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On the importance of prismatic/basal interfaces in the growth of $(\bar{1}012)$ twins in hexagonal close packed crystals

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The growth process of $(\bar{1}012)$ twins is studied in magnesium using atomistic simulations. It is shown that a specific interface, which places prismatic and basal planes face-to-face, plays an important role. This interface has a low energy, forming a cusp in the orientation-dependent interface energy of a twinned bicrystal. This interface appears in several published twin structures and, for instance, accommodates the large deviations of twin interfaces from $(\bar{1}012)$ planes reported recently (Zhang et al., Scr. Mater. 67 (2012) 862).

Keywords: Twinning; Hcp; Molecular dynamics; Plasticity

Twinning, a mechanism of plastic deformation by which a crystal sub-domain is reoriented by mirror symmetry, is of prime importance in low-symmetry materials, particularly hexagonal-close-packed (hcp) metals [1]. The mechanism of twinning is seen as the sequence of three phenomena: (1) nucleation, (2) transverse propagation and (3) thickening (i.e. growth perpendicular to the twin interface). As discussed in the seminal work of Partridge [2], twinning in hcp metals induces a shuffling of atoms, implying a more complex structure of the twinning dislocations, as for instance in face-centered cubic (fcc) crystals. A consequence is that hcp twinning dislocations extend over several atomic layers [3], and are referred to as disconnections [4]. Twinning dislocations form steps on the twinning plane, thus increasing or decreasing the twin thickness as they glide along the twin interface, much like kinks on high-Peierls stress dislocations [5].

Since the early 1950s [6], twinning has been the subject of several important studies aiming at understanding its activation and influence on other aspects of plasticity (for instance latent effects and transmutation). Focusing here on the onset of nucleation and propagation, early models have proposed different scenarios for the heterogeneous nucleation of twin domains, including the pole mechanism of Thompson and Millard [7] and the more general slip dislocation dissociation mechanism of Mendelson [3]. In recent years, atomistic simulations revealed several potential dislocation-based structures of twin nuclei. Most works considered the $(\bar{1}012)$ twin that is commonly activated in hcp metals. In Ref. [8], a twin nucleus was proposed, composed of a dipole of partial dislocations, which spontaneously forms a twin embryo in between the two partials. However, the growth process of this embryo was not studied in details.

With regards to twin growth (i.e. transverse propagation and thickening), the thickening mechanism, i.e. the motion of the twin perpendicular to the twinning plane, has attracted a lot of attention. It has been shown [9,10] that thickening is mediated by the glide of twinning dislocations along the twin planes. An alternative mechanism based exclusively on shuffling has been proposed [11] but it has led to some debate [12,13]. Interestingly, the process of transverse propagation of the twin, i.e. its extension in the twinning direction, has received far less attention and is the subject of the present study.

Twin growth is studied using molecular dynamics (MD) based on a semi-empirical potential. Magnesium

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is used as a paradigm hcp metal and interatomic interactions are modeled with the embedded atom method potential developed by Liu et al. [14]. Since the structure of the twin nucleus is still unknown, two hypothetical twin nuclei were considered. A volume containing a twinned subdomain was created by (1) mimicking the analytical method of Eshelby's inclusion problem [15] and (2) introducing a dipole of partial dislocations in an otherwise perfect crystal as proposed by Wang et al. [8].

It is found that in both cases, a specific interface, which places a prismatic and a basal plane face-to-face, plays an important role in the growth of the initial twin nucleus. In the following, this interface will be referred to as a prismatic/basal (PB) interface. As discussed below, PB interfaces appear in several atomic-scale structures published in the literature, both experimental and numerical, although, to the best of the authors' knowledge, the specific structure, stability and potential role of this interface in twin growth has not been discussed so far.

