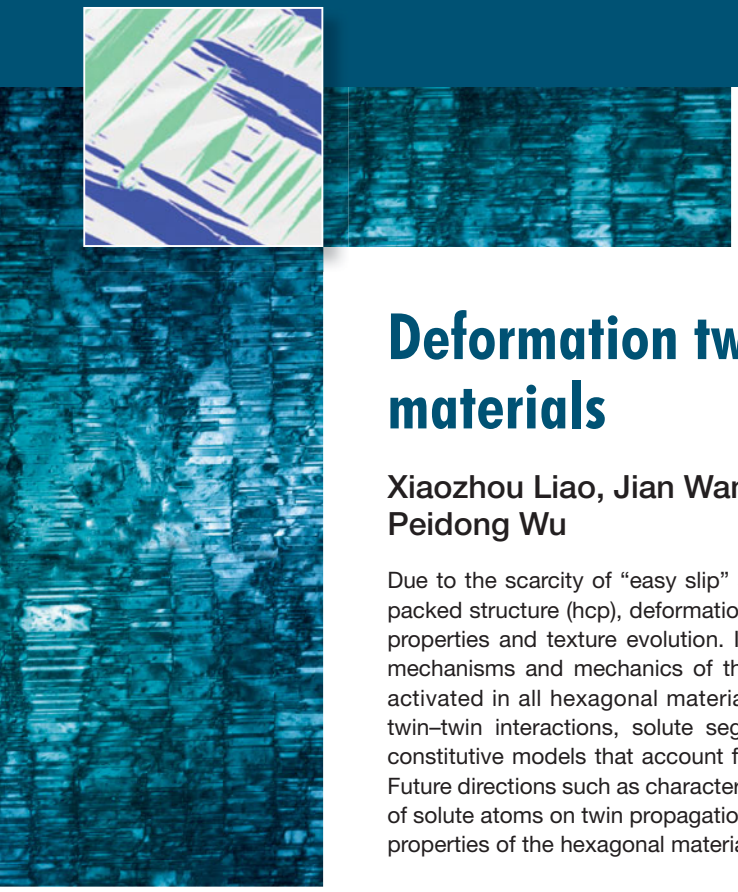


Deformation twinning in hexagonal materials

Xiaozhou Liao, Jian Wang, Jianfeng Nie, Yanyao Jiang, and Peidong Wu

Due to the scarcity of "easy slip" systems in hexagonal materials with a hexagonal close-packed structure (hcp), deformation twinning plays a crucial role in determining mechanical properties and texture evolution. In this article, we highlight the current understanding of mechanisms and mechanics of the twinning system $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$, which is commonly activated in all hexagonal materials for nucleation and propagation of deformation twins, twin–twin interactions, solute segregation at twin boundaries, and the development of constitutive models that account for the fundamental mechanisms of twinning/detwinning. Future directions such as characterizing the three-dimensional shapes of twins, the influence of solute atoms on twin propagation, and the influence of twin–twin junctions on mechanical properties of the hexagonal materials are discussed.

Introduction

Materials such as Mg, Zr, and Ti with a hexagonal close-packed (hcp) structure are used in automotive, nuclear, aeronautic, and defense technologies, among others.[1] The basic plasticity mechanisms associated with hcp structures are slip and twinning. The easiest dislocation slip is along the $\langle 11\bar{2}0\rangle$ close-packed directions on the (0001) basal plane or $\{10\bar{1}0\}$ prismatic planes.[2,3] These dislocations, however, do not generate deformation along the *c*-axis. The alternative mechanisms available for doing so are $\langle c+a\rangle$ slip on $\{10\bar{1}1\}$ pyramidal planes, tensile twins, or compressive twins where the twin planes vary with the material.[3] The activation of pyramidal slip requires a higher critical resolved shear stress than that of the basal and prismatic slip. Thus, $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning, which has a critical resolved shear stress close to the basal slip, is an important mode for accommodating strain along the *c*-axis.[4] The localized shear associated with twinning is partly the reason for the poor ductility and low deformability of Mg alloys.[4] The current emphasis for advancing applications of hexagonal materials is to improve deformability while preserving a high flow strength. The fundamental principle is to adjust the relative activity among slip and twinning systems.[5] Therefore, an in-depth understanding of mechanisms and mechanics of deformation twinning in hexagonal materials is essential.

Twinning in hexagonal materials is directional with a unique shear direction. Correspondingly, several specific characteristics are associated with hexagonal materials: (1) Rolled hexagonal metal plates exhibit a characteristic texture component with the crystal *c*-axis (the basal pole) preferentially aligned along the normal direction of the plates. (2) The flow-stress evolution shows strong anisotropy between the in-plane and through-thickness directions. (3) The in-plane flow stress is very different in tension from that in compression. Accompanying the reorientation of most grains by twinning, the aggregate shows an increase in hardening rate and continuous evolution of grain microstructure with deformation.

