



Editorial

Deformation twinning in magnesium: the role of phase transformations

Magnesium (Mg) and its alloys have attracted sustained interest as lightweight structural materials due to their extremely low density, high specific strength, and abundance in the Earth's crust. These attributes make Mg alloys particularly appealing for weight-sensitive applications in the automotive and aerospace industries, where reducing mass directly translates into improved fuel efficiency and lower emissions.

Despite these outstanding advantages, widespread adoption of Mg alloys cannot compete with aluminum (Al) or steel. Compared to these metals, Mg shows very poor room-temperature ductility and fracture toughness, strong plastic anisotropy and pronounced tension–compression asymmetry. These properties together translate to limited formability at room temperature and reliability. Since the 2000s, research on Mg has been intensely focused on enhancing the strength and ductility of Mg via alloying, precipitation, and heterostructured microstructures, with much success [1–5].

Mechanical properties like strength and ductility are a consequence of the microscopic mechanisms activated when the material is deformed. The motion of numerous dislocations, called slip, is the dominant carrier of plasticity in most metals and enables deformation without cracking. For cubic structured metals, like steel and Al, slip is the exclusive mechanism. Their ductility and near isotropic plasticity result from 12 to 48 independently oriented slip systems and nearly equivalent strengths (i.e., applied stresses needed to activate them). Mg, on the other hand, belongs to a class of metals called hexagonals, with a hexagonal close-packed (hcp) crystal structure, with a long $\langle c \rangle$ axis and short $\langle a \rangle$ axis. Mg relies on another mechanism, twinning, to accommodate strain along the $\langle c \rangle$ axis. While non-basal slip systems, called pyramidal $\langle c + a \rangle$ slip, can also be used, these slip systems usually cost more energy to activate than twinning.

Deformation twinning is inherently different from dislocation-mediated slip. Slip involves the motion of individual dislocations that shears the crystal without disrupting its order. Twinning not only shears the crystal but disturbs the order, manifesting as a crystallographic reorientation. A

boundary forms between the twinned and original regions of the crystal. There are at least seven twin modes, each with a distinct crystallographic plane and shear direction and providing its own precise amount of shear and lattice reorientation [6]. All twin modes have six variants each and are unidirectional, activated in either $\langle c \rangle$ -axis extension or contraction, but not the other way around. In Mg, experiments show that the most prevalent twin mode is the $\{10\bar{1}2\}\langle 10\bar{1}1 \rangle$ extension twin. When activated it stretches the crystal along the $\langle c \rangle$ axis, by an amount proportional to the size of the twin domain. The crystal is reoriented homogeneously throughout the domain by approximately 86° about the $\langle \bar{1}2\bar{1}0 \rangle$ axis. Contraction twin modes, such as the $\{10\bar{1}1\}\langle 10\bar{1}2 \rangle$ and $\{10\bar{1}3\}\langle 30\bar{3}2 \rangle$ modes, as well as double $\{10\bar{1}1\}$ – $\{10\bar{1}2\}$ twins, are also observed in Mg, particularly when deformed at high stresses and strain rates [7–12]. The unidirectional nature of twin activation causes the undesirable plastic anisotropy in Mg. Twins are also believed to limit ductility. The twinned regions concentrate shear, which can produce stress concentrations in the surrounding material and lead to voids and cracks [13].

Many strategies to enhance formability and ductility in Mg have targeted controlling deformation twinning. Efforts have ranged from suppressing twin nucleation and growth to twin proliferation in the form of 3D interconnected twin networks [14,15]. These approaches comprise ways to *manage* twinning, such as by confinement (fine grain sizes), promoting slip (lowering the barrier for competing pyramidal $\langle c + a \rangle$ slip), or providing obstacles to growth (precipitates) [16–19]. Few studies have even explored exploiting a pseudomorphic transition to the body-centered cubic (bcc) Mg phase, which intrinsically removes the troubling hcp structure [20]. However, much more efficient and effective ways to master deformation twinning in Mg would rely on understanding how twins form in the first place.

