe interfacial defects on TBs for twinning modes in hcp metals. However, the disconnection model does not answer a fundamental question: why the classical twinning theory generally well describes other twinning modes but fails on $\{10\bar{1}2\}$ mode?

Recently, Li and Ma [21] proposed that $\{10\bar{1}2\}$ mode is mediated solely by atomic shuffling and no twinning dislocations are involved in TB migration. Their simulations showed that this twinning mode is accomplished by the transformation of parent basal to twin prismatic, and parent prismatic to twin basal. More recently, Li and Zhang [15] proved that the magnitude of twinning shear s of $\{10\bar{1}2\}$ mode cannot be any finite value but zero because the twinning plane is not an invariant plane. To transform parent to twin, the structure of the twinning plane has to be distorted. Cayron [22] mathematically calculated the lattice transformation and showed that the twinning plane is indeed not invariant and no twinning shear should occur on the $\{10\bar{1}2\}$ twinning plane.

Most recently, Molodov et al. [23] experimentally measured $\{10\bar{1}2\}$ "twinning shear" in deformed Mg. A line marking on the surface of a specimen, which was found deflected after twinning, was used to determine s. The measured twinning shear was 12.6%, close to

* Corresponding author.
** Correspondence to: B. Li, Department of Chemical and Materials Engineering, University of Nevada, Reno, NV 89557, United States of America.
E-mail addresses: kehen888@163.com (X.Y. Zhang), binl@unr.edu (B. Li).

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the theoretical value 12.9%. This report adds more controversy to the mechanism of $\{10\bar{1}2\}$ twinning mode.

The purpose of this work is to demonstrate that line deflection, which is a manifestation of lattice correspondence or lattice transformation in deformation twinning, may occur even when *s* equals zero. Thus, observation of line deflection is insufficient to reach a conclusion of a finite twinning shear for $\{10\bar{1}2\}$ mode, unless a homogeneous simple shear indeed occurs on the twinning plane.

To understand the underlying physics of line deflection in twinning, we first introduce a key feature in deformation twinning – lattice correspondence. In his posthumous book, Christian stated that [24] there exists a one-to-one correspondence between vectors/planes in parent and twin. Thus, a plane of the parent must be transformed to a corresponding plane of the twin. As shown by Li and Ma [21], Li and Zhang [15], the lattice correspondence in $\{10\bar{1}2\}$ twinning is such that a parent basal is transformed to a twin prismatic and a parent prismatic to a twin basal. This lattice correspondence, although implicit, can be readily identified in atomistic simulations in the literature by numerous researchers [17,25–29]. Fig. 1 is the analysis of shearing and shuffling in $\{10\bar{1}2\}$ twinning reported by Khater, Serra and Pond [25]. The parent lattice (in solid symbols) and the twin lattice (in hollow symbols) were superimposed. To the right, an array of black arrows represents the homogeneous simple shear distributed on layer 0 to 4. Because a twinning shear is a simple shear, the magnitude of shear each atom undergoes is proportional to the distance from the atom to layer 0, as represented by the black arrows pointing to the shear direction, i.e. the η_1. But obviously, the parent atoms cannot be carried to the twin positions by the simple shear, for example, atom B must shuffle upward (denoted by the blue arrow) after shear, to reach the twin position B′. Similarly, atom A must shuffle downward after shear, to reach the twin position A′. Now we analyze to what plane the parent basal is transformed, and to what plane the parent prismatic is transformed after the shearing and shuffling, by adding auxiliary lines to the analysis by Khater et al. [25]. We mark out the trace of the parent basal with the dashed red line across the solid symbols. It can be readily seen that, these atoms reach the twin positions marked out by the double dashed purple lines across the hollow symbols, which is exactly the trace of the double-layered twin prismatic. Similarly, we mark out the trace of the parent prismatic with the double dotted red lines across the solid symbols. After shearing and shuffling, these atoms reach the twin positions marked out by the dotted purple line which is exactly the trace of the twin basal. Thus, the lattice transformation implied in the analysis by Khater et al. [25] can be described as: $(0002)_P \rightarrow \{10\bar{1}0\}_T$ and $\{10\bar{1}0\}_P \rightarrow \{0002\}_T$, which is exactly the Li-Ma mechanism [21]. If we drew a line marking along the trace of the parent basal, it would be deflected to the position of the twin prismatic; and a line marking along the trace of the parent prismatic would be deflected to the position of the twin basal. Hence, lattice correspondence in deformation twinning is the root cause of line deflection observed in the experiments.

