On basal-prismatic twinning interfaces in magnesium

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Abstract. The existence of basal-prismatic interfaces and their roles in twinning of hexagonal materials have recently attracted appreciable attention of scientific community. In this paper, we utilize molecular statics to investigate the formation of basal-prismatic facets in the \{10\bar{1}2\} twin boundary of magnesium. This interface is shown to be the consequence of a collective motion and interaction of twinning disconnections. By analyzing volume deformations caused by the migration of a single basal-prismatic interface, we show that the passage of this interface distorts the material equivalently to twinning shear.

1. Introduction

Twinning is a mode of plastic deformation that results in reorientation of lattice inside the twinned volume. Macroscopically, twinning can be thought as shear in the invariant (undistorted) plane \(K_1\) in the shearing (twinning) direction \(\eta_1\) [1]. In order to characterize the twinning mode, one often considers also a conjugate invariant plane \(K_2\) and the direction of shear, \(\eta_2\).

Twinning is an important mode of deformation in materials with hexagonal crystal structure due to smaller number of slip systems available in comparison to cubic materials [1,2]. Magnesium is a prospective light-weight material that can store large amounts of hydrogen. It crystallizes in hexagonal close-packed structure and displays significant twinning activity. Using intensive plastic deformation, one can obtain a fine-grained structure and thus improve mechanical properties of magnesium and its alloys [3,4]. These are a few reasons that make the understanding of the mechanism of twinning in magnesium an important research topic [5-10].

Twin boundaries are usually aligned along \(K_1\) planes [1]. Since these planes are invariant relative to the twinning shear, they represent the boundary between the twinned anduntwinned regions along which the two crystal orientations are well-matched. However, non-invariant plane twin boundaries are also observed. For instance, deviations from the twin boundary plane \(K_1\) are commonly observed at the tips of lenticular twins [11-13]. Recently, twin boundaries highly deflected from \(K_1\) were observed in cobalt [14] and magnesium [15]. These boundaries are associated with \{10\bar{1}2\} twins and match with the basal plane in one grain and with the prismatic plane in the other. The formation of these basal-prismatic (BP) interfaces was also observed in recent computer simulations of \{10\bar{1}2\} twin nucleation in magnesium [9,16]. Such interfaces also occur during twin growth [17] and as a result of the twin boundary interaction with bulk dislocations [18].

It was shown in [17] that the motion of the BP interface can be interpreted as a sequential glide of twinning disconnections along the \{10\bar{1}2\} plane. Consequently, it is natural to anticipate that the transformation of the lattice after the passage of the basal-prismatic interface is equivalent to twinning shear. However, this picture is not universally accepted and, instead, some authors report that no shear is observed in this case [15, 19, 20]. The objective of this paper is to provide further insight into this problem by employing molecular statics simulations. We show that the transmission of the BP interface through a small volume of the crystal, driven by the externally applied load, is equivalent to twinning
shear. This supports the view that the twinning in magnesium is a consequence of the glide of twinning disconnections.

2. **Experimental observation of twin boundaries**

In Fig. 1, EBSD map is presented for AZ31 magnesium alloy that shows twin boundaries deflected from the \{10\bar{1}2\} planes. This sample was annealed 1 hour at 350°C and then deformed in compression to 3.5% strain in order to obtain a high concentration of twin boundaries. It is clear from Fig. 1(b) that the boundary I is close to a \{10\bar{1}2\} plane. The directions \( I_T \) and \( I_M \) are deflected from the \{10\bar{1}2\} planes by approx. 7.5° and 9°, respectively.

The boundaries II and III can be considered as slightly distorted BP interfaces. In particular, the \( II_T \) direction is deflected from the trace of the (0001) plane by 4.5° and the \( II_M \) direction is deflected from the \{10\bar{1}0\} plane by 4.9°. The traces \( III_T \) and \( III_M \) are deflected from the traces of the prismatic and basal planes by 15.3° and 16.9°, respectively.

![Fig. 1](image)

Fig. 1. (a) The EBSD map showing various twins in AZ31 magnesium alloy. The grains corresponding to the untwinned crystal (matrix) and to the twin are designated as M and T, respectively. Three distinct orientations of the twin boundaries are observed; these are marked here as I, II and III. (b) Stereographic projection with the traces of \{10\bar{1}2\} planes shown in green, the traces of \{10\bar{1}0\} planes in red and those of the (0001) plane in blue. The orientations of I, II and III boundaries relative to both M and T grains are shown as green, red and blue circles, respectively.

3. **Atomistic studies of basal-prismatic interfaces**

Our studies of the formation of basal-prismatic interfaces were made similarly as in [17]. We used a rectangular simulation block with a \{10\bar{1}2\} boundary in the middle. The block size was 605.9 Å in the [\textsuperscript{10}11] direction, 239.9 Å in the direction normal to \{10\bar{1}2\} plane, and 19.2 Å in the [\textsuperscript{12}10] direction. Several twinning disconnections were inserted into the twin boundary, as shown in Fig. 2(a). These disconnections have the following Burgers vector [21]:

\[
b = \frac{3 - (c/a)^2}{3 + (c/a)^2} [\text{To11}]
\]

and the step height equal to two \{10\bar{1}2\} interplanar separations. The atomic interactions were described by the Liu et al. EAM potential [22]. This potential yields a stable hcp lattice with parameters \( c/a = 1.623 \) and \( a = 3.206 \) Å. From (1), the length of the Burgers vector is thus \( b = 0.494 \) Å. The LAMMPS simulation package [22] was used for molecular statics simulations.
and the OVITO code [23] for visualization. The shear strain was applied to the simulation block with the steps of 0.5% and the total energy of the system was minimized at each level of strain using conjugate gradients.