While the occurrence of twins is easy to detect in the deformation response or in microscopy, twinning is hard to understand compared to slip. The mechanisms underlying the nucleation and growth of deformation twins in hexagonals, like Mg, have been the subject of decades of theoretical and experimental investigation, and to date, much debate persists on how, when, and where twins form as Mg is being de-

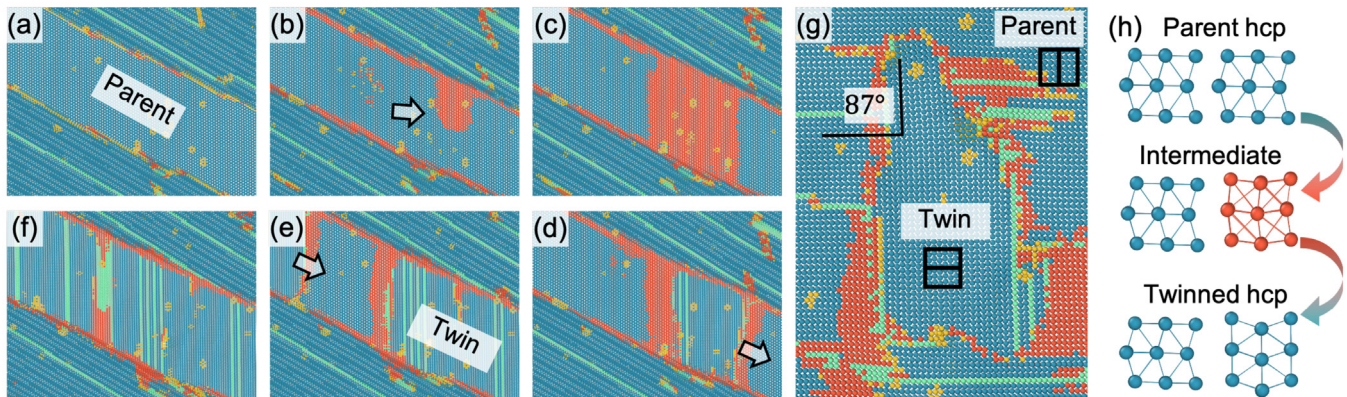


Fig. 1. MD simulation results showing the formation of $\{10\bar{1}2\}$ extension twins through (a, b) hcp-to- distorted bcc phase and (c, d) bcc-to-hcp martensitic phase transformations in Mg. The two formed $\{10\bar{1}2\}$ twin boundaries (e) migrate quickly and (f) react with each other and result in a few layers of fcc phase. (g) A close-up view shows the $\{10\bar{1}2\}$ twin orientation of the newly formed hcp phase with the parent hcp phase: 86° misorientation across a common (a) axis. In panels (a)–(g), hcp, bcc, fcc, and amorphous structured atoms are shown by cyan, red, green, and yellow colors, respectively, and the long lines of green atoms are partial stacking faults. (h) Schematic illustration of the twin formation process [44].

formed. The difficulty stems from the fact that twin nucleation is an atomic-scale and rare event. By the time twins become experimentally detectable, through techniques such as high-resolution transmission electron microscopy (HRTEM) or electron backscatter diffraction (EBSD), they have already nucleated and experienced much growth. The twin mode and variant of that mode have already been selected, obscuring the fundamental processes governing their initial formation.

Dislocation-based models represent a major advance in understanding deformation twinning in Mg. In these models, twin boundaries form and propagate through the collective motion of dislocations, often referred to as twinning dislocations or disconnections, which possess both a Burgers vector and step character [21,22]. This framework has been supported by transmission electron microscopy (TEM) observations of dislocation arrays at twin boundaries and by atomistic simulations revealing the nucleation and glide of disconnections [23–26]. Dislocation-based models explain the thickening of twins, the role of stress concentrations in twin variant selection, and the nucleation via dissociation reactions of slip dislocations into twin embryos or twinning dislocations. Other proposals describe the twin nucleus or embryo formation differently than growth. The boundary of $\{10\bar{1}2\}\langle 10\bar{1}1 \rangle$ twin embryos seen in HRTEM and MD deviate from the theoretical twin/matrix orientation relationship and consist of facets of prismatic or basal plane [27–30]. These observations support a “pure shuffle” theory in which the matrix transformed into an embryonic domain without shearing or dislocations but with transformations between the prismatic and basal planes [27,31]. The concept has been extended to explain embryo growth in grain boundaries and other twin modes [32–34]. However, these models first prescribe or start with a known twin mode.

