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Twinning and De-twinning via Glide and Climb of Twinning Dislocations along Serrated Coherent Twin Boundaries in Hexagonal-close-packed Metals

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The $\{\bar{1}012\}$ twin boundaries experimentally observed in hexagonal-close-packed metals are often serrated rather than fully coherent. These serrated coherent twin boundaries (SCTBs) consist of sequential $\{\bar{1}012\}$ coherent twin boundaries and parallel basal–prismatic planes serrations (BPPS). We demonstrated that the formation of BPPS is geometrically and energetically preferred in the SCTBs, and an SCTB thus migrates by glide and climb of twinning dislocations, combined with atomic shuffling. Particularly, the climb mechanism, combined with the density and the height of BPPSs in the SCTBs, could be crucial in controlling twinning and de-twinning, and twinning-associated hardening.

Keywords: Twin boundary, Disconnection, Climb, Shuffle, Hexagonal-close-packed metals

Twinning and de-twinning, which are the dominant deformation mechanisms in hexagonal-close-packed (hcp) metals, exhibit more complex nucleation and propagation mechanisms than those associated with dislocation slip [1–3]. Specifically, twinning and de-twinning are directional, involve atomistic shuffling, and they induce a strong crystallographic reorientation. Twin nucleation, a necessary first stage of twinning, seems to invariably take place at grain boundaries in hcp materials, and to involve complex dislocation reactions. There are eight predicted and observed twinning modes $\{\bar{1}01n\}$ and $\{\bar{2}01n\}$ ($n = 1, 2, 3, 4$) in hcp metals [1–3]. Of those, the $\{\bar{1}012\}$ twinning mode is one of the most commonly activated in hcp metals. Correspondingly, the nucleation, propagation, growth of deformation twins, and their role in plastic deformation have attracted many experimental and modeling at multiple length scales [1–21].

Most atomic scale modeling, including topological models, density functional theory (DFT) and molecular dynamics (MD) simulations [8–19], has focused on coherent twin boundaries (CTBs) [11–17] and symmetrical tilt grain boundaries (STGBs) [18,19]. The latter work on STGBs found that STGBs near the $\{\bar{1}012\}$ twin orientation could be represented as a $\{\bar{1}012\}$ CTB plus

an array of grain boundary dislocations (GBDs) [18]. However, even GBs with misorientation near an ideal twin misorientation may not be symmetric due to the GB-mediated plastic deformation and slip activity [15–20]. Accompanying the growth of a twin, slips are often activated. Lattice dislocations can glide toward CTBs and are impeded at CTBs, and can dissociate on CTBs or transmit across CTBs into the adjacent grain [10–16]. Also, lattice dislocations may nucleate at CTBs and glide away from them [17,20]. Accompanying these plastic deformation processes, the misorientation relation deviates from the ideal twin misorientation due to the residual dislocations left at CTBs [21], and the CTBs adopt a serrated configuration formed by CTB segments joined by dislocations or disconnections. Under mechanical loadings and/or thermal loadings, these residual defects within CTBs can accumulate to form pure steps or steps with disconnection characters to reduce the excess energy of a dislocated CTB, especially when the facets associated with the steps are low energy and thermodynamically stable [22–26]. As experimentally observed in Co, Mg, and Ti [22–24], steps are formed in the $\{\bar{1}012\}$ CTB, which are geometrically associated with a facet where the basal plane of one grain is nearly parallel to the prismatic plane

