Why are $\{10\bar{1}2\}$ twins profuse in magnesium?

Haitham El Kadiri^{a,b,*}, Christopher D. Barrett^{a,b}, Jian Wang^c, Carlos Tomé^c

^aDepartment of Mechanical Engineering, Mississippi State University, Mississippi State, MS 39762, USA

^bCenter for Advanced Vehicular Systems, Mississippi State University, Mississippi State, MS 39762, USA

^cMaterials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM, 87545, USA

Abstract

We show that $\{10\bar{1}2\}$ twinning in magnesium acts as an effective sink of basal dislocations without loss of mobility. The lattice dislocation decomposes into the $\mathbf{b}_{0/0}^{BP}$ dislocation recently identified by the present authors, and a residual dislocation. The $\mathbf{b}_{0/0}^{BP}$ dislocation in turn spontaneously decomposes into a Burgers vector content of the basal prismatic facet related disclination dipole, $\mathbf{f}_0^{BP}$, plus an associated number of twinning disconnections. The residual dislocation lies on the basal-prismatic facet and thus remains glissile should the twin boundary move forward or recede back. Importantly, the basal-prismatic facet absorbs any twinning disconnection gliding on one side of the twin boundary and releases another one to other side, enabling thereby the twin boundary to progress through forest of basal dislocations with no apparent decrease in mobility or loss of coherency. This mechanism explains why $\{10\bar{1}2\}$ twinning is profuse in hexagonal close-packed metals as slip induces the interfacial atomic structure to change favorably for twin propagation.

1. Introduction

The invasive growth capability of $\{10\bar{1}2\}$ twinning in hexagonal close packed (HCP) metals is one of the predominant attributes of this twinning mode, having profound consequences on the mechanical properties. However, no formal mechanism exists which explain this superior propagation ability compared to other twinning modes. For instance, in traditional wrought magnesium polycrystals, an adequate loading can induce $\{10\bar{1}2\}$ twins to consume the entire parent matrix in a fashion no other twin mode can achieve regardless of the c/a ratio of the HCP material in question [1–6].

There is, however, a difficulty in understanding this important issue from the perspective of classical literature. One may become in fact baffled by confusing two entirely different topics. The first one relates to the universality of $\{10\bar{1}2\}$ appearing in all HCP metals, while the second one, being the focus of this paper, relates to its ability to grow despite pre-existing and/or concomitant slip.

The first issue is actually connected to its particular ease of *nucleation* regardless of the c/a ratio, in contrast to all other twin modes which can be made to vanish by choosing an existing c/a ratio material. This phenomenon can be reasonably explained in terms of pure crystallography. Twinning on $\{10\bar{1}2\}$ plans offers an optimal combination of relatively low characteristic shear

*Corresponding author

Email address: elkadiri@me.msstate.edu (Haitham El Kadiri)

and very simple shuffles [7]. This explanation is somewhat vague because no relationship has been identified between the mobility of twin boundary (TB) and the magnitudes of shear and shuffle operating at the disconnection core [7]. Atomistic simulations by Serra et al. [8], Serra. et al. [9] cast further doubts on this rationalization as the core width of $\{11\bar{2}1\}$ twinning disconnection (TD) was computed to be much wider than that of $\{10\bar{1}2\}$ twinning, but still correlates with very slow twin propagation rates in Ti and Zr. With regard to either shear or shuffle alone, they could not provide any consistent explanation for the high mobility of $\{10\bar{1}2\}$ TDs, and ample counterexamples could be listed. For instance, the generally very low shear of $\{10\bar{1}1\}$ and $\{11\bar{2}2\}$ twinning and the minimum required shuffle in $\{11\bar{2}1\}$ twinning did not preclude their sluggish edgewise thickening.

Not least, the second issue essentially lies in the peculiar invulnerability of $\{10\bar{1}2\}$ twinning mode to concomitant slip and/or pre-existing dislocations. On one hand, slip has the potential to cause roughness of the twin boundary (TB), and thus provoke a severe loss of local coherency, both of which would impede twinning disconnection glide and thereby also impede further twin propagation. Recently, Wang et al. [10] showed $\{11\bar{2}1\}$ twins quickly developing roughness on one side of the boundary, which obstructed their propagation. On the other hand, inhomogeneous deformation that develops within both the twin and the parent should in principal induce the K_1 plane to rotate away from either sides of the twin composition plane, implying a tendency of the boundary to lose perfect coherency. Another plausible argument put forward by Asgari et al. [11] is the development of lattice curvature due to the inhomogeneous strain which has the effect of reducing the length scale over which deformation twins are formed. Thus, since smaller grains require higher twin nucleation stress, in-grains misorientation may significantly impede further twin nucleation and propagation.

Figure 1 shows inverse pole figures maps at three stages of in-plane compression of a rod-textured AM30 magnesium alloy obtained by high temperature extrusion. Before compression, the extrusion process induced substantial subgrains and lattice curvature gradients in grains (in blue) which did not completed their dynamic recrystallization process. In these grains, $\{10\bar{1}2\}$ twins were perfectly able to propagate despite the substantial in-grain deformation inhomogeneities. At 3% plastic strain, twins readily curved their boundaries to follow the complex path of the composition plane which meanders through dislocation substructures (Figure 1a). By 6% of plastic compression (Figure 1b), twins have already reached the coalescence stage, and finally, by 9% of plastic deformation they nearly consumed the entire parent structure (Figure 1c).