Challenges remain in explaining twin mode selection, particularly in heterogeneous polycrystalline structures with grain boundaries or complex loading conditions [35,36]. Studies of the crystallography, nucleation sites, and boundaries of

budding twin embryos suggest that local shear was not the driving force, as it is for nucleating dislocations [37–41]. As an alternative twinning mechanism, Bhattacharya et al. proposed that theoretically a two-step martensitic phase transformations can produce a twin in the same way as simple shear [42]. Recent MD simulations revealed the dynamic process of phase-transformation-mediated twinning (PTMT) in Mg [43–45]. Fig. 1 shows snapshots of the transformation pathway for the $\{10\bar{1}2\}\langle 10\bar{1}1 \rangle$ extension twin in Mg. A strain-stabilized, distorted bcc phase initially forms and subsequently transforms into an hcp lattice with a twinned orientation. In support, the intermediate phase, a distorted bcc phase, has been recently observed in Mg alloys by TEM and predicted by density-functional theory [46–48].

Mg does not undergo conventional solid–solid phase transformations and first-principles calculations predict that a bcc phase of Mg only becomes stable under very high pressure (>45 GPa) [49]. Thus, the hcp–distorted bcc–hcp transformation sequence for Mg $\{10\bar{1}2\}$ twinning in Fig. 1 represents a non-equilibrium, transient structural rearrangement that facilitates twin nucleation. Generally, the intermediate phase for the PTMT process is determined by 1) a crystallographic correspondence and 2) energy minimization. Regarding the first, there is a rigorous orientation relationship between the crystallographic planes of the parent, intermediate, and twin phases. Fig. 2 illustrates this relation for the $\{10\bar{1}2\}\langle 10\bar{1}1 \rangle$ extension twin in Mg, where the parent basal plane ($(0001)_{\text{hcp}}$) first transforms into the (100) plane of the bcc phase and then into the twin prismatic plane ($\{10\bar{1}0\}_{\text{twin hcp}}$), while the parent prismatic plane first transforms into the (010) plane and then into the twin basal plane. As a result, the $\{10\bar{1}2\}$ twin plane formed between the parent and twin hcp phases is found to correspond to the $\{110\}$ plane of the bcc phase. For the second criterion, the intermediate phase needs to be an allowable phase for the material at the corresponding thermodynamic or strain/stress conditions; otherwise, the corresponding twinning process cannot occur.

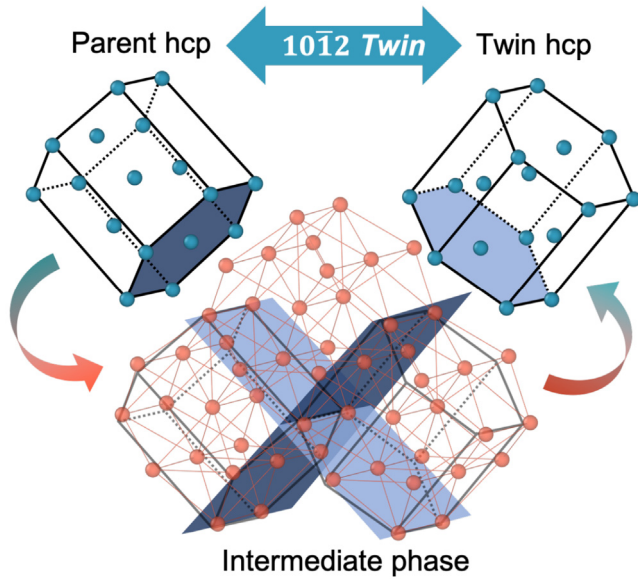


Fig. 2. Orientation relation of the parent hcp phase, metastable bcc phase, and twinned hcp phase. Dark blue represents the parent basal plane and bcc (100) plane, and light blue represents the twin basal plane and bcc (010) plane. The black lines in the intermediate bcc lattice are drawn to show the correspondence with the parent hcp lattice and twin hcp lattice [44].