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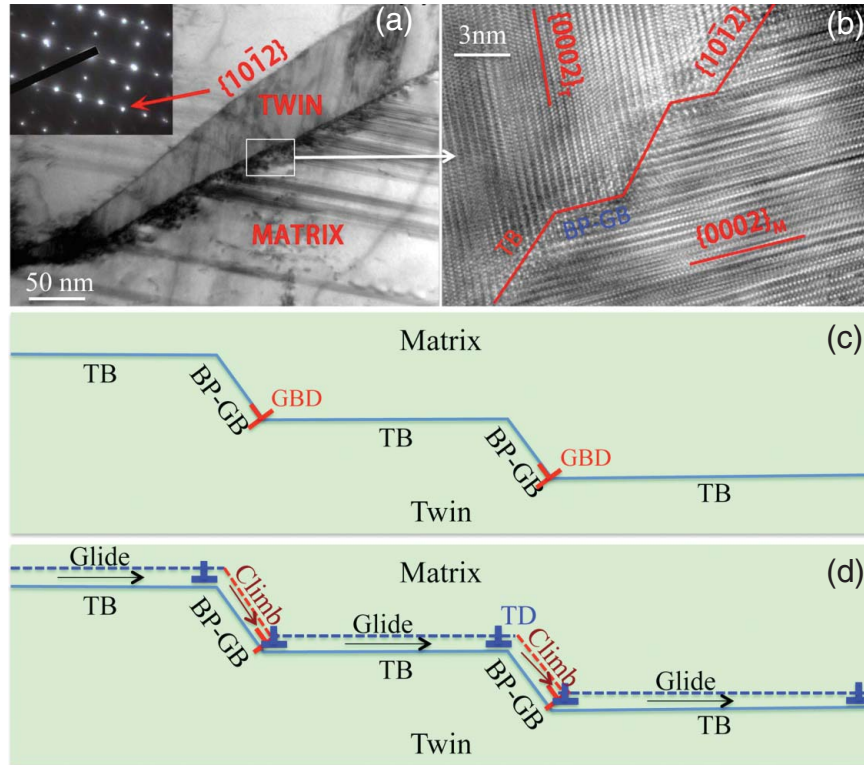


Figure 1. (a) and (b) Transmission electronic microscopic images showing the serrated twin boundary in Co. Two types of boundaries, TBs and BPPSs, are marked. Selected area electron diffraction (SAED) pattern inserted in (a) confirms the twin orientation relationship between the twin strip and the matrix. The beak direction is along $\langle 11\bar{2}0 \rangle$. (c) A schematically SCTB containing geometrically necessary dislocations and (d) the migration mechanism of a serrated TB via glide and climb of TDs.

of the other grain (Figure 1). In the following description, the facet is referred to as basal–prismatic planes serrations (BPPS) (B for basal plane and P for prismatic plane), and the serrated CTB is referred to as SCTB.

The formation of BPPSs is geometrically and energetically preferred. Corresponding to crystallographic characteristics of the $\{10\bar{1}2\}$ twin orientation, the twinned crystal is rotated nearly 90° (86.3° in Mg) with respect to the matrix, as a result, the basal plane in the matrix is nearly parallel to the prism plane in the twinned domain, and this parallelism geometrically favors the formation of a short segment of BPPS. In addition, atomistic simulations done for Mg show that the BPPS has a low formation energy of 170 mJ/m^2 , comparable to the CTB formation energy (122 mJ/m^2) and much lower than the formation energy of other STGBs ($>250 \text{ mJ/m}^2$) [18]. BPPSs are thus energetically preferred and result in an SCTB, rather than a symmetric tilt boundary. As observed in experiments, the boundary near the twin orientation is composed of two types of boundaries: $\{10\bar{1}2\}$ CTB and BPPS segment. In addition, geometrically necessary grain boundary dislocations or disconnections (GBDs) will be present in the serrated CTB (Figure 1(c)). If the bicrystal is in an ideal twin misorientation, the net Burgers vector of the GBDs required to accommodate the tilt is $|\mathbf{b}_{\text{GBD}}| = 2L \tan(\varphi/2)$ for a BPPS of the length L ($\varphi = 3.7^\circ$ for Mg). The condition for having a visible

GBD is that the Burgers vector equals the atomic plane separation $c/2$, and for Mg it means that a serration is present when the length of the BPPS is greater than 4 nm. For the shorter steps, the SCTB can migrate through a collective glide of twinning dislocations or disconnections (TDs) because GBDs are not necessary. If the misorientation relation of the bicrystal deviates from the ideal twin misorientation relation, GBDs must be present at the steps to accommodate the misorientation, impeding the glide of TDs. The number and the Burgers vector of GBDs are a function of the misorientation and the step height [21].

These steps presented in SCTBs play a crucial role in determining the mechanics of twin growth and twin shrinkage because TDs gliding on the CTB cannot continue gliding in the perfect crystal once they meet the step [8]. Atomistic simulations showed that the glide of TDs on the CTB corresponds to twinning and de-twinning. The TD has been characterized to have the step (two-layer thick) and the Burgers vector ($\mathbf{b}_{\text{TD}} = \lambda[10\bar{1}1]$, $\lambda = (3 - \kappa^2)/(3 + \kappa^2)$ and $\kappa = c/a$) [8,9]. Accompanying the glide of a TD, atomic shuffles must take place in the intermediate plane [8–15]. However, concerning the steps, it is not known what stress is required to propagate twin dislocations across non-contiguous crystal planes, or what are the energy barriers associated with the atomic shuffling taking place in the intermediate planes.

