Deviations from Theoretical Orientation Relationship Along Tensile Twin Boundaries in Magnesium

B. Leu, M. Arul Kumar, Y. Liu, and I. J. Beyerlein

Abstract

Deformation twinning is a prevalent mode of plastic deformation in hexagonal close packed (HCP) magnesium. Twin domains are associated with significant lattice reorientation and localized shear. The theoretical misorientation angle for the most common $\{10\bar{1}2\}$ tensile twin in magnesium is 86.3°. Through electron backscatter diffraction characterization of twinning microstructure, we show that the twin boundary misorientation at the twin tips is approximately 85°, and it is close to the theoretical value only along the central part of the twin. The variations in twin/matrix misorientation along the twin boundary control the twin thickening process by affecting the nucleation, glide of twinning partials, and migration of twinning facets. To understand this observation, we employ a 3D crystal plasticity model with explicit twinning. The model successfully captures the experimentally observed misorientation variation, and it reveals that the twin boundary misorientation variations are governed by the local plasticity that accommodates the characteristic twin shear.

Keywords

Deformation twins • Misorientation • Crystal plasticity • Local stresses • Magnesium

Introduction

Due to the scarcity of easy dislocation glide systems, deformation twins play a dominant role in the accommodation of plastic deformation of Mg and its alloys [1]. The formation and growth of twins create new sub-grain boundaries [2, 3], and characteristics of these boundaries control the local stresses and interactions with defects [4–7]. In this way, it significantly affects the mechanical properties of polycrystalline metals [8–11]. Thus, understanding the characteristics of twins and its boundaries is crucial for microstructure design and processing of advanced Mg alloys. In pure Mg, $\{10\bar{1}2\}$ tensile twins are the most common twin to be activated when the c-axis of the crystal is subjected to elongation [2]. All twins are associated with a characteristic lattice misorientation and twinning shear. For $\{10\bar{1}2\}$ tensile twins in Mg, the twin/matrix misorientation angle is 86.3° about $<11\bar{2}0>$ axis [12]. Very often, this theoretical relationship is used to identify twins within a deformed Mg microstructure.

Recently, the deviation in this twin/matrix orientation relationship was characterized by electron microscopy in several studies [13–18]. For example, Li and Zhang [15] showed that the misorientation angle of $\{10\bar{1}2\}$ tensile twin can range from 84° to 97° in Mg alloys rather than the theoretical value of 86.3°. They argued that the local atomic shuffling is the responsible for this deviation. Zhang et al. [16] also observed an approximately 4° deviation in the twinning misorientation relationship, and they ascertain this deviation as a result of local dislocation–twin interactions. Similar observations have been reported for other twin types, like $\{10\bar{1}1\}$ compression twins, and also in other material systems, like Ti and Co [17, 18]. Other proposals for this deviation in the twin/matrix misorientation in the existing literature include strain accommodation, twin–slip interactions, twin–twin interactions, and local atomic shuffling. These phenomena collectively are external factors that may

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contribute to the development of variation in the twinning misorientation relationship. The question still remains on whether the underlying mechanism could instead be intrinsic. The origin of this deviation would be important as there is the potential that it could affect further twinning processes, such as twin boundary migration.

To address these questions, in this work, first we experimentally measure the twinning misorientation along $\{10\bar{1}2\}$ tensile twins in HCP pure Mg. We observe similar deviations in the twin orientation relationship; that is the misorientation at the twin tip is approximately 1.5° lower than that of the middle. To interpret and quantify the effect on twin boundary migration, we employ a crystal plasticity fast Fourier transform (CP-FFT) model with the ability to model subgranular twin lamella explicitly [19, 20]. Using this model framework, we found that the accommodation of intrinsic twinning shear by dislocation plasticity can explain the observed variations in the twin/matrix misorientation. We also find that these deviations are associated with variations in the local stresses. Interestingly, these local stresses favor the formation of P/B facets and thus may help to migrate the twin boundaries, and eventually thicken the twins.