The orientation of the simulation cell is shown in Figure 1. Horizontal planes are $(\bar{1}012)$ twinning planes with the x-axis along the $[10\bar{1}1]$ twinning direction. The z-axis is parallel to the $[1\bar{2}10]$ direction. The $[1\bar{2}10]$ direction is contained in a second twinning plane, the $(10\bar{1}2)$ plane, which is almost perpendicular to the horizontal $(\bar{1}012)$ plane (the angle between the two $\{\bar{1}102\}$ planes is $2\tan^{-1}(\sqrt{3}a/c) = 93.7°$, with $c/a = 1.623$ for Mg). The $[1\bar{2}10]$ axis also belongs to the basal plane and to a prismatic plane, both shown in Figure 1. Periodic boundary conditions are used in all directions in a cell of dimensions $76.1 \times 38 \times 0.32\ \text{nm}^3$ containing 40,000 atoms.

In the first case, a twinned region is created by a procedure inspired from Eshelby's method for solving the inclusion problem in an elastic medium [15]. A region bounded by $(\bar{1}012)$ prismatic and basal planes as illustrated in Figure 1 is initially cut out. A mirror symmetry

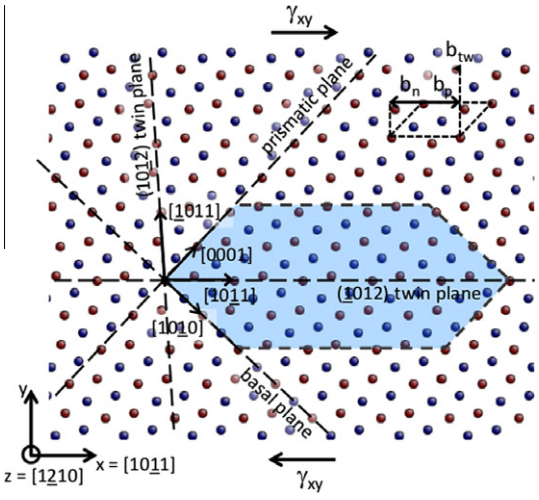

Figure 1. Crystallography of the simulation cell. Horizontal planes are $(\bar{1}012)$ twinning planes with the x-axis along the $[10\bar{1}1]$ twinning direction. The z-axis perpendicular to the plane of the figure is the $[1\bar{2}10]$ direction, at the intersection between two twinning planes, the basal plane and a prismatic plane. Also noted in the top right corner of the figure are the partial Burgers vectors $\boldsymbol{b_n}$ and $\boldsymbol{b_p}$ forming a stable stacking fault in the horizontal $(\bar{1}012)$ plane and the twinning partial Burgers vector $\boldsymbol{b_{tw}}$.

with respect to the $(\bar{1}012)$ twin plane is then applied to the atoms inside the cut-out region. The shape of the region after the symmetry operation is slightly different from the initial shape. In order to restore the initial shape, a shear is applied parallel to the $(\bar{1}012)$ planes in the $[10\bar{1}1]$ direction. Energy minimization is then used to relax the configuration. If no strain is applied to the simulation cell, the twinned region is unstable, shrinks and disappears during the energy minimization. However, if the initial nucleus is sufficiently large and a shear strain γ_{xy} is applied in the $[10\bar{1}1]$ direction parallel to the $(\bar{1}012)$ planes, the nucleus may be stabilized. Note that this strain and the corresponding stress depend on the size of the nucleus, as expected from nucleation theory.

Upon further increasing the applied shear strain, the nucleus becomes unstable and grows in the simulation cell. Several snapshots of the growth process are shown in Figure 2. The initial nucleus, shown in Figure 2a, was stabilized by application of 5.5% simple shear (the shear stress in the cell is then ~1200 MPa). The top and bottom planes of the nucleus are $(\bar{1}012)$ twin planes, while laterally the nucleus is bordered by interfaces at ~45° from the horizontal twin planes. Inspection of the atomic structure (see inset of Fig. 2a) shows that both interfaces place a prismatic and a basal plane face-to-face, one in the matrix and the other in the nucleus. They are therefore PB interfaces as introduced above. It should be noted that the appearance of these interfaces does not depend on the initial shape of the cut-out region. For instance, a nucleus initially bordered by only primary and conjugate $\{\bar{1}102\}$ planes will also form PB interfaces upon relaxation.