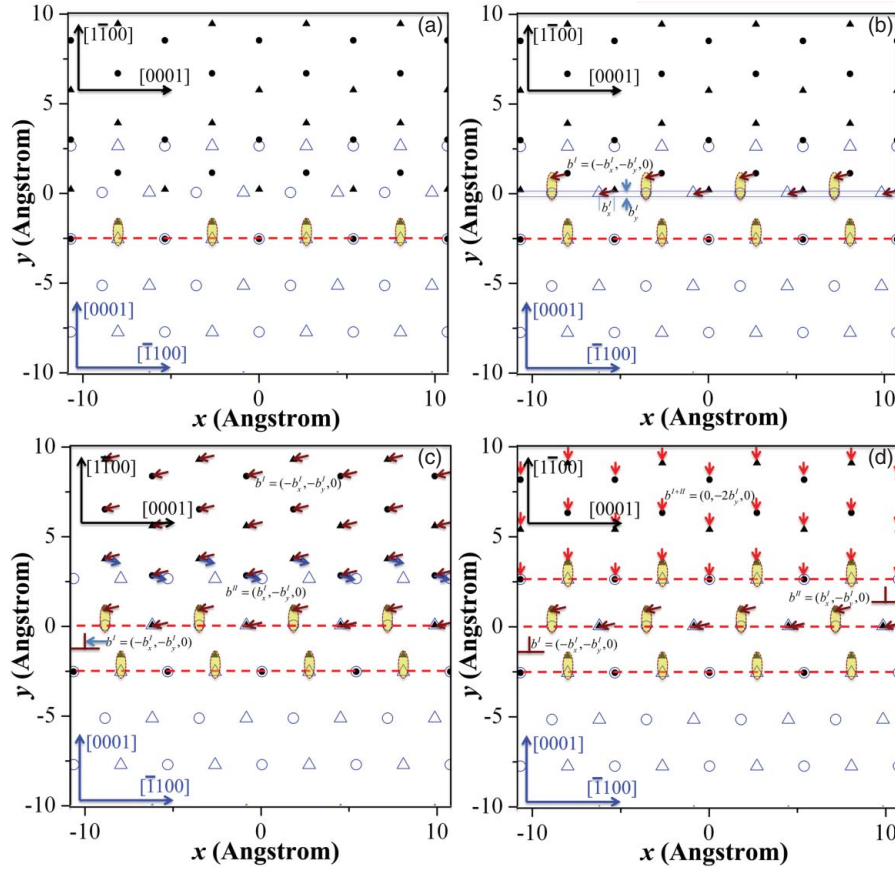


Figure 2. Mechanism 1 includes two one-layer interface disconnections with the opposite signed x-component. (a) The initial BPPS structure, (b) the definition of the first interface disconnection b^I are denoted by brown arrows, and (c) the top grain movement in association with the ID b^I and the definition of ID b^{II} are denoted by blue arrows. (d) The resultant structure in association with the migration of BPPS about two atomic layers through two IDs b^I and b^{II} . The top crystal denoted by the black solid symbols adopts the x-axis along $[1\bar{1}00]$ and the y-axis along $[0001]$. The bottom crystal denoted by blue empty symbols adopts the x-axis along $[0001]$ and the y-axis along $[1\bar{1}00]$. They share the common z-axis along $[11\bar{2}0]$ and relatively rotate 90° . The circle and triangle symbols indicate the $(11\bar{2}0)$ plane stacking along the z-axis.

In what follows we address the above-mentioned issues at the atomic scale by using topological models and MD simulations. The dichromatic pattern (Figure 2(a)) corresponding to the BPPS orientation relation in hcp metals suggests several possible mechanisms regarding the migration of the coherent BPPS. In Figure 2, the two crystals share the same z-axis along $[11\bar{2}0]$ and form a coherent BPPS. Within the boundary plane, the circles in both crystals overlap exactly, but the triangles do not because of the rumpled nature of the prismatic plane. However in real materials, they will occupy the same site in association with a low energy state after relaxation. Correspondingly, we marked them with the yellow ellipses in the topological model, representing the overlap. Figure 2(b) shows the minimum displacements required for the transformation of a prismatic plane to a basal plane. The displacements can be considered as a result of the motion of an interface disconnection (ID) that has the Burgers vector $b^I = (-b_x^I, -b_y^I, 0)$ and the step height of one atomic plane. Accompanying the