The shearing and shuffling analysis by Khater et al. [25] (Fig. 1) also reveals an important feature: during twinning, atoms must shuffle up or down off the twinning plane, indicating that the $\{10\bar{1}2\}$ twinning plane cannot be invariant. Li and Zhang [15] showed that the lattice transformations (Fig. 1) have to distort the twinning plane and thus no simple shear can occur on it. The breakdown of the invariant plane strain condition is denoted by the dashed zigzag lines across the atoms on layer 0. This is the very reason why TBs of $\{10\bar{1}2\}$ mode can entirely depart from the twinning plane, as observed in experiments and simulations.

The one-to-one lattice correspondence exists in any twinning mode, irrespective of a finite or zero *s*. We can now demonstrate why line deflection should not be used to determine the “twinning shear” for $\{10\bar{1}2\}$ mode. In the prediction of the classical theory, the misorientation angle equals 86.3° for Mg. The twinning shear is determined by the choice of the second invariant plane $K_2 = \{10\bar{1}\bar{2}\}_P$ of the parent which is transformed to the $K_2' = \{10\bar{1}2\}_T$ of the twin. The angle θ between these two planes can be used to calculate the twinning shear $s = 2\tan\frac{\theta}{2}$. However, as shown in Fig. 1, the $\{10\bar{1}2\}$ twinning plane cannot remain invariant during twinning. Thus, actually no

