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Twinning with zero twinning shear

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ABSTRACT

It is generally believed that the $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning shear in magnesium equals 0.129 and twin growth is mediated by twinning dislocations. Starting from these notions, we analyze, in great detail, the lattice transformation from parent to twin, and prove that the twinning shear cannot be any finite value but zero. Thus, no twinning dislocations should be involved in this twinning mode and the lattice transformation is solely accomplished by atomic shuffling. Atomistic simulations and high resolution transmission electron microscopy observations unambiguously confirm our conclusion.

1. Introduction

Mechanical twinning is an important deformation mode in hexagonal close-packed (hcp) metals [1–4]. Among all the twinning modes that were observed in hcp metals, $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ mode is the most commonly observed and plays a crucial role in the mechanical behavior of hcp metals. Consequently, this twinning mode has received much more attention than others. Historically, this twinning mode has been treated classically, i.e. a finite twinning shear is involved and twinning dislocations are needed in mediating twin boundary (TB) migration. In classical theory [5,6], the K_1 plane, i.e. the first invariant plane or the twinning plane is $\{10\bar{1}2\}$, and the second invariant plane K_2 is $\{10\bar{1}\bar{2}\}$. A homogeneous shear occurs along $\eta_1 = \langle 10\bar{1}\bar{1}\rangle$. It was suggested that the twinning dislocation is a two-layer zonal dislocation [6,7]. Serra et al. [8] proposed a disconnection model to describe the interfacial defects mediating TB migration. These two models differ fundamentally in that in the classical theory, a unique lattice correspondence can be established for each twinning mode by the homogeneous shear; whereas in the disconnection model, lattice correspondence is not considered, and twinning dislocations are defined purely from local geometry of the TB.

For $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ mode, the magnitude of twinning shear s can be computed as $(3-\gamma^2)/(\sqrt{3}\cdot\gamma)$, and the resultant Burgers vector of the elementary twinning dislocation b_T equals $(3-\gamma^2)\cdot a/(2\sqrt{3+\gamma^2})$ [7], where a is the lattice parameter and γ the c/a ratio. For magnesium (Mg), $b_T = 0.024$ nm which is very small, but the corresponding s is not small and equals 0.129. Thus, a significant shear strain (12.9%) should be produced during twinning. However, numerous experimental observations over the past five decades cast doubt on these widely accepted notions. For a typical example, the most recent in-situ transmission electron microscopy (TEM) observations of $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning in single crystal Mg [9] show that during twinning and detwinning, no shear offsets were observed on the specimen surfaces and thus zero shear strain was produced, even though the specimen was oriented such that any shear strain should be most readily observed with the twinning plane being edge-on. Other examples that deviate from classical twinning include: extremely incoherent TBs [10]; no well-defined misorientation angle [11–13]; reversible twinning [14,15]; presence of super-wide, anomalous stack faults (SFs) that may cross a whole twin without the activity of partial dislocations [16–19]; change of habit plane during twin growth and little interaction between migrating TBs and precipitates [20] etc. These abnormal phenomena cannot be accounted for by any twinning dislocation theories. Thus, it is of great importance to analyze and clarify, in great detail, the mechanism of $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning.

2. Analysis of lattice transformation

In classical twinning theory [5,6], a homogeneous shear linearly maps a plane/direction of the parent to another plane/direction of the twin, i.e. the homogeneous shear is an affine shear. Thus, a one-to-one lattice correspondence can be established between the parent and the twin lattice. The linear mapping can be described by a second rank tensor **S** [6]. Any vector **u** of the parent is linearly mapped to a vector **v** of the twin by **S** in reference to the coordinate system of the parent: **v** = **Su**. It should be noted that the homogeneous shear is accomplished under the "invariant plane strain (IPS) condition" which presumes

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that the twinning plane undergoes no structural change after the homogeneous shear occurs on it. Twinning dislocations are required to accomplish the shear deformation and they can only glide in the composition plane so that the lattice correspondence will not be disrupted [21]. For hcp metals, there are four major twinning modes. A complete calculation of the lattice correspondence of these twinning modes was recently conducted by Niewczas [22]. It was shown that, for $\{10\bar{1}2\}\langle10\bar{1}\bar{1}\rangle$ mode, the basal plane of the parent $(0002)_P$ is mapped to the prismatic plane of the twin $\{10\bar{1}0\}_T$, and the prismatic plane of the parent $\{10\bar{1}0\}_P$ is mapped to the basal plane of the twin $(0002)_T$. These planes share the zone axis $\langle1\bar{2}10\rangle$ with the twinning plane $\{10\bar{1}2\}$. However, the crystallography-based calculations [22] provided no details of lattice transformation in terms of the movements of individual atoms, for example, how a single-layered basal plane of the parent is transformed to a double-layered prismatic plane of the twin, which cannot be achieved by a homogeneous shear alone.

Following the classical theory, we start our analysis by examining how lattice transformation is accomplished by shear and shuffle in $\{10\bar{1}2\}\langle10\bar{1}\bar{1}\rangle$ twinning. So far, no detailed lattice correspondence analysis on the atomic scale of this very important twinning mode has been reported, yet such an analysis is the key to understanding the mechanism of any twinning mode in hcp metals. Bilby and Crocker [5], Christian and Mahajan [6] schematically showed some of the shuffles, but their analysis was incomplete and no details were provided. Wang et al. [23] defined a "shear type shuffle", but how a twinning dislocation and the "shear type shuffle" transform the parent to the twin was not analyzed.