For $\{10\bar{1}2\}$ twin nucleation, the $\langle a \rangle$ axis of the hcp lattice aligns with the $\langle 100 \rangle$ axis of the intermediate bcc phase, following a Pitsch–Schrader orientation relationship [50,51] for the hcp–bcc phase transformation. The four-fold symmetry of the bcc $\langle 100 \rangle$ axis naturally accounts for the geometry of the extension twin: the 86° misorientation of the $\{10\bar{1}2\}$ twin in Mg closely approximates the 90° rotation associated with this symmetry.

A similar PTMT process has been observed in MD simulations for the high-shear $\{10\bar{1}1\}$ contraction twin in Mg [43]. This mode follows a different orientation relationship: the zone axis of the $\{10\bar{1}1\}$ twin aligns with the $\langle 111 \rangle$ direction of the intermediate bcc phase, following the Burgers orientation relationship [51,52]. The six-fold rotational symmetry of the bcc $\langle 111 \rangle$ axis gives an expected 60° rotation, close to the 56° misorientation of the $\{10\bar{1}1\}$ twin. Ref. [43] further suggests that the high-shear (b4 disconnection) and low-shear (b2 disconnection) $\{10\bar{1}1\}$ modes are strongly connected. In >20 MD simulations using different loading conditions and interatomic potentials, $\{10\bar{1}1\}$ twin nucleation occurred predominantly through the high-shear b2 PTMT pathway, whereas subsequent twin growth often transitioned to the low-shear b4 disconnection mode. Direct nucleation of the low-shear mode was observed only in a case involving free surfaces, more representative of nanodot geometries than bulk materials. Furthermore, the MD simulations in Ref. [43] revealed that during twin growth or boundary migration, the low-shear b4 disconnections are composed of two high-shear b2 disconnections stacked together, with an intermediate bcc-like core. This is analogous to the dissociation of a perfect dislocation in an fcc lattice into two

partial dislocations separated by an hcp stacking-fault region. This analogy remains to be further validated, but it suggests that the high-shear PTMT pathway is not merely exceptional; rather, it may be important for $\{10\bar{1}1\}$ twin nucleation under high-stress or high-strain-rate conditions, consistent with the relative scarcity of this twin mode in experiments.

The PTMT framework is not limited to Mg, but may also extend to other hcp metals. MD simulations have revealed analogous PTMT pathways in titanium (Ti) and zirconium (Zr) for both $\{10\bar{1}2\}\langle 10\bar{1}1 \rangle$ extension twins and $\{10\bar{1}1\}\langle 10\bar{1}2 \rangle$ contraction twins [45,53]. Notably, PTMT also provides a plausible explanation for why $\{11\bar{2}2\}\langle 11\bar{2}\bar{3} \rangle$ contraction twins are absent in Mg, even though they are commonly observed in Ti and Zr. MD simulations show that this twin mode in Ti and Zr nucleates through an hcp– ω –hcp pathway [54]. The intermediate ω phase is stable or metastable in Ti and Zr under relevant conditions, whereas no corresponding ω phase is available in Mg. Consequently, the hcp– ω –hcp path required for $\{11\bar{2}2\}$ twinning is unavailable in Mg, thus disabling this twin mode [55].

Table 1 summarizes the PTMT processes identified in MD simulations to date. For completeness, we note that the phenomenon of PTMT is not restricted to hcp metals [56]. It has also been observed in bcc systems, such as β -Ti alloys and iron (Fe) [57]. These findings suggest that the feasibility of a specific twinning mode is governed by the existence of a viable intermediate phase, as well as the stability of that phase under the prescribed loading direction and thermal conditions.