Both this clear unyielding capabilities of the $\{10\bar{1}2\}$ TB to punch through dislocation structures and curve through strong in-grain misorientations indicate a special interaction mechanism between the TB and lattice distortions. Independently from the issues raised above, Serra and Bacon [12], Serra et al. [13], and Pond et al. [14] suggested based on results of atomistic simulations that $\{10\bar{1}2\}$ TB is able to convert intersecting slip dislocations into appropriate TDs, which was not found to be the case for other prominent twin modes such as $\{11\bar{2}1\}$ and $\{11\bar{2}2\}$. This is a very encouraging finding, which indicates a possible violation of classical theories ruling dislocation transmutation by the twinning shear at TBs [1, 15–17], and which may operate in a favorable scenario for twin propagation. The generation of TDs by virtue of slip–twin interactions was first reported by Thompson and Millard [18] on the basis of the crystallographic theory of the pole-based twin growth mechanism originally suggested by Cottrell and Bilby [19]. However, these authors postulated the creation of only two TDs as basal slip merges onto the $\{10\bar{1}2\}$, which was shown by Serra and Bacon [12] to not be the case as the perfect basal dislocation is actually equivalent

Figure 1: Inverse pole figure maps obtained by electron backscattered diffraction on deformed samples under simple compression up to (a) 3%, (b) 6%, and (c) 9% of plastic deformation. Note the substantial lattice curvature due to high dislocation density. The initial orientation condition corresponded to a rod texture typical of extrusion where the blue grains have their $\langle 0001 \rangle$ poles normal to the extrusion direction along which simple monotonic compression stress was applied.

to three TDs as required by minimization of the residual dislocation. To our knowledge, the first experimental evidence of slip producing TDs on the $\{10\bar{1}2\}$ corresponded to the work by Lay and Nouet [20] on zinc. However, despite the breakthrough finding by Serra et al. [13], a few gaps persist in explaining the brisk and implacable mobility of $\{10\bar{1}2\}$ TBs in HCP metals:

1. Very recently, through high resolution transmission electron microscopy (HRTEM) and MD simulations, [21–27] found that $\{10\bar{1}2\}$, $\{10\bar{1}1\}$, $\{2\bar{1}11\}$, and $\{2\bar{1}\bar{1}2\}$ TBs adopt serrated morphologies in cobalt, zirconium, titanium, and magnesium by extending along specifically selected asymmetric tilt boundaries. In particular, the $\{10\bar{1}2\}$ TBs facet along the asymmetric basal-prismatic (BP) boundary. The present authors recently established a formal theory for deformation faceting of compound twinning in HCP metals and identified all possible potential asymmetric boundaries for each twin mode [28]. This faceting may have important bearing on the mobility of $\{10\bar{1}2\}$ twinning. For instance, the three variants associated with BP and PB boundaries can in principal enable the $\{10\bar{1}2\}$ TB to curve in the lattice space which, as one may imagine, could be exploited by the TB to advance across in-grain misorientations. The existence of this morphology was first suggested by Serra and Bacon [12], Pond et al. [14]. However, their work does not explain TB faceting, although they describe a ‘boundary riser’ which would in current terms be analyzed as a new BP facet. Pond et al. [14] note many of the currently observed properties of the BP facet, such as its mobility along with the $\{10\bar{1}2\}$ twin and its ability to generate TDs. However, their analysis of the ‘riser’ as a disconnection with an extremely large step height complicates analysis and glosses over the core structure while requiring a somewhat awkward explanation of its low energy formation and movement.

2. In the event this hypothesis of faceting-enhanced twin mobility is accurate, the mechanisms through which the BP facet would nucleate on a TB advancing through slip dislocations and dislocation substructures are *a priori* unknown. It is not clear how the formation of BP facets will be favored under pre-existing or concomitant slip, and how these facets would enable the twin to overcome lattice barriers. The present authors showed through atomistic simulations that a twin facet can nucleate on a BP boundary by relaxation of several of $\mathbf{b}_{2/2}^{BP}$ type disconnections [29]. An analogous scenario could be celebrated for the nucleation of a BP facet along the $\{10\bar{1}2\}$ TB, which would instead involve TDs. However, this assumption requires a mechanism that involves locking of TDs on the TB, which is rather counter-intuitive and may not happen in normal cases except for areas where the twin terminates. Barrett and El Kadiri [28] in fact reproduced by MD simulations nucleation of BP facets by relaxation of TDs at the edgewise periphery of a twin terminating at the free surface at which point they were able to pile-up.
3. The creation of the BP interface implies the creation of a disclination dipole. Thus, upon their passage along the faceted interface, TDs will merge into a rotational distortion barrier, which is supposed to affect their mobility. This problem was not addressed in the twin growth model by Serra and Bacon [12] who considered the entire facet as a single defect. Thus, while they analyzed the Burgers vector content of the entire facet and TD mobility through it, the evolution of the core structure and energy of the facet are unclear.
4. If the generation of TDs by intersecting slip is all that is needed for the twin to overcome lattice distortions and slip, other twin modes would experience profuse growth as well. For instance, $\{10\bar{1}1\}$ twinning can generate TDs upon interactions with screw lattice dislocations [13, 30]. In magnesium $\{10\bar{1}1\}$ twinning is observed at fairly large strains where screw dislocations are expected to be substantial. However, $\{10\bar{1}1\}$ twinning is still one of the most sluggish twin modes known a priori. It is usually correlated to a needle-like shape morphology. The fact that a dislocation interacting with the $\{10\bar{1}1\}$ twin boundary can only produce one single TD [12, 31, 32] compared to five for $\{10\bar{1}2\}$ is still not sufficient to explain the large difference in propagation rates between the two twin modes. Moreover, $\{10\bar{1}1\}$ twinning could still be profuse in highly deformed lattices that could supply enough interaction dislocations. As such, further mechanisms must be involved in slip-twin interactions which appear to prominently favor $\{10\bar{1}2\}$ twinning.