Fig. 1 displays the homogeneous shear and the shuffles that are involved for the parent atoms to reach the twin positions. The parent (red atoms of the bottom crystal) and the twin (blue atoms of the top crystal) were obtained in molecular dynamics simulations of magnesium (Mg) after relaxation. The twins satisfy the $86.3°\langle1\bar{2}10\rangle$ twin relationship. The viewing direction, i.e. the zone axis, is along the $\langle1\bar{2}10\rangle$. Only a small portion of the twins is shown. The twin boundary (TB) is denoted by the red, dashed line, and the boundary plane is exactly the $\{10\bar{1}2\}$ twinning plane. To the right, the trace of the K_2 plane $\{10\bar{1}\bar{2}\}$ of the parent is denoted by the green line. After the homogeneous shear, the K_2 plane is sheared to the K_2' plane of the twin, invariantly. The homogeneous shear is denoted by the little red arrow.

Since the shear on the twinning plane is homogeneous, any planes/directions of the parent must undergo the same homogeneous shear as does the K_2 plane. We first examine the transformation of the parent basal plane and analyze the movements of the atoms on this plane. To the left of Fig. 1, the trace of the parent basal plane $(0002)_P$ is denoted by the green line, and three atoms 1, 2, and 3 below the twinning plane are selected. The homogeneous shear for these three atoms is displayed by the three red arrows. After shear, the corresponding positions of these three atoms in the twin are denoted by the three dashed circles filled with yellow, i.e. 1′, 2′, and 3′. However, it is clearly revealed that these positions 1′, 2′, and 3′ do not exactly fall on the twin positions. Hence, shuffles are needed. For position 1′, the atom must shuffle downward off the twinning plane; for position 2′, the atom must shuffle to the left. The magnitude of these shuffles is about twice the magnitude of the elementary twinning dislocation. The shuffles are denoted by the three black arrows. After the shear and shuffles, the basal plane of the parent is transformed to the prismatic plane of the twin: $(0002)_P \rightarrow \{10\bar{1}0\}_T$. The shuffles for the atoms on the parent basal plane are similar to the analysis in [5,6], but with more details showing how the shuffles are required and accomplished.

Because the atoms of the prismatic plane of an hcp lattice actually reside on two separate planes, it is necessary to analyze how the parent prismatic plane is transformed to another plane of the twin by the homogeneous shear. This analysis is represented by the double lines in Fig. 1. The trace of the prismatic plane of the parent $\{10\bar{1}0\}_P$ is now denoted by the two green lines. Three atoms 4, 5 and 6 of the parent experience the same homogeneous shear that is shown by the three red arrows. After the homogeneous shear, the corresponding positions of these three atoms in the twin are denoted by the three dashed circles filled with yellow, i.e. 4′, 5′, and 6′. But these positions are far off the atomic sites of the twin. Hence, large and complex shuffles are needed, as denoted by the black arrows. For position 4′, the magnitude of the shuffle is about four times that of the elementary twinning dislocation, and the direction of the shuffle is off the twinning plane and not in the direction of the shear. For position 5′, this atom must shuffle against

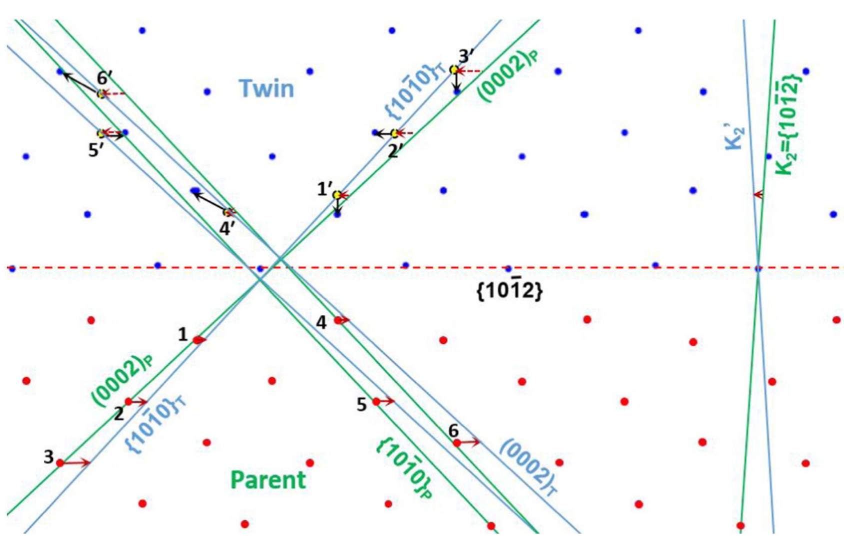

Fig. 1. Analysis of shear and shuffle in $\{10\bar{1}2\}\langle10\bar{1}\bar{1}\rangle$ twinning. The misorientation angle is 86.3°, and the TB (indicated by the dashed red line) is coherent. To the right, the K_2 (in green) undergoes a homogeneous shear (indicated by the little red arrow) to reach the position of the K_2' plane (in blue). To the left, the parent basal $(0002)_P$ plane experiences the same homogeneous shear (indicated by the solid, red arrows). Atom 1, 2, and 3 are sheared to 1′, 2′, and 3′ (indicated by the dashed circles filled with yellow). However, these atoms do not land on the twin positions. They must shuffle to reach the twin positions as indicated by the black arrows. After shear and shuffles, the parent basal plane is transformed to the twin prismatic plane. Transformation of the parent prismatic plane is indicated by Atom 4, 5, and 6 which reside on two slightly separated planes. They are homogeneously sheared to 4′, 5′, and 6′ (indicated by the dashed circles filled with yellow). As indicated by the black arrows, complex and large shuffles must be involved to bring the atoms to the correct positions. After shear and shuffles, the parent prismatic plane is transformed to the twin basal plane. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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