The disconnections move along the twin boundary when the strain is applied. An obstacle was inserted into boundary to prevent the leading disconnection from leaving the block. This obstacle was created by zeroing the forces on the boundary atoms to the right of the leading obstacle. Figs. 2(a-c) show different stages of the development of the BP interface, which occurs by accumulation of the twin disconnections at the obstacle. The leading disconnection immobilized by the obstacle exerts back-stresses on other disconnections that may pass through it in parallel \{10\bar{1}2\} planes. The resulting stable configuration is represented by a wall of disconnections deflected approx. 45° from the \{10\bar{1}2\} plane. A further increase of the applied strain results in nucleations of new twinning disconnections that increase the length of this boundary. Eventually, this 45° wall becomes unstable and transforms to the BP boundary with local misorientation of 90°. The wall of disconnections can be also considered as a disclination dipole with two disclinations located at the junctions of the \{10\bar{1}2\} plane with the BP facet.
Fig. 2. Formation of a BP interface from twinning disconnections (projection in the [12\bar{1}0] direction). (a) Initial configuration with 6 disconnections along the twin boundary. (b) Simulation block strained to 2.5% of shear. (c) Simulation block strained to 3% of shear showing the BP facet with a wall of twinning disconnections.
4. Discussion
From their recent in-situ compression experiments on a magnesium nanopillar, Liu et al. [20] concluded that the observed twinning produces a tetragonal deformation instead of simple shear. Moreover, the twinned and parent (untwinned) regions were bounded by a series of basal-prismatic and prismatic-basal facets instead of by the \{10\bar{1}2\} boundaries. These observations led them to assert the existence of a new mechanism of plastic deformation, which is different from classical \{10\bar{1}2\} twinning mediated by twinning disconnections. However, our calculations reported in the previous section demonstrate that the formation of BP interfaces takes place by the glide of twinning disconnections. Consequently, the mechanism of the formation of the BP facets agrees with the existing models of twinning.

Fig. 3. Transmission of the BP interface through a volume represented by polygon ABCD. (a) Initial configuration with undeformed selected polygon ABCD; (b) the BP interface meets an edge of the selected polygon; (c) the BP interface migrates through the selected polygon; (d) final configuration with fully transformed polygon ABCD.
Fig. 4. Schematic of relationship between tetragonal deformation and twinning shear. Twinning simple shear on \{10\overline{1}2\} plane is equal to combination of tetragonal deformation and 3.7° rotation. Green and red rectangles are obtained from ABCD by simple shear and tetragonal deformation, respectively.

The tetragonal macroscopic deformation of the sample observed in [20] is pure shear. The difference in deformation caused by the pure and twinning (simple) shears is only 3.7° rotation about the [\overline{1}2\overline{1}0] axis. In the following, we show that the migration of the BP interface produces simple shear.

A few characteristic snapshots of the migration of the BP interface are shown in Fig. 3. These are obtained by the same process as that used to obtain Fig. 2 but now the applied strain is increased beyond the value corresponding to Fig. 2(c). The BP boundary does not migrate as a whole, but step-like defects move along it and shift the boundary forward. The polygon ABCD shown in Fig. 3 lies originally inside the matrix but it is converted to the twin by the passage of the BP facet. The analysis of the changes of the vectors AB and BC and the angles of the ABCD polygon shown in Fig. 3(a) and (d) give the following results:

\[
\begin{align*}
\frac{|AB_T| - |AB_M|}{|AB_M|} &= 0.067, \\
\frac{|BC_T| - |BC_M|}{|BC_M|} &= -0.062 \\
\angle (AB_T, AB_M) &= 3.3°, \\
\angle (BC_T, BC_M) &= 3.7°
\end{align*}
\]  

(2)

The twinning shear parallel to the invariant plane \{10\overline{1}2\} can be accomplished by two successive processes [25]: (i) a combination of ~6.7% extension in the [0001] direction and ~6.3% contraction in the [1\overline{0}1\overline{0}] direction and (ii) ~3.7° rotation about the [\overline{1}2\overline{1}0] axis (Fig. 4). The deformation and angular misorientations identified in (2) are close to the values obtained from the procedures (i) and (ii), which implies that the dominant mechanism is the \{10\overline{1}2\} twinning simple shear rather than the tetragonal deformation. The small differences of these values can be due to strong elastic fields of disclinations that are probably located at the junctions of two BP facets. Consequently, the migration of BP interfaces cannot explain tetragonal deformation of the sample, as suggested in [20]. The observations of tetragonal deformations of the nanopilar [20] may well be due to surface effects or due to simultaneous activation of two \{10\overline{1}2\} twin variants sharing the [1\overline{2}1\overline{0}] axis. Simple shear deformations produced by these two twin variants can be described by the same process of contraction and extension as in (i) and counter ±3.7° rotations about the [1\overline{2}1\overline{0}] axis. The tetragonal deformation may then be a consequence of averaging the deformation produced by these two variants.

5. Conclusions

Basal-prismatic interface can be formed by the glide of twinning disconnections. The mechanism of its formation agrees with the existing models of twinning. The migration of a BP interface produces a simple shear deformation that transforms the matrix to the twin. These observations suggest that the migration of the BP interfaces observed in the experiments on magnesium nanopillars [20] cannot explain tetragonal deformation of the sample whose existence is asserted therein.

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