This paper focuses on filling these gaps by identifying the intricate mechanisms governing the well known supremacy of $\{10\bar{1}2\}$ twinning, which is still one of the most difficult conundrums for the experts dealing with the fundamentals of deformation in HCP metals. We base our work on the formal geometrical concept inherent to interfacial defect theory, which is exploited to critically evaluate and analyze results obtained by MD simulations of slip–twin interactions.

2. MD Methodology

Using LAMMPS [33] with an embedded-atom method potential by Liu et al. [34], $\{10\bar{1}2\}||\{10\bar{1}2\}$ TBs were first relaxed with periodic boundary conditions in the two dimensions spanned by the boundary and free surfaces on the dimension normal to the boundary. After relaxation, a lattice dislocation pile-up composed of four $\frac{1}{3}\{\bar{1}2\bar{1}0\}$ basal mixed dislocations were introduced into one crystal using the anisotropic elastic solution for a bicrystal [35, 36] (Figure 2a). The four dislocation pile-up induced a stress which was sufficient to drive the lead dislocation, $\mathbf{b}_m$, to the boundary.

The boundary was again relaxed and equilibrated before applying a positive shear strain in the yz twinning shear plane along the twinning direction, but one which would induce the pile up to move away from the boundary. The dislocation line direction was taken to be in the paper. However, the resolved shear stress on the glide plane was calculated to be very low. The shear strain was increased in small increments until the resolved stress on the twin plane reached about 100 MPa, at which point the stress on the cell was held constant. As the positive shear stress requires the TB to move upward toward the dislocation pile-up (Figure 2a), the top crystal is considered to be the parent crystal and is denoted black, μ , so the bottom crystal, the twin, is denoted by λ . The third lattice generated by faceting is denoted by κ .

We have limited this paper to studying interactions of $\{10\bar{1}2\}$ with only basal slip. Interactions with other slip modes is of considerable importance, but too complicated for inclusion in a single paper. We prefer to begin by treating basal slip as experimental evidence has accumulated that threshold stresses of basal slip in all commercial HCP metals, except for Zr and Ti, is smaller at least by a factor of two and an order of magnitude compared to the other observed slip modes such as prismatic $\langle a \rangle$ and pyramidal $\langle c + a \rangle$, respectively. Even for Zr and Ti where prismatic $\langle a \rangle$ slip is the easiest, basal slip is still noticeably active.

3. Results and discussions

3.1. Summary of the basal dislocation- $\{10\bar{1}2\}$ twin boundary interaction

Figures 2-3 expose the behavior of the TB when struck by the two incoming Shockley partials. (The other three lattice dislocations moved away from the boundary and eventually out of the simulation box.) The reaction scenario could be divided into five main sequences of interfacial reactions:

1. The incoming $\mathbf{b}_m$ dislocation induced the $\{10\bar{1}2\}$ TB to conservatively nucleate a $B^\mu P^\kappa$ facet with a length of $8d_{(0001)\kappa}$ by emitting a pair $\mathbf{b}_{2/2}^{TB}$ TDs¹ on either side of the facet. (The $B^\mu P^\kappa$ facet, unlike the $\{10\bar{1}2\}$ TB, lies on the basal plane of the parent and is able to directly absorb the lattice dislocation to lower its strain energy.) The $B^\mu P^\kappa$ facet formation from $\mathbf{b}_{2/2}^{TB}$ TDs has been previously elaborated [29]. The process observed here is similar; four TDs are emitted and the four opposite sense disconnections collect to form the facet. This process nucleates a pristine facet with a coherency strain. The $\mathbf{b}_m$ dislocation is superimposed on the facet to generate the complete picture of the process. The $\mathbf{b}_m$ disconnection partially annihilates with the coherency strain of the pristine facet, which explains why the formation is favorable on the boundary in response to the incoming dislocation. The pair of TDs on the left of the facet glided away along the boundary encouraged by the applied stress, while the pair of TDs on the right were not able to glide away under the applied stress and relaxed into a small $P^\mu B^\kappa$ facet which was $4d_{(10\bar{1}0)\kappa}$ long. The relaxation occurred by a similar mechanism studied in Barrett and El Kadiri [29].
2. The $B^\mu P^\kappa$ boundary emitted a $\mathbf{b}_{2/2}^{TB}$ disconnection from the upper disclination. This is the third TD which was able to glide away to the left, so the facet is now approximately $10d_{(0001)\kappa}$ long.

¹This notation was previously [28, 37] found useful to describe deformation faceting behavior of asymmetric tilt boundaries

Figure 2: Results of molecular dynamics simulations of lattice basal dislocation interaction with the $\{10\bar{1}2\}$ twin boundary showing (a) extended Shockley dislocations heading toward a $\{10\bar{1}2\}$ twin boundary under the pile-up stress in the yz plane of the simulation box. The Shockley partials were introduced on the basal plane of the upper lattice after relaxation. The shear is held at constant stress while the dislocations move into the boundary. Partially fixed surfaces are maintained in the x and y dimensions while the z dimension is periodic. (b) Upon entering the twin boundary, the dislocation dissociates, emitting two twinning disconnections on the left hand side, a basal-prismatic facet with a misfit dislocation accommodating the coherency strain, and two sessile TDs, which relaxed into a small immobile PB facet.