To simulate the growth process, the nucleus was destabilized by applying an additional 0.5% shear strain. The growth process, shown in Figure 2b–e, was simulated using MD at 50 K, keeping the applied strain constant. This low temperature was chosen in order to focus on the growth process and avoid perturbations by other thermally activated processes, such as nucleation of dislocations from the twin nuclei. Note that the same growth process was observed in 0 K simulations.

The twin grows in a conservative manner, both vertically (thickening in the $\pm y$-directions) and laterally (transverse propagation in the $\pm x$-directions). Transverse propagation of the twin is faster than thickening, resulting in an overall extension of the twin in the $[10\bar{1}1]$ direction. The nucleus initially grows in a direction at an angle with respect to the horizontal direction. There are therefore geometric steps on the $(\bar{1}012)$ interfaces to accommodate this slight deviation. In the lateral directions, the twin front is made of three interfaces: the conjugate $(10\bar{1}2)$ twinning plane and two PB interfaces, as indicated in Figure 2b. Since the rotation associated with the twin is close to 90°, but not exactly, the basal and prismatic planes across the PB interfaces should not be perfectly parallel. The two loci of intersection between the three planes bounding the twin front (i.e. PB interface/conjugate $(10\bar{1}2)$ twin boundary and conjugate $(10\bar{1}2)$ twin boundary/PB interface) are therefore expected to be characterized by incompatible elastic distortions due to the rapid transition in misorientation. These are likely to have a discrete representation equiv-

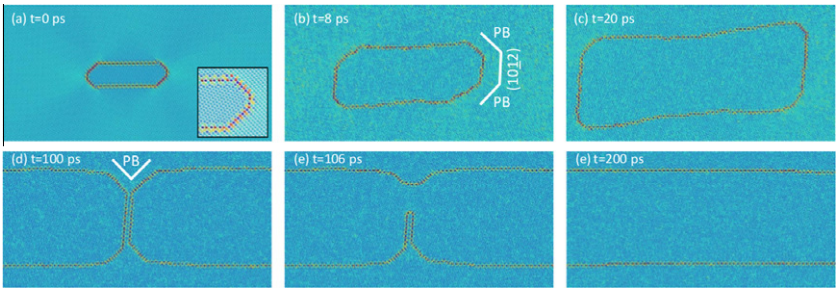

Figure 2. Growth process of a twin from a defect-free twin nucleus simulated by MD at 50 K. Colors scale with atomic energies, from blue at low energy to red at high energy (see text for details). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

alent to a disclination dipole. Such will be the subject to future studies.

Lateral motion of the twin front occurs via the nucleation and glide of steps, i.e. disconnections, along the PB interfaces. Step instances are visible in Figure 2b and c. Their height is $2c$, i.e. they comprise two basal planes. PB interfaces can be interpreted as slanted walls of twinning dislocations [8,16], aligned along either a basal or a prismatic plane. In this context, we see that PB interfaces do not move by the simultaneous motion of all the twinning dislocations it contains, but rather by the motion of some dislocations in the interface forming a step, which then runs along the interface. Thickening of the twin also occurs by the nucleation and propagation of steps along the upper and lower $(\bar{1}012)$ interfaces. Examples are visible in Figure 2b and c.

Figure 2d and e shows the end of the growth process when both ends of the nucleus meet through the periodic boundary conditions. PB interfaces are again involved since the two twinned regions meet along the conjugate $(10\bar{1}2)$ twinning plane but are bordered by PB interfaces. After coalescence and retraction of the PB interfaces, a single twinned layer parallel to the $(\bar{1}012)$ plane is obtained. This layered structure is similar to that considered in the works of Serra and co-workers [9,10] on the motion of twinning planes perpendicular to their interfaces, i.e. their thickening. It is also similar to the structure observed experimentally in Ref. [17].