Twin shear localizes in a defined domain of a grain. Twin nucleation in hexagonal materials is driven by local stress states and local atomistic configurations at grain boundaries (GBs).[6,7] Twin growth, including propagation and thickening, is driven by long-range stress states across grains through the motion of twin boundaries (TBs), either by the gliding of twinning dislocations on the twin plane along the twinning direction (propagation) or migration of TBs normal to the twin plane (thickening) via nucleation and gliding of twinning dislocations on the twin plane. This motivated the study of structural characteristics of TBs and the pinning effect of solute atoms on the migration of TBs.[8] Corresponding to the

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crystallography of hexagonal structures, twin variants on different twin planes nucleate and grow during deformation. These twin variants interact and react with each other, forming twin–twin junctions that influence twin propagation and thickening during loading, as well as detwinning and nucleation of secondary twins during unloading.[9] For a comprehensive understanding of nucleation and growth of twins, and twin–twin interactions, atomic-level characterization of the structures of TBs and twin–twin junctions and their influence on mechanical properties at the micro- and mesoscales are essential.

In this article, we highlight the current understanding of the mechanisms and mechanics associated with the twinning system $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$, which is commonly activated in all hexagonal materials. Discussions are concentrated on the nucleation and growth of deformation twins, twin–twin interactions, solute segregation at TBs, and the development of constitutive models that account for the fundamental mechanisms of twinning/detwinning.

Nucleation and propagation of deformation twins

Recent studies of twin nucleation in hexagonal metals using topological analysis, molecular static/dynamics, and density functional theory (DFT) show that a twin nucleus must consist of multiple atomic layers for it to be stable.[10] Twinning dislocations can only glide on preexisting TB planes and are always accompanied by atomic-shuffle accommodation. Two important conclusions from these studies can be reached: (1) The traditional pole mechanism based on the gliding of a single twinning dislocation is not feasible for twin nucleation in hexagonal metals, because a single twinning dislocation does not exist alone in a perfect hcp structure; and (2) homogeneous nucleation of twins inside a grain is energetically and kinetically difficult, because it involves a zonal dislocation with multiple atomic layers. Extensive experimental electron backscatter diffraction data support the notion that twins always start at GBs.[11]

These results motivated the investigation of the relationship between twin nucleation and GBs. Molecular dynamics simulations show that low-angle symmetrical tilt GBs favor twin nucleation when lattice dislocations approach the GBs.[12,13] The Burgers vectors of GB dislocations within symmetrical tilt GBs are larger than that of the zonal twinning dislocation, and can potentially react with incoming lattice dislocations or dissociate into partials to produce the defects needed for a stable twin nucleus formation (**Figure 1**a). Most importantly, twin nucleation was characterized as a pure-shuffle mechanism: a 90° rotation about the zone axis by atomic shuffling or atoms in a prismatic plane in the matrix transforming into a basal plane in the twin (Figure 1b).[14,15] Correspondingly, the prism plane in the parent is nearly parallel to the basal plane in the twin (the prism-basal boundary is called PB), or the basal plane in the parent is nearly parallel to the prism plane in the twin, in which case the basal-prism boundary (BP) results.[15,16] This mechanism deviates from the classic dislocation-based nucleation mechanisms. Thus, a twin nucleus in hexagonal materials is surrounded by the PB and BP interfaces instead of conventional coherent TBs (CTBs). This crystallographic feature was confirmed in recent high-resolution transmission electron microscopy (TEM) observations (Figure 1c).[17,18]

The finding of PB and BP interfaces inspired researchers to revisit twin growth. High-resolution TEM analysis of TBs in hexagonal materials showed that TBs are serrated and composed of both CTB, PB, and BP boundaries (Figure 1d).[16,19] Atomistic simulations further demonstrated that coherent PB and BP boundaries are energetically stable, and their formation is associated with the pileup of twinning dislocations. It has been concluded that the propagation and thickening of