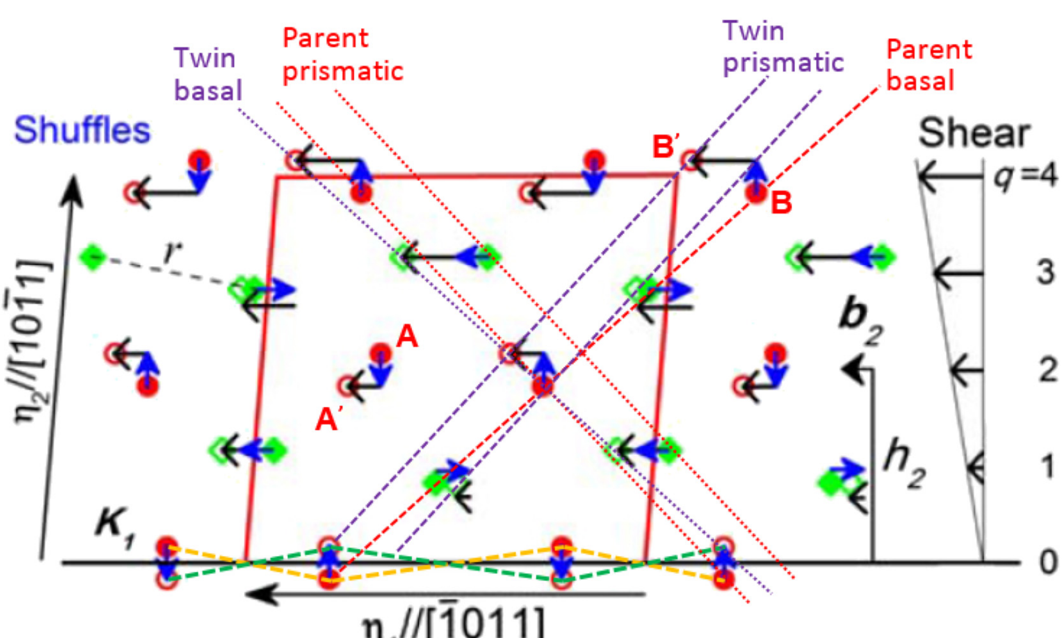

Fig. 1. Lattice correspondence analysis on the report by Khater et al. [25] (with permission of Taylor and Francis: www.tandfonline.com). Note layer 0 of the parent and the twin do not coincide as indicated by the dashed, zigzag green and yellow lines. Some shuffles (the blue arrows) are off the twinning plane. We add the broken lines to the original figure to show that the parent basal (the dashed red line across the solid symbols) is transformed to the twin prismatic (the dashed double purple lines across the open symbols) by the shearing and shuffling, i.e. $(0002)_P \rightarrow \{10\bar{1}0\}_T$; and the parent prismatic (the dotted double red lines across the solid symbols) is transformed to the twin basal (the dotted purple line across the open symbols), i.e. $\{10\bar{1}0\}_P \rightarrow \{0002\}_T$. This transformation is the same as the Li-Ma model [21]. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

homogeneous simple shear can occur on the twinning plane, although a finite value of θ can still be measured in experiments. On the other hand, as shown in our TEM observations [12–15,30] (and shown below), the misorientation angle θ varies over a range of values and the actual TB can be extremely incoherent on the atomic scale. Irrespective of variation in the misorientation angle and TB morphology, the lattice correspondence remains exactly the same. Therefore, microscopically, one could draw a line marking on the surface of a specimen before deformation. After twinning, one could observe and measure the value of deflection angle θ, but the magnitude of "twinning shear" obtained from such line deflection has no physical significance unless a homogeneous simple shear indeed occurs on the twinning plane.

In the following, we present high resolution TEM observations of TBs in an AZ31 Mg alloy which was dynamically compressed at room temperature, to further clarify our point. More experimental details of the testing and TEM characterization can be found in [16]. Fig. 2 shows a HRTEM micrograph of $\{10\bar{1}2\}$ twins with a misorientation angle ~86° which is close to the theoretical value. The $\{10\bar{1}2\}$ twinning plane is denoted by red line. Note the actual TB is highly incoherent and largely departs from the twinning plane. The K_2 plane $\{10\bar{1}\bar{2}\}_P$ in the parent is transformed to the K_2' plane $\{10\bar{1}2\}_T$ in the twin, i.e. $K_2 \rightarrow K_2'$. However, because the actual TB is highly incoherent and entirely deviates from the $\{10\bar{1}2\}$ twinning plane, no simple shear can occur on the twinning plane. Thus, if we drew a line marking along the K_2, it would be deflected to the K_2'. The angle θ between these two planes equals ~7.3° which gives a "twinning shear" of ~12.8%. Obviously, such a value measured from line deflection is not produced by a homogeneous simple shear which should occur on the twinning plane, but by atomic shuffling that transforms the parent to the twin.

Fig. 3 shows $\{10\bar{1}2\}$ twins with the TB being highly incoherent and composed of small facets (<5 nm). The misorientation angle equals ~89°, and a split (~3°) between the twinning planes of the parent and the twin can be seen. Obviously, no twinning shear on the twinning planes can occur. But if we drew a line marking along the $K_2 = \{10\bar{1}\bar{2}\}_P$, then after twinning, it would be deflected to the $K_2' = \{10\bar{1}\bar{2}\}_T$.