Experimental Characterizations

Commercial purity polycrystalline Mg is used in this study. The material has a strong basal texture resulting from prior rolling. To activate $\{10\bar{1}2\}$ tensile twins, Mg material is subjected to compression at 10^{-3}/s strain-rate along an in-plane direction at room temperature. To activate a sufficient number of twins, sample was compressed to 1% strain. The deformed microstructure was imaged using electron backscatter diffraction (EBSD) technique with a step size of 0.25 μm. An EBSD image of a representative region of the deformed Mg with the activation of several tensile twins is shown in Fig. 1a.

From these twins, we analyze further the twins that have terminated inside the grain, and not at the grain boundary. Those that terminate at grain boundaries could have their morphology affected by the properties of the neighboring grain. Figure 1b–d displays three different twins and the corresponding measured misorientation angle along the twin boundaries. For reference, the theoretical value is shown as a dashed line. For all three twins shown in Fig. 1, the measured misorientation angle in the middle of the twin away from the twin tip is close to the theoretical value. In contrast, at the twin tips, the misorientation angle is approximately 1°–1.5° lower than the theoretical value. Although similar misorientation variations have been reported in the literature, here the spatial variation in the misorientation angle along the twin boundaries is reported for the first time.

Numerical Calculations

To understand and interpret the measured misorientation angle variation shown in Fig. 1, a CP-FFT model is employed here [19, 20]. This model was originally developed to calculate and relate the effective and local responses associated with inter- and intra-granular stress states resulting from the heterogeneity in elastic and plastic properties between grains in polycrystalline materials [21, 22]. Recently, it was extended to model deformation twin lamellae explicitly [20]. The twinning portion of the model is briefly reviewed here. The constitutive behavior of an elasto-visco-plastic material under an infinitesimal strain approximation with twinning shear transformation can be written as

$$\boldsymbol{\sigma}(x) = \boldsymbol{C}(x) : \boldsymbol{\varepsilon}^{\mathrm{el}}(x) = \boldsymbol{C}(x)\left(\boldsymbol{\varepsilon}(x) - \boldsymbol{\varepsilon}^{\mathrm{pl}}(x) - \boldsymbol{\varepsilon}^{\mathrm{tr}}(x)\right) \quad (1)$$

where $\boldsymbol{\sigma}(x)$ is the Cauchy stress, $\boldsymbol{C}(x)$ is the elastic stiffness tensor, and $\boldsymbol{\varepsilon}^{\mathrm{el}}(x)$ is the elastic strain at a material point x. In this work, we consider deformation twinning as the shear transformation process. The elastic strain can be written as the difference between the total strain $\boldsymbol{\varepsilon}(x)$ and the plastic strain $\boldsymbol{\varepsilon}^{\mathrm{pl}}(x)$ due to dislocation slip and the transformation strain $\boldsymbol{\varepsilon}^{\mathrm{tr}}(x)$ associated with twinning. We solve the problem for the local stress field at material point x by using an implicit time discretization of the form:

$$\begin{aligned}\boldsymbol{\sigma}^{t+\Delta t}(x) = \boldsymbol{C}(x) : \big(&\boldsymbol{\varepsilon}^{t+\Delta t}(x) - \boldsymbol{\varepsilon}^{\mathrm{pl},t}(x) - \dot{\boldsymbol{\varepsilon}}^{\mathrm{pl},t+\Delta t}(x, \boldsymbol{\sigma}^{t+\Delta t})\Delta t \\ &- \boldsymbol{\varepsilon}^{\mathrm{tr},t}(x) - \Delta\boldsymbol{\varepsilon}^{\mathrm{tr},t+\Delta t}(x)\end{aligned} \quad (2)$$

where

$$\dot{\varepsilon}^{\mathrm{pl}}(x) = \sum_{s=1}^{N} m^s(x)\dot{\gamma}^s(x) \text{ and } \Delta\boldsymbol{\varepsilon}^{\mathrm{tr}}(x) = \boldsymbol{m}^{\mathrm{tw}}(x)\Delta\gamma^{\mathrm{tw}}(x). \quad (3)$$