motion of the ID, the BPPS migrates upwards one atomic plane (Figure 2(c)). From a strictly geometric perspective, the boundary can continue to migrate through the second ID that has the Burgers vector $b^{II} = (b_x^{II}, -b_y^{II}, 0)$ (blue arrows in Figure 2(c)). In association with the glide of the two IDs, the BPPS moves upwards two atomic planes and the top crystal shrinks with a net displacement $(0, 2b_y^I, 0)$ (Figure 2(d)). We call this operation as Mechanism 1. Notice, however, that the continuous operation of Mechanism 1 requires alternating changes of the shear direction because the x-component of b^{II} is opposite to that of b^I . Therefore, this mechanism may be operative during thermal annealing but not under applied stresses.

Unlike in Mechanism 1, the migration of the BPPS can be accomplished through the climb of the ID b^{IV} which is two-layer thick and the Burgers vector $b^{IV} = (0, -2b_y^I, 0)$ (Figure 3(a)), corresponding to a combination of the IDs b^I and b^{II} . Accompanying the climb, atoms in the first layer experience collective shuffles. The top crystal grows downwards, resulting in a structure

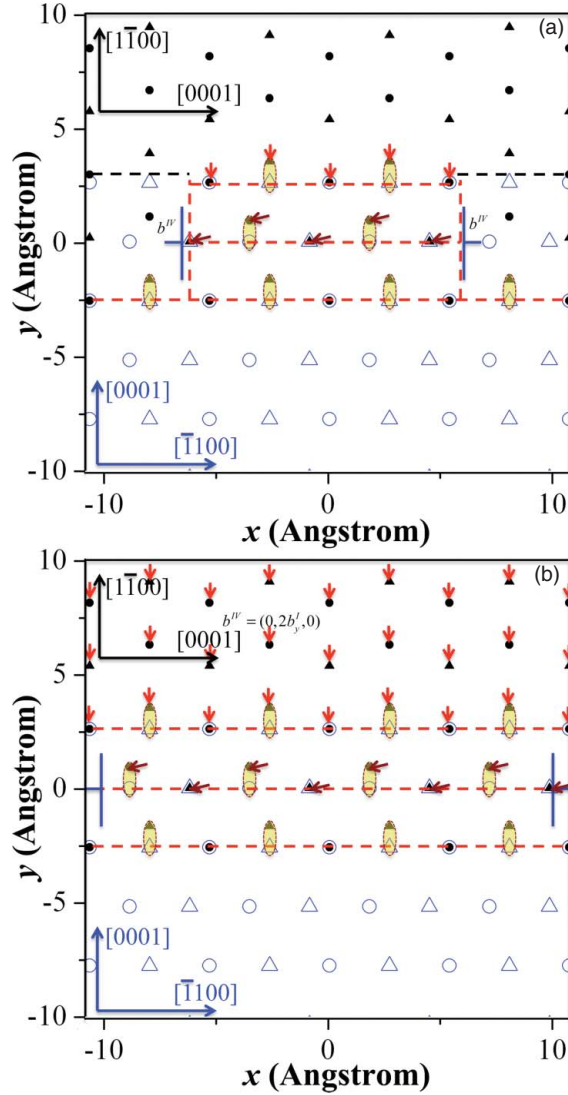


Figure 3. Mechanism 2 includes one two-layer interface disconnection b^{IV} denoted by the red arrows. (a) Disconnection dipole and (b) the resultant structure.

(Figure 3(b)) which is the same as that shown in Figure 2(d). This operation works under the normal stress with no requirement for shear stress and the net Burgers vector is smaller than those in Mechanism 1. We call this as Mechanism 2. A third possibility (Mechanism 3) is the glide of an ID b^{III} , indicated by the green arrows in Figure 4(a), which has the Burgers vector $b^{III} = (-b_x^{III}, -b_y^{III}, \pm a/2)$, much greater than any of the ones in Mechanisms 1 and 2. The resultant structure is shown in Figure 4(b).