The transferability of MD-observed PTMT pathways to experimental conditions remains an important open question. MD simulations typically involve much higher strain rates and much smaller simulation domains than real polycrystalline Mg alloys, which contain micrometer-scale grains, grain boundaries, precipitates, solute clusters, and heterogeneous stress fields. These differences may influence the formation, stability, and lifetime of the intermediate phase. In particular, high strain rates and nanoscale dimensions may make the transient intermediate phase more visible in MD simulations by stabilizing it over a larger volume or for a longer time than would be accessible experimentally.

Table 1
Summary of twinning modes via PTMT pathways in MD simulations.

Material	Twinning mode	Path (parent-intermediate-twin)	Temperature
Mg, Ti, Zr	$\{10\bar{1}2\}\langle 10\bar{1}1 \rangle$ extension	hcp– distorted bcc –hcp	N/A
	$\{10\bar{1}1\}\langle 10\bar{1}2 \rangle$ contraction	hcp– distorted bcc –hcp	N/A
Ti, Zr	$\{11\bar{2}2\}\langle 11\bar{2}\bar{3} \rangle$ contraction	hcp– ω –hcp	Low
	$\{10\bar{1}1\}\langle 10\bar{1}2 \rangle$ contraction	hcp– distorted bcc –hcp	High
β -Ti, Fe	$\{112\}\langle 11\bar{1} \rangle$ anti-twinning	bcc–hcp–bcc	Low
	$\{112\}\langle \bar{1}\bar{1}1 \rangle$ twinning	bcc–fcc–bcc	High

This limitation, however, does not necessarily imply that PTMT and conventional disconnection-based twinning descriptions are distinct or competing mechanisms. Rather, they may describe the same twinning process from different perspectives. Both connect the same parent and twinned crystallographic states and produce the same net shear, shuffle, and twinning elements. Indeed, MD simulations and previous studies of $\{11\bar{2}2\}$ twinning in Ti [58], where twin growth is mediated by disconnections whose cores adopt the ω phase, suggest that phase transformation and disconnection formation can be intrinsically linked. During PTMT, the intermediate phase forms locally, and disconnections naturally emerge at the interface between the intermediate phase and the parent hcp lattice. In this sense, disconnections may be viewed as an interfacial manifestation, or natural consequence, of the underlying phase-transformation pathway rather than as evidence for a separate mechanism.

An analogy can be drawn to stacking faults and deformation twinning in fcc metals. Small grain sizes and high strain rates can make extended stacking faults more prominent, even in metals with intermediate or relatively high stacking-fault energies. However, whether the stacking fault is narrow or extended, it remains part of the same extended-dislocation framework. Similarly, PTMT may reveal the transient atomistic structure underlying a twinning process that appears experimentally as disconnection-mediated nucleation or growth.

The PTMT concept provides explanations for several longstanding experimental questions. It naturally accounts for the extremely rapid kinetics of twin nucleation, often occurring on sub-microsecond timescales, since martensitic transformations proceed much faster than thermally activated dislocation processes. The PTMT mechanism also explains the temperature dependence of twinning modes. In Ti and Zr for instance, $\{11\bar{2}2\}$ twinning, via hcp- ω -hcp transformations, only occurs at low temperature because ω -Ti is a high-pressure/low-temperature phase. In contrast, the $\{10\bar{1}1\}$ twin, which forms via hcp-bcc-hcp transformations, only occurs at high temperature because its intermediate bcc phase is a high-temperature phase in Ti. More broadly, the absence of certain twinning modes in specific hexagonal metals may reflect the lack of a viable intermediate phase or transformation pathway, as discussed above for the absence of $\{11\bar{2}2\}$ contraction twins in Mg despite their occurrence in Ti and Zr.

More generally, the PTMT framework may provide a predictive route for identifying possible twinning pathways. A PTMT pathway is likely to be feasible when an intermediate phase satisfies three conditions: it crystallographically connects the parent and twinned lattices, it is energetically accessible under the relevant local stress, strain, temperature, or chemical environment, and the kinetic barrier for the parent-intermediate-twin transformation is sufficiently low during deformation. This perspective helps rationalize several known observations as discussed earlier in this editorial. Correspondingly, identifying metastable phases that satisfy crystallographic, energetic, and kinetic requirements may provide a useful strategy for predicting and controlling twinning modes.