The shear rate of slip system s is written as,

$$\dot{\gamma}^s(x) = \dot{\gamma}_0\left(\frac{|\boldsymbol{m}^s(x) : \boldsymbol{\sigma}(x)|}{\tau_c^s}\right)^n \times \operatorname{sgn}(\boldsymbol{m}^s(x) : \boldsymbol{\sigma}(x)) \quad (4)$$

where $\boldsymbol{m}^s = \frac{1}{2}(\boldsymbol{b}^s \otimes \boldsymbol{n}^s + \boldsymbol{n}^s \otimes \boldsymbol{b}^s)$ is the symmetric part of the Schmid tensor, and $\boldsymbol{b}^s$ and $\boldsymbol{n}^s$ are the unit vectors along the slip direction and normal to the glide plane. The resistance τ_c^s is the critical resolved shear stress associated with slip system s, and n is the stress exponent. Note that the $\Delta\varepsilon^{\mathrm{tr}}(x)$ in Eq. 2 is zero outside of the twin domain.

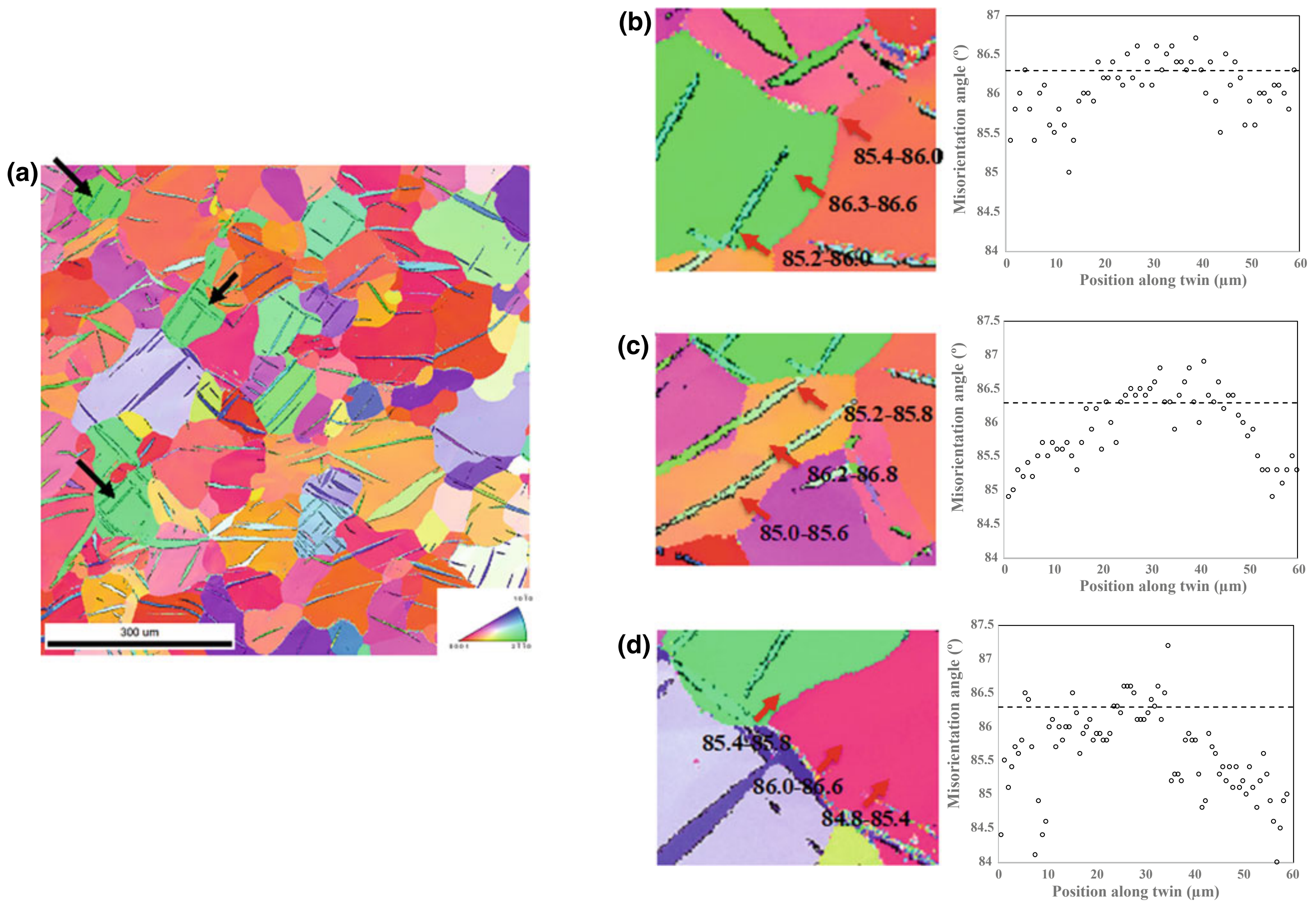

Fig. 1 Experimentally observed variation in the twin misorientation relationship. **a** EBSD image of deformed microstructure shows the activation of $\{10\bar{1}2\}$ tensile twins. **b–d** Three sample twins with the misorientation profile along the twin boundary. The deviation in twin misorientation relationship is significant at twin tips compared to twin middle

The tensor $\boldsymbol{m}^{\mathrm{tw}} = \frac{1}{2}(\boldsymbol{b}^{\mathrm{tw}} \otimes \boldsymbol{n}^{\mathrm{tw}} + \boldsymbol{n}^{\mathrm{tw}} \otimes \boldsymbol{b}^{\mathrm{tw}})$ is the symmetric part of the Schmid tensor associated with the twinning system, where $\boldsymbol{b}^{\mathrm{tw}}$ and $\boldsymbol{n}^{\mathrm{tw}}$ are unit vectors along the twinning direction and the twin plane normal, respectively. The number of increments required to reach the characteristic twinning shear s^{tw} is