So far the topological model suggests four possible IDs: b^I , b^{II} , b^{III} and b^{IV} . The undefined components of these Burgers vectors are calculated to be $b_x^I = \frac{\sqrt{3}}{6}a$, $b_y^I = \frac{\sqrt{3}-\kappa}{2}a$, and $b^{III} = \frac{\sqrt{3}}{3}a$. For $\kappa < \sqrt{3}$, the prismatic planes transform into the basal plane and the top crystal grows downwards through their motion along the BPPS, driven

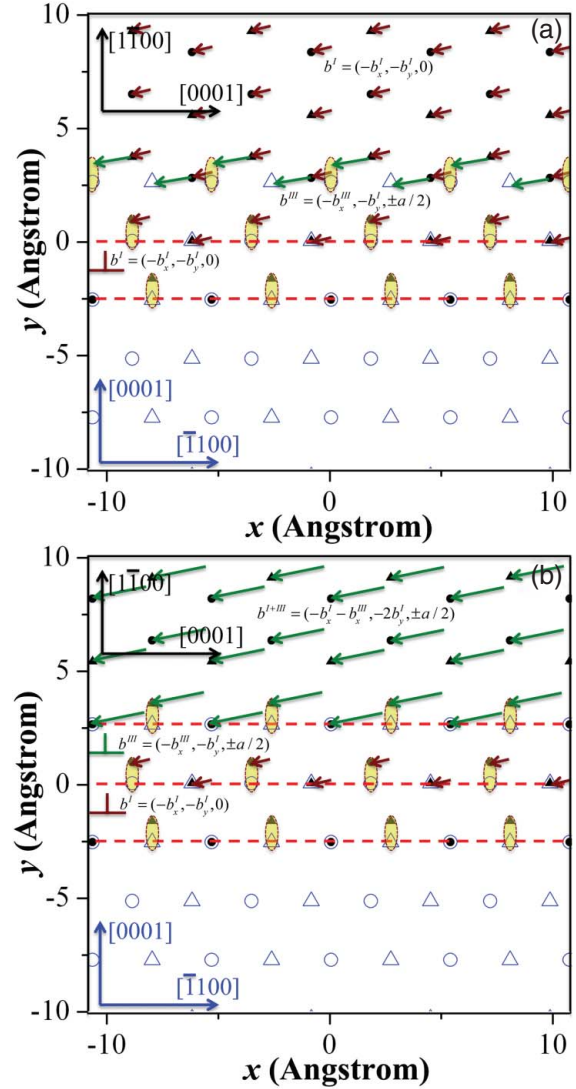


Figure 4. Mechanism 3 involves two interface disconnections, one one-layer interface disconnection b^I (brown arrows) and another one-layer interface disconnection b^{III} (green arrows). (a) The BPPS migrates upwards one atomic layer via ID b^I and the definition of ID b^{III} . (b) The resultant structure in association with the migration of BPPS about two atomic layers through two IDs b^I and b^{III} .

by compression normal to the BPPS. Under tension, four disconnections with Burgers vectors of opposite signs will transform the basal planes into the prismatic planes. On the other hand, for $\kappa < \sqrt{3}$, the prismatic planes transform into the basal planes under compression and the transformation reverses direction under tension. Since these disconnections do not move perpendicular to the BPPS, heterogeneous nucleation of IDs dipoles on a BPPS is necessary during the migration of the BPPS. Under mechanical loading, elastic strain energy is released because the transformation between the basal and prismatic planes alters the lattice spacing. For example, in Mg, the transformation is from the prismatic

to the basal plane under compression, corresponding to a decrease in the interplanar spacing. For tension, the interplanar spacing increases corresponding to the transformation from the basal to the prismatic plane.

Atomistic simulations are performed for Mg with reliable empirical interatomic potentials [27], which has been proven in recent atomistic simulations [8–10,28], to examine these mechanisms. A bicrystal model is constructed with periodic boundary conditions in the three dimensions. Two identical semi-coherent BPPSs are created in the x - z plane. The equilibrium, relaxed model has the dimensions of 49.8 nm in the x -direction, 15.98 nm in the z -direction, and 15 nm for each crystal in the y -direction. Due to the mismatch of lattices in the x -direction ($2(\sqrt{3} - \kappa)/(\sqrt{3} + \kappa)$), the semi-coherent BPPS contains an array of misfit dislocations, which can be described as $\langle 0001 \rangle \{ \bar{1}100 \}$ with respect to the prismatic plane or $\langle \bar{1}100 \rangle \{ 0001 \}$ with respect to the basal

plane (Figure 5(a)). The average spacing is 8.3 nm, suggesting that the misfit dislocation would not be present in a short BPPS (Supplementary Information, Figure S1). We first performed MD at temperature 10 K under the shear stress parallel to the BPPS plane. We did not observe the migration of the BPPSs via IDs b^I , b^{II} , and b^{III} . Instead, $\langle a \rangle \{ 0001 \}$ dislocations nucleate at the BPPS from the misfit dislocations, implying that Mechanisms 1 and 3 are unlikely, and the nucleation of IDs under shear stresses is more difficult than the nucleation of $\langle a \rangle \{ 0001 \}$ dislocation.