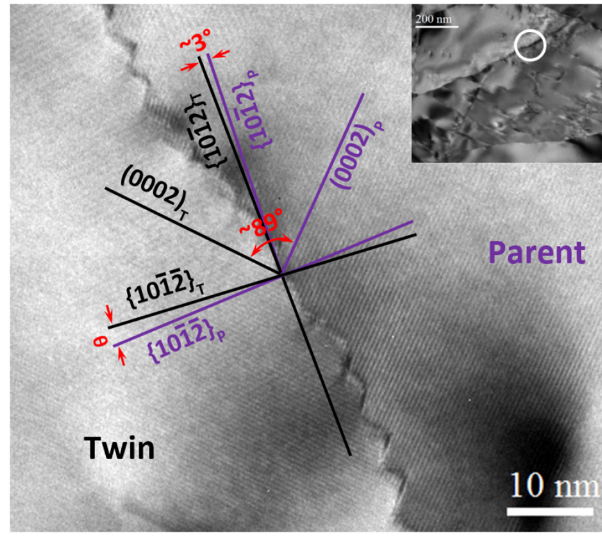

Fig. 3. HRTEM micrograph of $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twins in an AZ31 Mg alloy. The TB at a low magnification is shown in the inset. The HRTEM is the magnified view of the circled region in the inset. Zone axis $\langle 1\bar{2}10\rangle$. The misorientation angle equals ~89°. The TB is composed of small facets (<5 nm). The split in the twinning plane equals ~3°. If we measured the "twinning shear", $\theta \approx 4.7°$, and $s \approx 8.2\%$ would be obtained.

If we measured the angle θ between the K_2 and the K_2', a value of ~4.7° would be obtained. This gives a "twinning shear" ~8.2% which has no physical significance.

For further clarification, we examine a rather commonly observed misorientation angle 90° which deviates from the theoretical value of 86.3°, as shown in Fig. 4. This 90° misorientation angle can be readily identified in numerous atomistic simulations [26–28] and experiments [30]. The actual TB, denoted by the red lines, is extremely incoherent and composed of small facets that are basal-prismatic interfaces. It can be seen that the $\{10\bar{1}2\}$ twinning planes of the parent and the twin do not coincide, as indicated by the split angle (~4°) between the traces

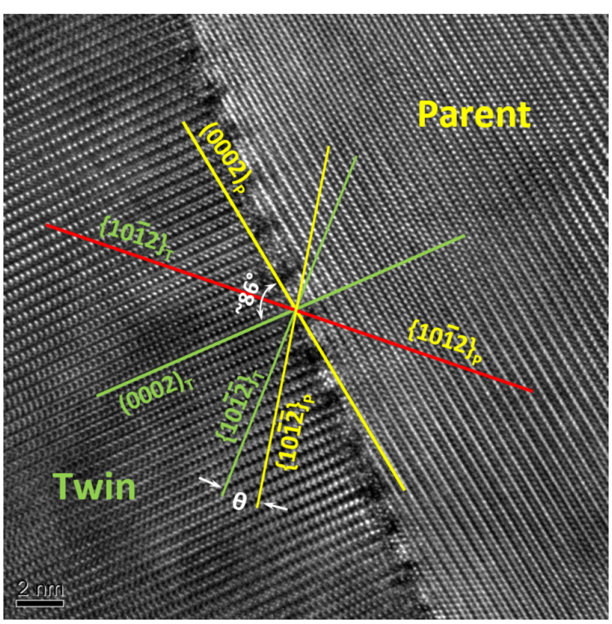

Fig. 2. HRTEM micrograph of $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twins in an AZ31 Mg alloy. Zone axis $\langle 1\bar{2}10\rangle$. The misorientation angle equals ~86°. The TB is highly incoherent and entirely deviates from the twinning plane (the red line). If we measured the "twinning shear", a value of 12.8% would be obtained. Obviously such a value is not a result of a homogeneous simple shear on the twinning plane. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