$$\Delta\gamma^{\mathrm{tw}}(x) = \frac{s^{\mathrm{tw}}}{N^{\mathrm{twincr}}} \tag{5}$$

The time increment and the number of increments to achieve the twinning transformation N^{twincr} are set sufficiently low and high, respectively, to ensure convergence.

Results and Discussion

In this work, we embed the tensile twin inside a grain to model twins that have terminated inside the grain and away from the neighbor. The simulation unit cell with a tensile twin is shown in Fig. 2a, which is discretized into 3 × 510 × 510 voxels. The c-axis of the central grain is oriented along the Z-direction, which corresponds to the Euler angles of (0°, 0°, 0°) in Bunge convention. A buffer layer, representing a material with random orientation, five voxels thick, surrounds the grain. We first apply compression along the Y-direction, thus providing a sufficiently high resolved shear stress to activate the $(01\bar{1}2)[0\bar{1}11]$ tensile twin. We then introduce this tensile twin in the pre-selected voxels by reorienting the crystal following twinning relationship and by imposing characteristic twinning shear. The volume fraction of the twin domains is taken as 1%. Deformation at all stages of the simulation is accommodated by a combination of anisotropic elasticity and visco-plasticity. The anisotropic elastic constants of Mg at room temperature in GPa are: C_{11} = 58.58; C_{12} = 25.02; C_{13} = 20.79, C_{33} = 61.11, and C_{44} = 16.58 [23]. The plasticity is accommodated by basal <a>, prismatic <a>, and pyramidal <c+a> slip modes, and the corresponding critical resolved shear stress (in MPa) for its activation is 3.3, 35.2, and 86.2, respectively [24].