3. The $B^\mu P^\kappa$ emitted a second $\mathbf{b}_{2/2}^{TB}$ disconnection which is the fourth TD gliding away to the left as required by the shear sign, so the facet is now approximately $12d_{(0001)^\kappa}$ long.
4. As soon as this TD moved away, the unstable $P^\mu B^\kappa$ facet relaxed into the $\{10\bar{1}2\}$ TB by reacting with the $B^\mu P^\kappa$ facet and shortening them both by $4d$. The $B^\mu P^\kappa$ facet length is back now to $8d_{(0001)^\kappa}$.
5. The $B^\mu P^\kappa$ facet emitted a third $\mathbf{b}_{2/2}^{TB}$ positive edge disconnection being the third and last one to extend this facet to $10d_{(0001)^\kappa}$ by gliding to the left. This length was found to correspond to the final stage of slip-twin interactions as no TDs could then nucleate unless the stress was increased by at least a factor of two.

The simulations showed that the basal dislocation, $\mathbf{b}_m$, ended its interaction with the twin boundary by decomposing into five effective TDs along with other defects corresponding to the creation of a $B^\mu P^\lambda$ facet $10d_{(0001)^\kappa}$ long. This reaction shall be written as:

$$\mathbf{b}_m = 5\mathbf{b}_{2/2}^{TB} + \mathbf{f}_0^{5BP} + \mathbf{b}_r \quad (1)$$

where $\mathbf{f}_0^{5BP}$ is the dislocation content (BV) of the disclination dipole (DD) associated with the formation of a $(5 \times 2d_{(0001)^\kappa})$ $B^\mu P^\kappa$ facet on the TB, and $\mathbf{b}_r$ is the residual dislocation content of the entire dissociation process. A general expression of $\mathbf{f}_0^{iBP}$, where the superscript i counts the number of TDs generated with the BP facet, could be provided from the fundamental equation of interfacial defect theory by Pond and Hirth [38] as illustrated in Barrett and El Kadiri [37]:

$$\mathbf{f}_0^{iBP} = \mathbf{R}\mathbf{l}_i - \mathbf{l}_i \quad (2)$$

where $\mathbf{R}$ represents the rotational symmetry operation of the trichromatic complex defining the disclination, and $\mathbf{l}_i$ is the facet length vector of the disclination dipole bounding the $B^\mu P^\kappa$ facet and normal to the tilt axis. We shall mention a possible confusion in Barrett and El Kadiri [29] between the BV content of the DD represented by $\mathbf{f}$, and the definition of the original Frank vector; $\boldsymbol{\omega}$ introduced by Nabarro [39], Nabarro and Argon [40], Romanov and Kolesnikova [41], Das et al. [42], Kroupa and Lejček [43]. The Frank vector $\boldsymbol{\omega}$ represents the strength of the disclination from the mutual rotation of the undeformed surfaces of the cut bounded by the disclination line, so it could simply be written as:

$$\boldsymbol{\omega} = \frac{1}{3a} \arccos \left(\frac{1}{2} (\text{Trace}(\mathbf{R} - 1)) \right) [1\bar{2}10] \quad (3)$$

Here $[1\bar{2}10]/3a$ is the normalized eigenvector of $\mathbf{R}$ corresponding to an eigenvalue of unity.

3.2. Analysis of the transient stages of the interaction process

Equation 1, however, does not reflect that $B^\mu P^\kappa$ stabilized after several transient stages. At an early stage, four TDs were first generated and then evolved into two separate processes: (1) the glide of only one pair of TDs, and (2) the coalescence of the other pair of TDs, which piled-up and relaxed on the right-hand side of the TB portion onto which the basal dislocation has merged from the parent. The simultaneous glide to the left of the first four TDs is probably less energetically favorable, because a potential TD relaxation would have led to a high energy TB- $P^\mu B^\kappa$ - $B^\mu P^\kappa$ -TB configuration of facets. However, a PB facet could immediately collapse if it is smaller than $8d_{(0001)^\kappa}$.

So to stabilize the facet at this length, the neighboring TB segment of $2\boldsymbol{\eta}_1$ vector extended into two small $P^\mu B^\kappa$ - $B^\mu P^\kappa$ facets by relaxation of a pair of TDs in a similar fashion described by Barrett and El Kadiri [28, 29], and such that:

$$2\boldsymbol{\eta}_1 = 2[0001]^\mu + 2[0001]^\kappa \quad (4)$$

At first sight, this mechanism does not upset the BV vector of the initial DD given by $\mathbf{f}_0^{ABP}$. In fact, on one hand, there is no rotational distortion, e.g. no interfacial disclination required to accommodate the lattice transition from the $B^\mu P^\kappa$ to the $P^\mu B^\kappa$ facet. On the other hand, the next transition from the $P^\mu B^\kappa$ to the TB facet is mediated by a disclination with BV content equal to $\mathbf{f}_0^{1BP}$ plus a counterclockwise $\pi/2$ rigid body rotation. The only difference is the higher surface energy adopted by the extension of the TB segment. To reflect this mechanism, the initial reaction could be written as:

$$\mathbf{b}_m = 4\mathbf{b}_{2/2}^{TB} + \mathbf{f}_0^{3BP} + R_{90^\circ}\mathbf{f}_0^{1PB} + \mathbf{b}_r \quad (5)$$

where R_{90° is the 90° basic matrix rotation around the common tilt axis of the facet. However, the right-hand sides of both Equation 1 and Equation 5 are equal.