Mechanism 2 is examined under compression and tension, respectively. Notice that a shear stress on the twin plane would produce such a compressive or tensile stress on the BPPS. During compression, the nucleation and motion of IDs commence at a compressive stress of 1.5 GPa (Figure 5(b)). The analysis of the relative displacements [29] confirms that IDs are $2n$ -layer thick and

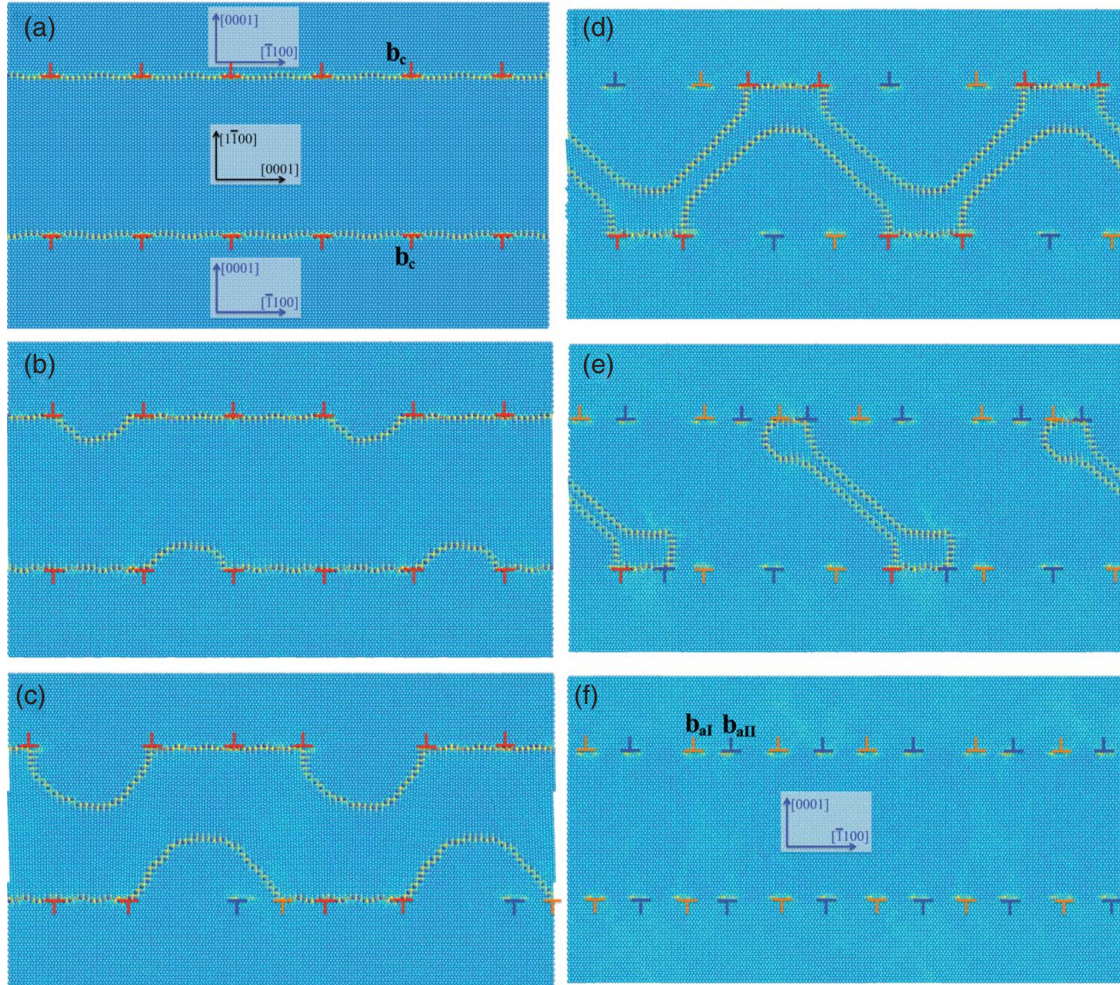


Figure 5. Snapshots of BPPSs migration during atomistic simulations for Mg show (a) to (e) the migration of BPPSs under compression. The misfit dislocations are denoted by b_c . For easy visualization of the nucleation, climb and annihilation of interface disconnections, we show $\langle 1\bar{1}00 \rangle$ -oriented grain in the middle under compression. Accompanying the nucleation, climb, and annihilation of interface disconnections, the bicrystal transforms to a single crystal containing a couple of dislocations dissociated from the misfit dislocations. b_{aI} and b_{aII} are $\langle a \rangle \{ 0001 \}$ 30° basal dislocations with z -components of opposite signs.