The second method used to generate a potential twin nucleus consists in introducing a dipole of particular partial dislocations within the system and letting the system relax via energy minimization. The Burgers vector of the partials is $\pm\boldsymbol{b}_n$ with the $\boldsymbol{b}_n$ vector shown in Figure 1. When the initial dipole width is larger than ~5 nm, the relaxed dipole structure consists of small twinned regions near the partial dislocation cores connected by a stacking fault in the horizontal $(\bar{1}012)$ plane, as shown in the inset of Figure 3a. When a shear strain on the order of a few per cent is applied, the twinned regions coalesce, remove the stacking fault and generate the structure presented in Figure 3a. This nucleus has a similar shape previously, being bordered by $(\bar{1}012)$ planes and PB interfaces. The difference is that there are dislocation cores at both extremities of the nucleus. This nucleus is stable if the applied strain is reduced back to zero and becomes unstable if the applied strain is instead increased. The growth process is shown in Figure 3b–d using MD at 50 K. Motion of PB interfaces is again involved, in particular near the

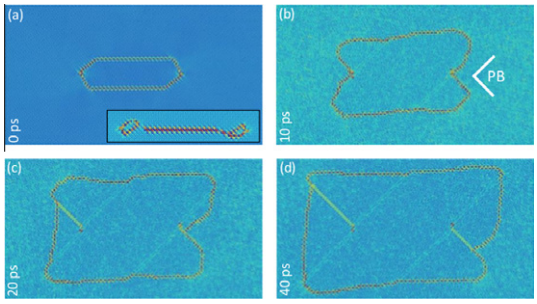

Figure 3. Growth process of a twin from a dipole of partial dislocations, as proposed in Ref. [8]. The color code is the same as in Figure 2. The dipole initial width is 20 nm. The dipole was initially relaxed under an applied shear strain of 5.4% and then subjected to an increment of 0.2%. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

partial dislocation cores. We note that in all our simulations, the partial dislocations remained sessile. The twin front had to bypass them and left behind stacking faults in prismatic planes of the twinned region, visible in Figure 3c and d. The latter could be an artifact of Liu's potential, which predicts a stable stacking fault in prismatic planes in contrast with first-principles calculations [18].

When the initial nucleus, whether the homogeneously twinned region (i.e. method 1) or the partial dislocation dipole (i.e. method 2), is too narrow, i.e. not extended enough in the x-direction, the nucleus grows mostly vertically and not in the x-direction, resulting in twinned regions parallel to the conjugate $(10\bar{1}2)$ planes, which are almost perpendicular to the direction of the applied shear, a very counterintuitive result. It is therefore very important to consider wide enough initial nuclei.

If the misorientation across the PB interface is exactly 90°, a prismatic and a basal plane are perfectly parallel to the interface. The corresponding geometry is represented in Figure 4a. The elementary prismatic and basal unit cells placed against each other are rectangular, with no lattice mismatch along their common $[1\bar{2}10]$ direction and a mismatch of $2(\sqrt{3}a - c)/(\sqrt{3}a + c) \approx 6.5\%$ in the orthogonal direction. Misfit dislocations are required to accommodate this mismatch. Since coherency is almost restored when 14 basal unit cells are placed against 15 prismatic unit cells ($14\sqrt{3}a/15c = 0.996$), we expect one misfit dislocation along the $[1\bar{2}10]$ direction every 14 basal unit cells. The Burgers vector of this dislocation will