The natural trichromatic pattern (NTP) introduced by Barrett and El Kadiri [28] and Barrett and El Kadiri [37] and illustrated in Figure 4 enables a more elegant derivation and understanding of the residual defect $\mathbf{b}_r$. Interestingly, for the general case of i number of TDs, where $i = 4$ for the immediate interaction between basal slip and the $\{10\bar{1}2\}$ TB, this defect is found to be equal to:

$$\mathbf{b}_r = \mathbf{b}_m - i \left(\mathbf{b}_{2/2}^{TB} + \mathbf{f}_0^{1BP} \right) = \mathbf{b}_m - i\mathbf{b}_{0/0}^{BP} \quad (6)$$

where $\mathbf{b}_{0/0}^{BP}$ is the dislocation identified by Barrett and El Kadiri [29] corresponding to the residual dislocation content upon nucleation of $(a\gamma)^\kappa$ small $B^\mu P^\kappa$ facet:

$$\mathbf{b}_{0/0}^{BP} = \frac{\gamma - \sqrt{3}}{\sqrt{\gamma^2 + 3}} \begin{pmatrix} 0 \\ -\sqrt{3} \\ \gamma \end{pmatrix}, \quad h = 0 \quad (7)$$

Remarkably, $\mathbf{b}_r$ disconnection is glissile as it lies on the $B^\mu P^\lambda$ facet and has no step character. Hence, the $B^\mu P^\kappa$ facet will be able to move upward should the twin grow in the matrix.

Following the nucleation stage of the facet, the $\mathbf{b}_r$ motivated upward motion of the upper disclination to further reduce the Burgers vector content on the facet. This motion generated a new TD which glided toward the left similarly to the first pair of TDs during nucleation. Emission of dislocations during disclination motion results from the fundamental characteristic that the Frank vector is conserved along the disclination line, similarly to the Burgers vector conservation along the dislocation line [44, 45]. The production of TD could also be understood from the perspective of the plastic deformation contributed by the motion of the upper disclination [41]. To accommodate this plastic deformation, a TD nucleated and glided at the upper junction of the facet. The mathematics related to this mechanism was treated in length in Barrett and El Kadiri [29] and Barrett and El Kadiri [28] for the cases of $\{10\bar{1}2\}$, $\{10\bar{1}1\}$, and $\{10\bar{1}3\}$ faceting. The disclination must move by an increment vector of magnitude equal to c^κ in the direction of the facet normal to the tilt axis:

Figure 3: Results of molecular dynamics simulations of lattice basal dislocation interaction with the $\{10\bar{1}2\}$ twin boundary showing growth stages of the basal-prismatic facet which was governed by the motion of the upper disclination under stress provoking (a) emission of a third TD which glided to the left as imposed by the shear, then (b) elimination of the high energy interfacial disclination by absorbing the PB facet, and finally (c) emission of a fifth disconnection where the BP facet reached the final most stable length.

$$\mathbf{r}_1 = a \begin{pmatrix} 0 \\ -\frac{\gamma^2}{\sqrt{\gamma^2+3}} \\ \frac{\sqrt{3}\gamma}{\sqrt{\gamma^2+3}} \end{pmatrix} \quad (8)$$

The BV content of the DD augments then by a magnitude derived from Equation 2 by setting $i = 1$:

$$\mathbf{f}_0^{1BP} = a \begin{pmatrix} 0 \\ -\frac{\sqrt{3}\gamma-\gamma^2}{\sqrt{\gamma^2+3}} \\ -\frac{\sqrt{3}\gamma-\gamma^2}{\sqrt{\gamma^2+3}} \end{pmatrix} \quad (9)$$

At the same time, the residual dislocation inherent to the $B^\mu P^\kappa$ facet nucleation augments by the same value given in Equation 7 (of a magnitude equal to $(a\sqrt{3})^\mu - c^\kappa$). However, conservation of the Burgers vector upon disclination motion requires the generation of a disconnection equal to:

$$\mathbf{b}_g = \mathbf{b}_{0/0}^{BP} - \mathbf{f}_0^{1BP} = \frac{3-\gamma^2}{\sqrt{3+\gamma^2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \mathbf{b}_{2/2}^{TB}, \quad h = \frac{\gamma\sqrt{3}}{\sqrt{\gamma^2+3}} \quad (10)$$

which is exactly the $\{10\bar{1}2\}$ TD observed to glide away to the left.

The upper disclination kept moving by the same rate and, thereby, sequentially emitted two more TDs. Before the last TD was emitted from the upper disclination, the lower disclination moved rapidly up by distance equal to $4d_{(0001)^\kappa}$. This motion triggered emissions of two TDs to the right, but having an opposite sign to that of the first TD pair which caused the formation of the $P^\mu B^\kappa$ facet. Therefore, dislocation/disclination annihilation took place causing the small $B^\mu P^\kappa$ - $P^\mu B^\kappa$ to constrict and collapse back into the original TB segment.