Conventional strategies for suppressing twinning, such as grain refinement, alloying additions, and precipitate addition, can also be reinterpreted within the PTMT framework. In addition to increasing the apparent nucleation stress, hindering disconnection glide, or impeding twin-boundary motion, solute atoms may suppress twinning by altering the local thermodynamic and kinetic conditions required for the intermediate phase to form [15,59]. Further, at a higher, micro-length scale, the constraints on the twin shear provided by neighboring grains and stiffer precipitates can limit expansion of the twin domain or twin “thickening” [60,61]. This effect has been used to rationalize the critical embryo size or can lead to a grain size effect on twinning [32,62]. While the PTMT concept does not change the characteristic twin shear fundamental to these explanations, it identifies an essential intermediate transformation strain. Grain boundaries and precipitate/matrix interfaces may disrupt the crystallographic correspondence needed for the hcp-intermediate-hcp pathway, relax the transformation strain, and destabilize the intermediate structure. These viewpoints suggest additional alloy-design strategies: solute additions or precipitate/matrix interfaces could be selected not only to obstruct disconnection glide, but also to disrupt the relevant intermediate phase or increase the kinetic barrier for its formation.

Despite these potentially detectable signatures, PTMT in Mg still requires further experimental validation. However, recent experimental studies increasingly support this twinning mechanism in other hcp metals. HRTEM and STEM observations of deformed Ti have revealed residual ω -phase embryos [63] or ω -like structural units [58] at $\{11\bar{2}2\}$ twin boundaries and twin tips. These observations are consistent with the PTMT picture, in which the ω and α'' phase forms transiently during twinning and may, in some cases, become kinetically trapped at twin boundaries or twin tips. Alloying may further stabilize such metastable structures, as demonstrated in metastable bcc alloys, making retained intermediate phases more experimentally detectable. These residual phases are difficult to explain using a purely dislocation-based model but can be naturally rationalized from a phase-transformation-mediated perspective.

Several challenges remain before PTMT can be fully validated as a general twinning mechanism. First, the picosecond and nanometer-scale nature of PTMT observed in MD simulations makes direct observation difficult, even using state-of-the-art HRTEM or ultrafast X-ray/neutron diffraction techniques. Second, the strain rates accessible to MD simulations are orders of magnitude higher than those in most experiments, and the strain-rate dependence of PTMT remains unclear. Third, most atomistic simulations use single-crystal or bicrystal cells only tens of nanometers in size, whereas real polycrystals contain micrometer-scale grains, grain boundaries, precipitates, solute clusters, and heterogeneous stress fields. These features may promote PTMT by creating local stress concentrations and favorable nucleation sites, or suppress it by relaxing transformation strain, disrupting crystallographic correspondence, or destabilizing the intermediate phase. Thus, while MD simulations establish the atomic fea-

sibility of PTMT, its prevalence in real polycrystals and at practical strain rates remains an open question.

In summary, the phase transformation-mediated viewpoint has the potential to unify deformation twinning, martensitic phase transformations, and twinning disconnections within a single physical framework. By recognizing that lattice transformations can occur at the nanoscale during twinning, this mechanism provides a coherent explanation for twin nucleation kinetics, mode selectivity, and observed metastable phases in deformed hcp metals. Continued advances in in-situ characterization, high-fidelity simulations, and integrated multiscale modeling are expected to play a crucial role in developing a more unified understanding of twinning, ultimately enabling the design of Mg alloys with improved ductility, reduced anisotropy, and enhanced structural reliability.

Declaration of competing interest

Irene J. Beyerlein is an editorial board member for the Journal of Magnesium and Alloys and was not involved in the editorial review or the decision to publish this article. All authors declare that there are no competing interests.

CRediT authorship contribution statement

Lei Cao: Writing – original draft, Visualization, Formal analysis, Conceptualization. **Irene J. Beyerlein:** Writing – original draft, Project administration, Funding acquisition, Conceptualization.

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