be contained in the interface, corresponding to a c vector of the prismatic unit cell, in contrast with the twinning dislocations in which the Burgers vector intersects the interface at an angle close to 45°. We used a bicrystal with 14 prismatic unit cells on top of 15 basal unit cells with periodic boundary conditions to compute the interface energy. The resulting atomic structure is shown in Figure 4b. The surface energy is ~170 mJ m^{-2}, above but close to the twin energy along a $\{\bar{1}102\}$ plane, ~120 mJ m^{-2}. In addition, we computed the surface energy of a twinned bicrystal as a function of the angle θ between its interface and the $[10\bar{1}1]$ direction, as noted in the inset of Figure 4c. The energy curve is shown in Figure 4c for θ between 0° and 93.7°, i.e. between the two conjugate $\{\bar{1}102\}$ planes. Three cusps are visible. The ones at $\theta = 0°$ and $\theta = 93.7°$ correspond to the primary and conjugate twinning planes, which are equivalent with the present setting. The cusp at $\theta = \tan^{-1}(\sqrt{3}a/c) = 46.9°$ corresponds to the PB interface, confirming the relative stability of this interface. Actually, the PB interface is so stable that in the vicinity of the PB orientation, the interface decomposes into segments of PB interfaces connected by steps, as illustrated in the inset of Figure 4c. The stability of the PB interface can also be judged by comparison with the symmetric tilt grain boundary energies [19] that are on the order of 250 mJ m^{-2}, with cusps for singular orientations down to between 100 and 150 mJ m^{-2}, i.e. only slightly below the PB interface energy.

Interestingly, PB interfaces appear in several atomic-scale structures published in the literature, but had never been mentioned or studied before. For instance, the simulated twin boundaries near $\boldsymbol{b_n}$ dipoles in Figures 3 and 4 of Ref. [8] and Figures 8 and 9 of Ref. [16] are composed of PB interfaces. Also, a PB interface is visible in the twinned region reported in Ref. [19], which nucleated at a symmetric tilt grain boundary after absorption of a four-dislocation pile-up. PB interfaces are also visible in the atomic-scale simulations of tractions along the c-axis performed by Qi et al. [20], which involve an interplay between twinning and dislocation plasticity. More importantly, Zhang et al. [21] reported very recently twin boundaries with large deviations from $\{\bar{1}102\}$ twinning planes and the inset of Figure 2b of this work shows that the deviation is accommodated by a succession of PB interfaces in both of their equivalent perpendicular orientations. Such decomposition (faceting) is expected from the low energy of PB interfaces compared to other twin plane orientations.

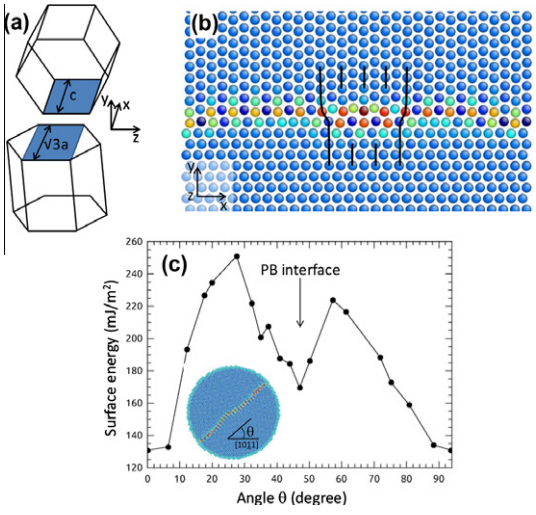

Figure 4. Structure and energy of a prismatic/basal (PB) interface: (a) basal and prismatic unit cells placed face-to-face across the PB interface, (b) relaxed structure of the interface with the core of a misfit dislocation highlighted (same color code as in Figs. 2 and 3), (c) energy of a twin interface as a function of its angle θ with respect to the horizontal $[10\bar{1}1]$ direction. An example of atomic configuration is shown in the inset. A cylindrical geometry was used with free boundary conditions on the outside. Energies were computed in an inner cylinder to avoid surface effects. Atoms not accounted for form a ring of light blue atoms visible on the outside of the cylinder. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

In conclusion, we have seen that a particular interface, often seen but never reported, plays an important role in the growth of a twin. The twins considered here are hypothetical but the real nature of the twin nucleus is still unknown. We may expect that heterogeneous nucleation from grain boundaries is more likely [19], but this process has not been clearly explained nor simulated so far and in all cases, we can conclude from the present work that the front of a growing twin, independently of the initial nucleus, will be made of PB interfaces and $\{\bar{1}102\}$ twin planes because they are of much lower energy than all other twin interfaces. Their combined mobility will therefore control the overall kinetics of twin propagation.

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