After that, the $B^\mu P^\kappa$ facet reached the stable interaction length corresponding to $i = 5$ and with a final residual dislocation of:

$$\mathbf{b}_r = \mathbf{b}_m - 5\mathbf{b}_{0/0}^{BP} = \mathbf{b}_{\text{final}} = \begin{pmatrix} -\frac{1}{2} \\ \frac{10\sqrt{3}\gamma-27}{2\sqrt{\gamma^2+3}} \\ -\frac{\gamma(10\gamma-9\sqrt{3})}{2\sqrt{\gamma^2+3}} \end{pmatrix} \quad (11)$$

3.3. Growth model

The BP facet was observed to nucleate TD dipoles from the facet junctions by a similar process indicated by Serra and Bacon [12]. However, we only observed this when the stress was tripled, i.e. ≈ 300 MPa. This type of TD emission was rather due to a synchronized movement of the two DD partners, which did not cause the facet to lengthen. As can be clearly noted in Figure 4, the movement of the upper disclination partner is motivated by the minimization of the residual defect from the interfacial reaction, $\mathbf{b}_r$, which decreases monotonically upon extension of the $B^\mu P^\kappa$ facet up to a length of approximately $16d_{(0001)^\lambda}$, where it increases back. However, this lengthening is

Figure 4: Natural trichromatic pattern (NTP) for the basal slip interaction with the $\{10\bar{1}2\}$ twin boundary showing the decomposition of the perfect basal into i number of twinning disconnections, a basal-prismatic ($B^\mu P^\kappa$) disclination dipole characterized by its Burgers vector content $\mathbf{f}_0^{iBP}$, and an interaction residual defect $\mathbf{b}_r^{iBP}$ related to the residual $B^\mu P^\kappa$ nucleation defect $\mathbf{b}_{0/0}^{iBP}$. The $\mathbf{b}_r^{iBP}$ lies in the $B^\mu P^\kappa$ interface and thus enables the disclination dipole to move with twin boundary if required. Inset A and Inset B corresponds to initial $B^\mu P^\kappa$ length and stable lengths, respectively. Inset A highlights the required twinning disconnection transformation if the disclination dipole is to move normal to its plane, which was not observed in the present simulations.

counteracted by the increase of the DD energy which scales with the facet length square, such that the balanced compromise is reached at a length of $10d_{(0001)\kappa}$.

An important note can be given concerning the Burgers vector of the residual “defect” found by Serra and Bacon [12] upon the interaction of basal slip with the TB producing i number of TDs. This residual “defect”, denoted by $\mathbf{b}_{-(2i-1)/-2i}$ is equal to $-(\mathbf{f}_0^{iBP} + \mathbf{b}_r)$ in our notations, and it is obviously not the correct strength of the defect resulting from the decomposition of the basal dislocation. In fact, Serra and Bacon [12] did not consider the disclination dipole nucleating during the interaction, and as such overlooked its BV content, which entered the equation governing the interfacial reaction. Serra and Bacon [12] did mention that “it was surprising” that the residual “defect” moved with the TB as it does not lie on the “interfacial step”. This “interfacial step” is the $B^\mu P^\kappa$ facet in our terminology. Thus, while the total BV of the “defect” observed by Serra and Bacon [12] is confirmed by our work and equal to the BV of the DD plus the residual dislocation, the fact that they did not decompose it into a DD and a dislocation obstructed the rest of the analysis, leading to some inaccurate conclusions. Namely, the rationale given to explain $i = 3$ upon nucleation of the “interfacial step” is not valid. While $i = 3$ is correct for Ti, which Serra and Bacon [12] studied, a same reasoning would predict $i = 4$ for Mg, while in actuality, $i = 5$ at equilibrium. This is because the energy of the DD is less than an equivalent disconnection. Thus, the facet tends to continue lengthening to decrease the residual dislocation BV at the expense of increasing the DD BV.

On the other hand, our simulations did not show a spontaneous nucleation of TD dipole from either sides of the DD. We did observe this growth mechanism, but at rather a much higher shear stress, in the range of 300 MPa, than that required for the $B^\mu P^\kappa$ nucleation and growth. So the easy propagation of $\{10\bar{1}2\}$ may not be explained by this mechanism as suggested in Serra and Bacon [12].

We emphasize that there are two questions which must be answered to explain the predominance of $\{10\bar{1}2\}$ twinning in HCP metals. The first question is how does this twinning mode overcome slip barriers? In this paper, the simulations showed that $\{10\bar{1}2\}$ TB spontaneously destroys basal slip dislocations by converting them to very short $B^\mu P^\kappa$ facets (along with some minimum shifting of the TB), which we will call here interaction facets. The $B^\mu P^\kappa$ facet finds a way to quickly and readily grow to a stable length. This phenomenon naturally segues to the second question: how could then a serrated TB with a substantial number of interaction BP facets move swiftly in the parent lattice? In other words, what is the fate of TDs once they merge onto a TB- $B^\mu P^\kappa$ interfacial disclination? This question is of important consideration for a realistic growth model even if TDs would to nucleate at the interfacial disclinations, as they would have to overcome neighboring interaction $B^\mu P^\kappa$ facets. Otherwise, one has to unrealistically assume that a TB may only contain a single TB- $B^\mu P^\kappa$ facet.

Figure 5 exhibits simulation results of the behavior of a TD driven to $B^\mu P^\kappa$ facet. The behavior of this TD was such that TB accomplished an adequate propagation from both sides of the $B^\mu P^\kappa$ facet which readily followed the overall motion (Figure 5c). However, before the TD reappeared on the other side of the TB, the BP facet increased in length by a distance of $2d_{(0001)\kappa}$ (Figure 5b).