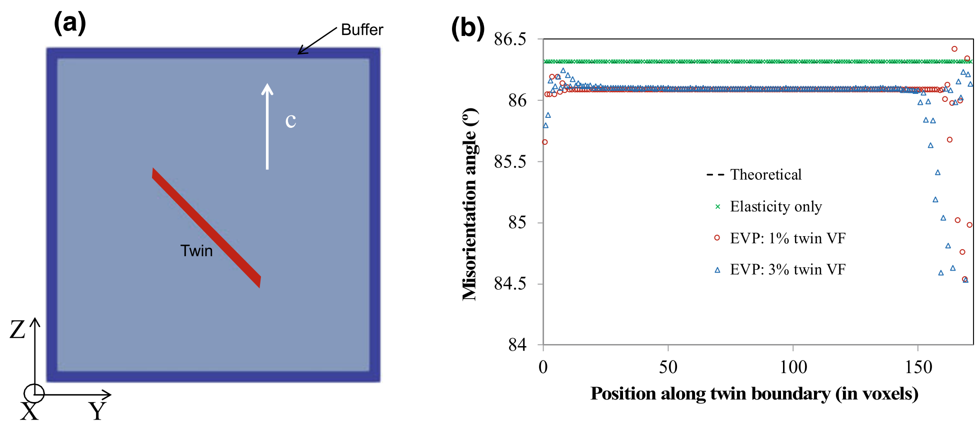

Fig. 2 **a** EVP-FFT model setup for $\{10\bar{1}2\}$ tensile twin simulations. The central grain orientation is $(0^{\circ}, 0^{\circ}, 0^{\circ})$ in Bunge convection, which aligns the grain c-axis with Z-direction. **b** Model predicted twin misorientation angle profile along the twin boundary for only elasticity and for elasto-visco-plastic formulation. Theoretical relationship is shown in dashed line

Origin of Twin Misorientation Variation

Figure 2b shows the variation of the misorientation angle along the tensile twin boundary calculated by the CP-FFT model. For reference, the theoretical misorientation value, which is 86.3°, is also shown in dashed line. To understand the independent effect of elasticity and dislocation plasticity on twin misorientation variation, the results of simulations that assume only elasticity are also plotted in Fig. 2b. The simulation with only elasticity does not alter the twinning misorientation angle from the theoretical one. The calculated result with elasto-visco-plasticity, however, predicts a variation in the twin/matrix misorientation angle. In particular, the misorientation angle is approximately 1.5° lower than the theoretical value at the twin tip, but not in the middle of the twin away from the tip. This variation is due to the accommodation of twinning shear by dislocation plasticity. This model prediction agrees well with the experimental observation as presented in Fig. 1. This analysis clearly demonstrates that the accommodation of twinning shear by plasticity gives rise to the variation in the twinning misorientation angle, and not anisotropic elasticity alone.

Further to understand the effect of twin volume fraction on this twinning misorientation variation, we have repeated the calculation with 3% twin volume fraction. We increase the volume fraction by increasing the twin thickness but without changing grain and twin dimensions. The calculated variation in the twin/matrix misorientation for both 1 and 3% volume fraction cases is shown in Fig. 2b. It suggests that the twin volume fraction does not alter the nature of variation in the twinning misorientation angle.

Effect of Misorientation Variation on Boundary Migration

Twin growth in HCP metals is accomplished by the migration of twin boundaries in the parent crystal. Several mechanisms have been proposed for twin boundary migration [25–31]. The most commonly accepted mechanism is the migration of coherent twin boundary (CTB) by the formation and gliding of twin facets [28, 30–32]. Along CTBs, two types of facets are observed, such as the prismatic–basal (P/B) and basal–prismatic (B/P) [33–35]. In the P/B facet, the prismatic plane of the matrix grain is parallel to the basal plane of twin domain and vice versa for the B/P facet. The nature of stress required to the formation and gliding of these facets depend on the crystallographic configuration. The interplanar separation between basal and prismatic planes in pure Mg is 5.21 Å and 5.55 Å, respectively. Thus, in order to grow the twin by the migration of P/Bs or B/Ps, a normal compressive or tensile stress, respectively, needs to act on their planes.

