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

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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, thereby enabling the twin boundary to progress through a 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.

Keywords: Twin mobility; Slip–twin interaction; Hexagonal

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 that can 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 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 – the focus of this paper – relates to its ability to grow despite pre-existing and/or concomitant slip.

The first issue is 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 and very simple shuffles [7]. This explanation is somewhat vague because no relationship has been identified between the mobility of a 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 doubt 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 counter-examples can 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.

The second issue essentially lies in the peculiar invulnerability of the $\{10\bar{1}2\}$ twinning mode to concomitant slip and/or pre-existing dislocations. On the one hand, slip has the potential to cause roughness of the 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

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deformation that develops within both the twin and the parent should in principal induce the K_1 plane to rotate away from either side 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 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-grain misorientation may significantly impede further twin nucleation and propagation.

Fig. 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 complete 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 (Fig. 1a). By 6% plastic compression (Fig. 1b), twins have already reached the coalescence stage, and finally, by 9% plastic deformation, they have consumed nearly the entire parent structure (Fig. 1c).

The clear unyielding capabilities of the $\{10\bar{1}2\}$ TB to both 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 [15–17,1], 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 to three TDs, as required by minimization of the residual dislocation. To our knowledge, the first experimental evidence of slip producing TDs on the $\{10\bar{1}2\}$ was reported 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 and molecular dynamics (MD) simulations, [21–27] found that $\{10\bar{1}2\}$, $\{10\bar{1}1\}$, $\{2\bar{1}\bar{1}1\}$ 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 an 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 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, in current terms, would 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 the analysis and glosses over the core structure, while requiring a somewhat awkward explanation of its low-energy formation and movement.
2. In the event that 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, or how these facets would enable the twin to overcome lattice barriers. The present authors have shown through atomistic simulations that a twin facet can nucleate on a BP boundary by relaxation of several of $\mathbf{b}^{BP}_{2/2}$-type disconnections [29]. An analogous scenario could be envisaged 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, using MD simulations, reproduced 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 of 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 [30,13]. 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 morphology. The fact that a dislocation interacting with the $\{10\bar{1}1\}$ twin boundary can only produce a single TD [31,32,12], 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