The fate of a TD encountering a TB- $B^\mu P^\kappa$ facet was recently addressed by the present authors in [28]. Depending on complex energetic consideration defining the sense of wedge disclination motion, the TD can interact in a couple of ways with the facet disclination. If the disclination line prefers to move normal to the facet plane, then the required rotational distortion imposes an addition of a BV content equal to:

Figure 5: Results of molecular dynamics simulations showing the behavior of a $\{10\bar{1}2\}$ twinning disconnection (a) gliding on the twin boundary and meeting a $B^\mu P^\kappa$ facet, (b) where the upper disclination migrated upward upon absorbing the disconnection, and the (c) the lower disclination moved up to restore the stable facet length by releasing a twinning disconnection which continued gliding to the right.

$$\mathbf{f}_2^{1BP} = \begin{pmatrix} 0 \\ \frac{\sqrt{3}(\gamma-\sqrt{3})}{\sqrt{\gamma^2+3}} \\ -\frac{\sqrt{3}(\gamma-\sqrt{3})}{\sqrt{\gamma^2+3}} \end{pmatrix} \quad (12)$$

This distortion can be formally understood in the inset C of the NTP (Figure 4). The facet normal motion requires the white lattice, λ to rotate to the red lattice, κ through $\mathbf{f}_2^{1BP}$. In this case the reaction with $\mathbf{b}_{2/2}^{TB}$ leads to the creation of a new disconnection with a double step height able to synchronize the motion of the TB and $B^\mu P^\kappa$ facet:

$$\mathbf{b}_{2/2}^{BP} = \mathbf{b}_{2/2}^{TB} + \mathbf{f}_2^{1BP} = \begin{pmatrix} 0 \\ \frac{\sqrt{3}\gamma-\gamma^2}{\sqrt{\gamma^2+3}} \\ -\frac{\sqrt{3}(\gamma-\sqrt{3})}{\sqrt{\gamma^2+3}} \end{pmatrix} \quad (13)$$

Although this reaction was observed in the deformation scenario studied in [29], it did not occur in the more realistic case of twin propagation studied in this paper, where the TB encounters slip and the resulting interaction $B^\mu P^\kappa$ facets are bounded by TBs from both sides. Instead, the disclination line at which the TD merged, moved up along the plane of the facet (Figure 5b), requiring an extension of the rotational distortion by $\mathbf{f}_0^{1BP}$ given in Equation 2, and an increase in residual content of BP nucleation by $\mathbf{b}_{0/0}^{1BP}$ given in Equation 6. As the DD separation distance increased beyond the stable threshold, the simulations showed that as soon as the upper disclination moved up, the lower disclination followed by the same rate. This latter motion decreases back the BV content by $\mathbf{f}_0^{1BP}$, so the conservation of the Burgers vector dictates an emission of a $\mathbf{b}_{2/2}^{TB}$ TD given by Equation 10.

Therefore, TDs, regardless of their nucleation site, are able to spontaneously cross over the interaction $B^\mu P^\kappa$ facets and accommodate twin propagation without any problem. Pond et al. [14] first reported this behavior, calling it compensated climb. By newly identifying the action of faceting in this situation, we are able to confirm that the process is actually disconnection transformation and glide on a new interface plane. Figure 6 provides a summary sketch of the entire mechanism of $\{10\bar{1}2\}$ twin propagation in HCP crystals undergoing prior or concurrent slip.

4. Conclusions

Molecular dynamics simulations of interaction between basal slip and $\{10\bar{1}2\}$ twinning in magnesium revealed a complex interfacial reaction which led to the complete absorption of the lattice dislocation in the twin boundary. This absorption consisted in the gradual dissociation of the basal dislocation into a final configuration which can be described by:

1. An interaction disclination dipole with a Burgers vector content $\mathbf{f}_0^{5BP}$ which rotated the white lattice into the red lattice to bring about a $B^\mu P^\kappa$ facet of $5 \times 2d_{(0001)\kappa}$ in length,
2. Emission of a total of nine twinning disconnections, $\mathbf{b}_{2/2}^{TB}$, where four of which mutually annihilated and the remaining five gradually glided away to effectively accommodate the progress of the twin boundary in the parent matrix μ ,

3. A residual defect $\mathbf{b}_r^{5BP}$ which lies on the BP facet, thus glissile should the twin boundary grow in the matrix μ . The residual defect was found to relate to the $\mathbf{b}_{0/0}^{5BP}$ dislocation previously reported by [28, 29]

Importantly, when a TD was motivated to glide and merge on the basal-prismatic facet, it disappears on the first disclination dipole partner but rapidly reappears again on the other side of the second disclination dipole partner, where it continues threading and advancing the twin boundary. This disappearance-reappearance was governed by the extension of the facet as the TD was absorbed by the upper disclination, but the dipole attraction motivates the lower disclination to move up in an effort to keep a stable separation distance of $10d_{(0001)\kappa}$, and thereby releasing back the twinning disconnection. This mechanism is believed to be responsible of the high growth rates uniquely associated with $\{10\bar{1}2\}$ twinning mode in all hexagonal close-packed metals. Furthermore, as can be noted from Figure 6, the interaction faceting enables the twin to adopt a large macroscopic curvature consistent with the experimental observations.

Acknowledgments

Authors are substantially grateful to Professor Surya R. Kalidindi who triggered this work after a fruitful and stimulating discussion with HEK.