no shear deformation is associated with the motion of IDs. At the constant compression of 1.5 GPa, Figure 5(c)–(e) shows that IDs nucleate, climb, react, and finally annihilate, resulting in a single crystal (Figure 5(f)) that contains $\langle a \rangle \{0001\}$ basal dislocations (Compression.mov in the Supplementary Material). It is worth mentioning that (1) IDs nucleate in the prismatic planes and is two-layer thick, (2) accompanying the motion of IDs, the six misfit dislocations in the original BPPS do not climb with the BPPS together, and they finally dissociate into 12 $\langle a \rangle \{0001\}$ mixed basal dislocations with z -components of opposite signs (also see Figure S2 in the Supplementary Material). The net Burgers vector is conserved. Similar processes are observed during the tension simulations, as shown in Supplementary Information, Figure S3 and Tension.mov in the Supplementary Material. IDs are two-layer thick and Burgers vector is equal to $-b^{\text{IV}}$.

However, there are two differences. First, the nucleation of ID is observed at the tensile stress of 2.0 GPa. Second, nucleation occurs on the basal plane.

The difference in the critical stress between compression and tension could be ascribed to the kinetics anisotropy from a geometric point of view. During compression, the less compact plane $\{\bar{1}100\}$ is transformed to the most compact plane $\{0001\}$. But during tension, the $\{0001\}$ plane is transformed to $\{\bar{1}100\}$. We examined this transformation by performing the chain-of-state calculation [30]. A two-layer ID b^{IV} is introduced in a coherent BPPS, and climbs one periodicity along the x -direction. The initial and final structures are shown in Figure 6(a) and 6(b). Figure 6(c) and 6(d) shows the change in potential energy and the effective climb force as a function of the equivalent climb distance. It is obvious that the energy curve is unsymmetrical. The peak force (6.0 N/nm) in