The stress component normal to P/B and B/P facets along the twin boundary is plotted in Fig. 3a and b, respectively. Here, we show the normal stresses before and after the formation of the tensile twin. In the secondary vertical axis, the calculated twin/matrix misorientation angle is plotted for reference. Before twinning, the stress normal to P/B and B/P facets along the twin boundary is constant at approximately −40 MPa (compressive) and 2 MPa (tensile), which favors the formation of tensile twin. After twinning, the normal stresses are varying along the twin boundary and particularly more heterogenous at the twin tip. The normal stress at the

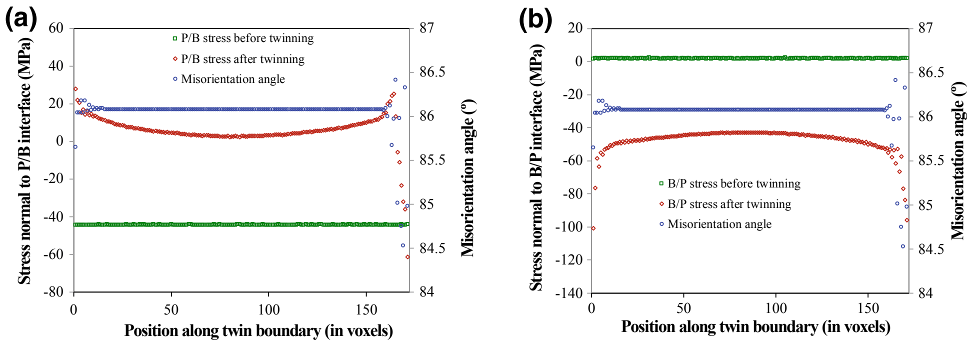

Fig. 3 Variation in the driving stress for the formation of **a** P/B and **b** B/P facets along the twin boundary. The driving stresses are shown before and after twin formation. For comparison, the misorientation profile also shown in the second vertical axis

twin middle for both the P/B and B/P facet changed its nature and does not favor further twinning. The change in stress state (compression to tensile and vice versa) is associated with the stress-reversal due to twinning shear accommodation [19, 20, 36]. This is commonly referred to as the twin backstress. As a result, twin growth is only possible by imposing further favorable loading [19, 20, 37]. However, we see a compressive P/B normal stress at the twin tip, which can favor the formation and migration of P/B facets locally at the twin tip. A similar possibility for the formation and migration of B/P facet is, however, not observed. More interestingly, we see a favorable stress state for the migration of P/B facet in a material point where we have observed the deviation in the twinning misorientation angle. It suggests that the local dislocation plasticity-induced deviation in the twinning misorientation angle may favor the twin growth process by the formation and migration of twin facets.

Summary

In this work, we have experimentally and numerically characterized the deviation in the twinning misorientation angle along $\{10\bar{1}2\}$ tensile twin boundaries in pure Mg. From the EBSD measurements, we found that the twinning misorientation at the twin tip is approximately 1.5° lower than that of the twin middle. Using a full field CP-FFT based twinning model, we show that the accommodation of intrinsic twinning shear by dislocation plasticity, not by the anisotropic elasticity, generates the changes in the twinning misorientation observed in the experiment. Also, we found that the thickness of the twin does not change the nature of the variation in the twinning misorientation. Using the model predicted stresses, we show that local stresses, where we observed the deviation in twinning misorientation, favor the formation of P/B facets, thus, may help to migrate the twin boundaries, and eventually thicken the twin.

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