References

- [1] El Kadiri, H., Oppedal, A.L.. J Mech Phys Solids 2010;58(4):613–624.
- [2] El Kadiri, H., Kapil, J., Oppedal, A., Hector Jr, L., Agnew, S.R., Cherkaoui, M., et al. Acta Mater 2013;61(10):3549–3563.
- [3] El Kadiri, H., Baird, J., Kapil, J., Oppedal, A., Hector Jr, L., Cherkaoui, M., et al. Int J Plast 2013;44:111–120.
- [4] Oppedal, A.L., El Kadiri, H., Tomé, C.N., Kaschner, G.C., Vogel, S.C., Baird, J.C., et al. Int J Plast 2012;30–31:41–61.
- [5] Oppedal, A., El Kadiri, H., Tomé, C., Vogel, S.C., Horstemeyer, M.. Philosophical Magazine 2013;93(35):4311–4330.
- [6] Ma, Q., El Kadiri, H., Oppedal, A.L., Baird, J.C., Horstemeyer, M.F., Vogel, S.C.. Int J Plast 2012;29:60–76.
- [7] El Kadiri, H., Barrett, C., Tschopp, M.. Acta Mater 2013;61:7646–7659.
- [8] Serra, A., Bacon, D.J., Pond, R.C.. Acta Metall 1988;36:3183–3203.
- [9] Serra, A., Pond, R.C., Bacon, D.J.. Acta Metall Mater 1991;39(7):1469–1480.
- [10] Wang, L., Barabash, R., Bieler, T., Liu, W., Eisenlohr, P.. Metallurgical and Materials Transactions A 2013;44(8):3664–3674.
- [11] Asgari, S., El-Danaf, E., Kalidindi, S.R., Doherty, R.D.. Metall Mater Trans A 1997;28(9):1781–1795.
- [12] Serra, A., Bacon, D.J.. Philos Mag A 1996;73(2):333–343.
- [13] Serra, A., Bacon, D.J., Pond, R.C.. Metall Mater Trans A 2002;33(3):809–812.
- [14] Pond, R., Serra, A., Bacon, D.. Acta Mater 1999;47(5):1441–1453.
- [15] Yoo, M.H.. Trans Met Soc AIME 1969;245:2051–2060.
- [16] Basinski, Z.S., Szczerba, M.S., Niewczas, M., Embury, J.D., Basinski, S.J.. Rev Metall / Cah Inf Tech 1997;94(9):1037–1043.
- [17] Niewczas, M.. In: Nabarro, F.R.N., Hirth, J.P., editors. Dislocations in Solids. Elsevier Science; 2007, p. 263.
- [18] Thompson, N., Millard, D.. Philos Mag 1952;43:422–440.
- [19] Cottrell, A.H., Bilby, B.A.. Philos Mag Series 7 1951;42(329):573–581.
- [20] Lay, S., Nouet, G.. Philosophical Magazine A 1994;70(2):261–275.
- [21] Metallurgical and Materials Transactions A 2014;doi:10.1007/s11661-014-2481-0.
- [22] Scripta Materialia 2014;9091(0):41 – 44.
- [23] Tu, J., Zhang, X., Wang, J., Sun, Q., Liu, Q., Tomé, C.N.. Appl Phys Lett 2013;103(5):051903–051903.
- [24] Li, Y., Chen, Y., Walmsley, J., Mathinsen, R., Dumoulin, S., Roven, H.. Scr Mater 2010;62(7):443 – 446.
- [25] Wang, J., Liu, L., Tomé, C., Mao, S., Gong, S.. Materials Research Letters 2013;1(2):81–88.

- [26] Xu, B., Capolungo, L., Rodney, D.. *Scr Mater* 2013;68(11):901–904.
- [27] Weatherly, G., Perovic, A., Perovic, V.. *Philosophical Magazine A* 1999;79(9):2071–2082.
- [28] Barrett, C.D., El Kadiri, H.. *Acta Materialia* 2014;70:137–161.
- [29] Barrett, C.D., El Kadiri, H.. *Acta Materialia* 2014;63:1–15.
- [30] Serra, A., Bacon, D.J.. *Acta Metall Mater* 1995;43(12):4465–4481.
- [31] Wang, J., Beyerlein, I., Hirth, J.. *Modelling and Simulation in Materials Science and Engineering* 2012;20(2):024001.
- [32] *International Journal of Plasticity* 2014;56(0):156 – 172.
- [33] Plimpton, S.. *J Comput Phys* 1995;117(1):1–19.
- [34] Liu, X., Adams, J., Ercolessi, F., Moriarty, J.. *Modell Simul Mater Sci Eng* 1996;4:293.
- [35] Barnett, D., Lothe, J.. *Journal of Physics F: Metal Physics* 1974;4(10):1618.
- [36] Barnett, D., Lothe, J.. *Journal of physics F: Metal physics* 1974;4(5):671.
- [37] Barrett, C.D., El Kadiri, H.. *Scripta Materialia* 2014;84:15–18.
- [38] Pond, R., Hirth, J.. *Solid State Phys* 1994;47:287–365.
- [39] Nabarro, F.R.. *Theory of crystal dislocations*. Clarendon Pr.; 1967.
- [40] Nabarro, F., Argon, A.. *Physics of strength and plasticity*. 1969.
- [41] Romanov, A., Kolesnikova, A.. *Prog Mater Sci* 2009;54(6):740–769.
- [42] Das, E., Marcinkowski, M., Armstrong, R., De Wit, R.. *Philosophical Magazine* 1973;27(2):369–391.
- [43] Kroupa, F., Lejček, L.. *Solid State Phenomena* 2002;87:1–14.
- [44] Friedel, J., Vassamillet, L.. *Dislocations*; vol. 3. Pergamon Press Oxford; 1964.
- [45] Romanov, A., Vladimirov, V.. *Dislocations in solids* 1992;9:191.