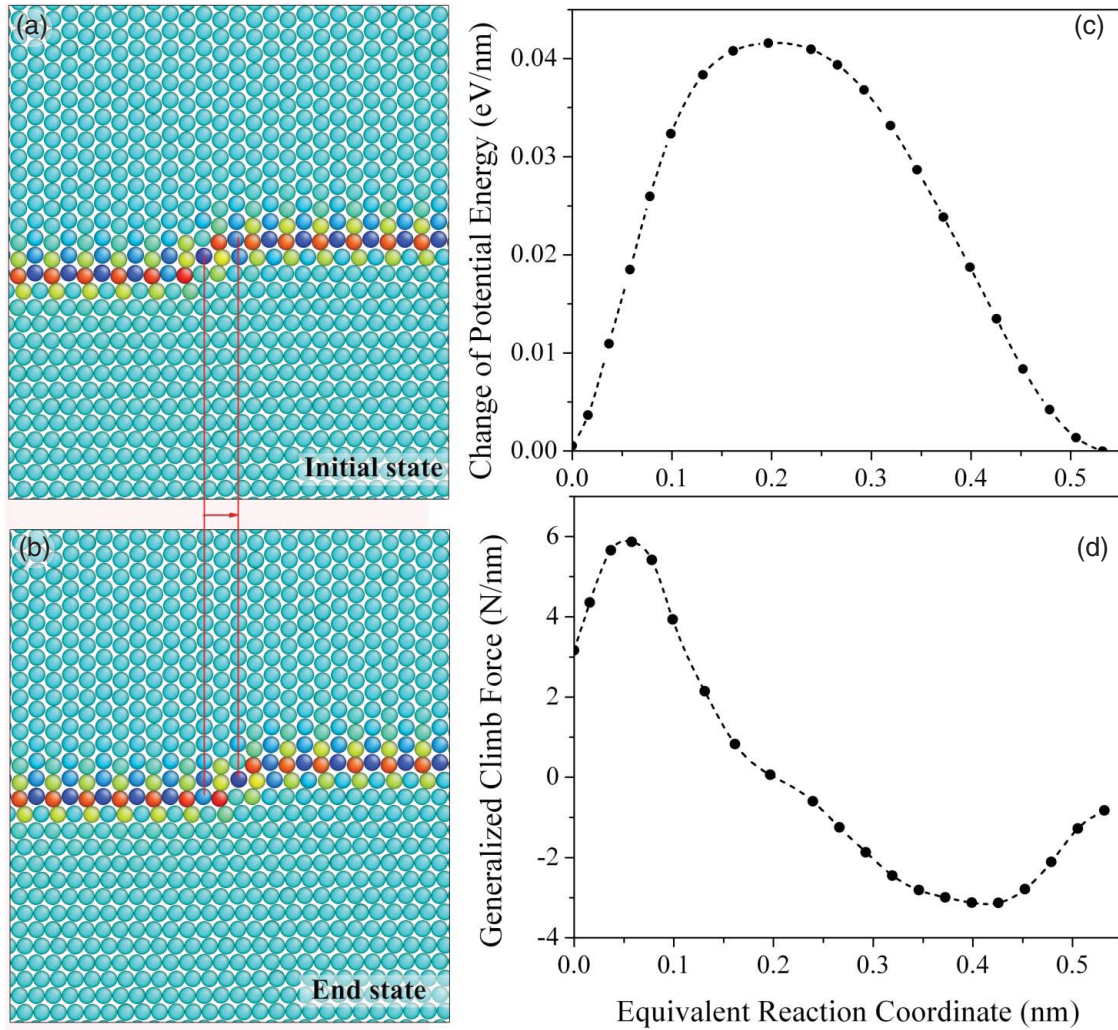


Figure 6. Climb kinetics of interface disconnection, (a) and (b) atomic structures of coherent BPPS containing one interface disconnection at two different locations separated by one periodicity. The chain-of-state results show that (c) the change in potential energy and (d) the effective climb force as a function of the equivalent climb distance. The disconnection is climb from the left to the right corresponding to the horizontal-axis direction.

association with the transformation of the basal plane to the prismatic plane is greater than that (3.1 N/nm) in association with the inverse transformation.

The migration of the SCTBs can be postulated as follows. For twinning or de-twinning, the maximum shear stress is on the twinning plane, and the maximum normal stress is on the BPPS. TDs gliding on CTBs are impeded at the steps (Figure 1(d)). The projection of a TD on the normal direction of the BPPS plane $|b_{\text{tw}}|_{\text{BP-GB}}$ is approximately equal to the Burges vector of ID b^{IV} . The ratio $|b_{\text{tw}}|_{\text{BP-GB}}/|b^{\text{IV}}|$ is equal to $(\sqrt{3}\kappa + \kappa^2)/(3 + \kappa^2)$, 0.95 for Be (with the minimum κ), 1.04 for Cd (with the maximum κ), and 0.97 for Mg ($\kappa = 1.623$), where $|b_{\text{tw}}|_{\text{BP-GB}}$ can be calculated by $|b_{\text{tw}}|(\sqrt{3}/(\sqrt{3} + \kappa^2))$. Under normal stress, TDs can climb along the BPPS plane, resulting in the migration of the SCTBs as schematically shown in Figure 1(d). Accompanying the migration of the BPPS, GBDs can move with the BPPS together through climb.

In summary, the SCTBs migrate through TDs by gliding along CTBs and climb along BPPSs, corresponding to twinning and de-twinning. Assuming that the glide of TDs is activated by relatively low shear stress, the density and the height of BPPSs in the SCTBs will play a crucial role in opposing the growth of twinning/de-twinning, and thus affect the twinning-associated hardening [31]. One could envisage a twin growth process that starts with an interrupted CTB which, as deformation progresses and the twin grows, incorporates an increasing number of serrations. The latter are the result of the reaction of gliding dislocations at the interface, which alters the perfect twin-matrix misorientation. In addition, the anisotropic kinetics in association with the climb process could correlate with the difference in the flow stress between twinning and de-twinning in hcp metals during cyclic loading [32]. Further experimental evidence is required, particularly, *in situ* high-resolution transmission electron microscopy observations in single crystals that can provide insights into kinetic processes at the atomic scale [33,34] and/or *in situ* measurements of the critical stresses and velocities in association with the migration of twin boundaries during twinning and de-twinning in single crystals by using transmission electron microscopy that can provide insights into understanding the anisotropic kinetics and the twinning-associated hardening at meso scale [35–38].

Supplementary online material. A more detailed information on experiments is available at <http://dx.doi.org/10.1080/21663831.2013.779601>

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