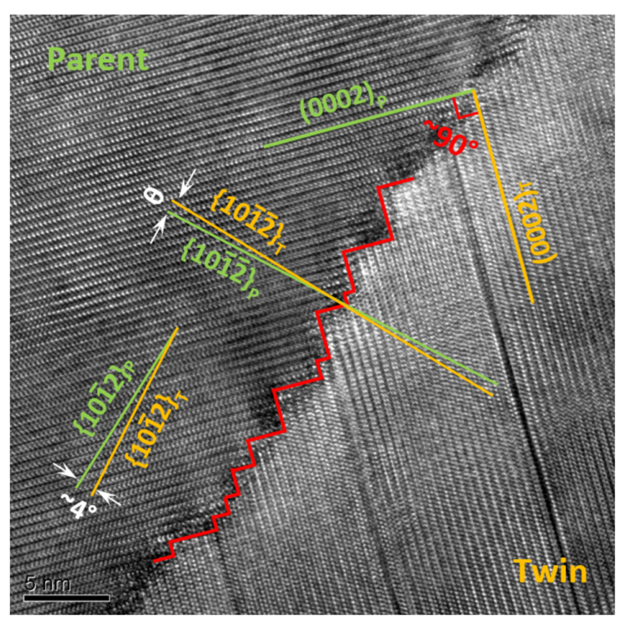

Fig. 4. HRTEM micrograph of $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twins in an AZ31 Mg alloy. Zone axis $\langle 1\bar{2}10\rangle$. The misorientation angle equals ~90°. The TB is composed of small facets. The angle θ between the $K_2 = \{10\bar{1}\bar{2}\}_P$ and the $K_2' = \{10\bar{1}\bar{2}\}_T$ now equals ~2.7°. If we drew a fiduciary line along the K_2 and measured the "twinning shear", a value of 4.7% would be obtained, but the twinning shear should be zero [15].

of the twinning planes. Irrespective of the misorientation angle, the lattice correspondence of this twinning mode remains the same. However, because the misorientation angle equals 90°, the parent basal is parallel to the twin prismatic, and the parent prismatic parallel to the twin basal. Thus, the twinning shear should be zero because any non-zero twinning shear would destroy the two parallelisms [15]. In this particular case, if we drew a line marking along the trace of the parent basal or the parent prismatic, no deflection would occur after twinning. If we drew a line marking along the trace of the K_2, it would be deflected to the K_2' by twinning, and the angle θ between the K_2 and the K_2' now equals ~2.7°. Thus, the measured "twinning shear" would be 4.7%, which has no physical significance as well.

The HRTEM micrographs in Figs. 2–4 clearly demonstrate that, if a line marking is randomly placed on the surface of a specimen before $\{10\bar{1}2\}$ twinning, a deflection will most likely be observed after twinning as a result of the one-to-one lattice transformation, but such deflection does not indicate a finite twinning shear which should be unique-valued and must occur on the first invariant plane.

Among the major twinning modes in hcp metals, $\{10\bar{1}2\}$ mode is the only one that largely deviates from the classical twinning behavior. As a matter of fact, the classical theory correctly predicted the twinning elements of $\{10\bar{1}1\}$ and $\{11\bar{2}1\}$ modes [1], despite that the details of how shear and shuffle transform parent to twin are missing. Thus, although the classical twinning theory did not correctly predict the anomalous properties of $\{10\bar{1}2\}$ mode, by no means this indicates that the classical theory is incorrect and unable to properly describe the twinning modes. On the contrary, as shown in [31], if one properly performs lattice correspondence analysis inside the framework of the classical theory, the twinning mechanisms can be revealed without ambiguity. The incorrect predictions in the classical theory for some twinning modes in hcp metals are actually owing to the intuitive assumptions in regard to shear and shuffle, and the lack of consideration of atomic interaction which is a dominating factor for TB energy, TB morphology and twinning dislocation structure. A thorough and detailed discussion on this important issue will be provided in future work.

To conclude, we demonstrate that line deflection observed in $\{10\bar{1}2\}$ twinning is solely a result of lattice transformation. Because the $\{10\bar{1}2\}$ twinning plane is not invariant, a homogeneous simple shear cannot occur, but line deflection can still be observed microscopically due to the lattice correspondence. Thus, caution should be exercised when line deflection is used to determine the magnitude of twinning shear.

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