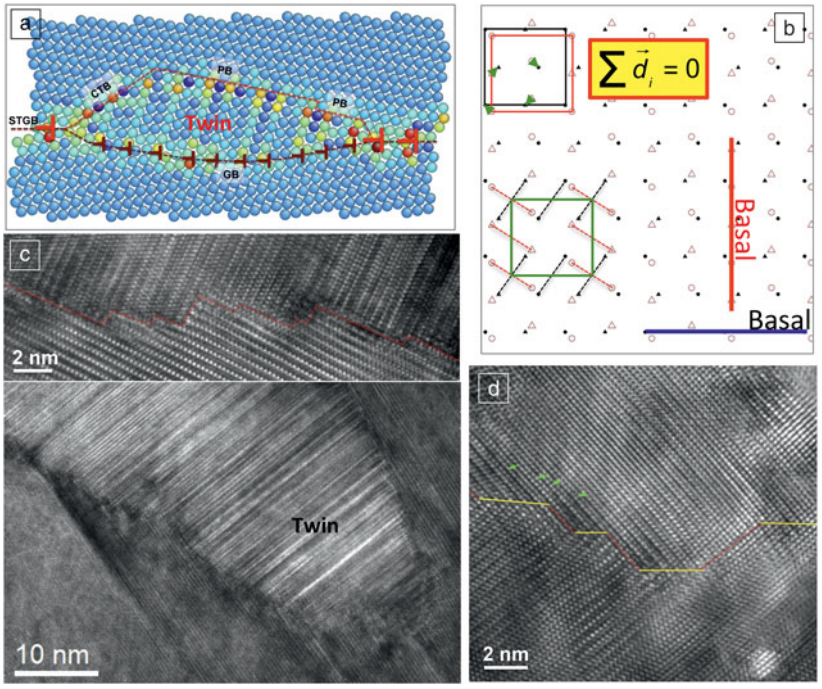


Figure 1. (a) Atomistic structure of a twin nucleus nucleated at a symmetrical tilt grain boundary (STGB) and outlined by coherent twin boundary (CTB) and prismatic-basal boundaries (PBs).[16] (b) Dichromatic complex of twin (red symbols) and matrix (black symbols) in Mg showing the pure-shuffle nucleation mechanism.[18] The green square indicates the coincidence lattices of the twin and matrix crystals. The red and black squares outline the real crystals. The green arrows show the displacements associated with the pure-shuffle nucleation. (c) A transmission electron microscope (TEM) image of a small twin showing that the twin is surrounded by PBs and basal-prism boundaries (BPs), as magnified at the top of (c). The red solid lines indicate PBs and BPs. Reprinted with permission from Reference 17. © 2012 Macmillan Publishers Ltd. (d) A TEM image of twin boundaries of a large twin consisting of CTBs (yellow lines) and PBs and BPs (red lines).[18] The green arrows in (d) indicate stacking faults of basal planes.

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twins involve the motion of twinning dislocations, PB, and BP boundaries.[16,19–21] The motion of PB and BP boundaries can be accomplished through either collective gliding of twinning dislocations or transformation between basal and prism planes that dictate the overall twin mobility.[16] Under some circumstances, the migration of BP and PB boundaries can dominate twin growth,[22,23] resulting in significant deviations of the TB away from the $\{10\bar{1}2\}$ plane.[17,22,23]

Crystal plasticity-based modeling of twinning

Crystal plasticity-based approaches for modeling the constitutive behavior of textured hexagonal alloys have proliferated over the past decade or so. Early materials models considered slip as the major plastic deformation mechanism.[24] Simulation models, including twinning for hexagonal materials, have been developed to mainly describe the reorientation and hardening evolution associated with twinning under monotonic loading conditions.[25–28] The crux of the problem has involved correctly accounting for the behavior of twinning and detwinning (TDT) mechanisms: twin nucleation and twin growth.

Twin nucleation is empirically treated in these simulation models by introducing a small twin volume when the resolved shear stress on the twin plane exceeds a critical level. More importantly, these models do not account for the statistical nature of twin nucleation. Commonly used criteria for constitutive models lead to significant discrepancy between modeling results and experimental observations.[29]

To improve the predictive capability of the models, a probability model[30] for twin nucleation was recently developed with inspiration from atomistic simulations of dislocation-GB interactions.[13,14] In this nucleation model,[30] twins originate from statistical distributions of GB dislocations that may vary in spacing, Burgers vector, and line direction. A stochastic Poisson process describes the number of GB dislocations, and the rate of this process increases with both local stress and GB area. As either factor increases, the rate of nucleation increases. Nucleation occurs when the local resolved shear stress on a given twin variant exceeds the statistically assigned nucleation threshold stress. In this way, for a bulk polycrystalline hexagonal material under a prescribed loading condition, the nucleation model dictates when nucleation occurs, in which grains, with which variant, and the number of twins.[30] Unlike nucleation, subsequent growth of the twin variants is assumed to be deterministic and is treated by a separate model, such as the visco-plastic self-consistent model[26] or the elastic visco-plastic self-consistent (EVPSC) model.[31]

Recently, it was shown that the EVPSC model, with the TDT description,[32–34] is able to simulate TDT in hexagonal materials and capture key macroscopic features observed experimentally in rolled plates,[35] extruded cylinders,[36] and extruded plates.[37] The TDT model assumes that a grain has four potential operations associated with TDT (**Figure 2**): twin nucleation, twin growth, twin shrinkage, and retwinning. Twin nucleation and twin growth increase the twin volume fraction, corresponding to twinning. Twin shrinkage decreases the twin volume fraction, corresponding to detwinning. Retwinning splits the twin band through detwinning or secondary twinning, decreasing the volume fraction of the original twin variant while increasing the volume fraction of the other twin variant.

It is important to point out that the EVPSC-TDT model considers a twin as a new grain. The orientation of the new grain is initially related to that of the parent through the crystallographic–twin relationship, which reorients the *c*-axis by 86.3° under extension twinning. However, it is worth mentioning that the twin only "interacts" with its parent during subsequent straining steps. Furthermore, there is no special enforcement equilibrium or compatibility between the twin and the parent. Rather, the twin and the parent are forced to satisfy equilibrium and compatibility with the homogeneous equivalent medium that surrounds each of them.

More specifically, the TDT model is designed to enforce a sort of pseudo-TB between the twin and its parent grain. The crystallographic lattices for the parent grain and the twin are mirrored across the TB. If an applied stress drives the migration of the pseudo-TB into the parent via the gliding of twinning dislocations, it increases the twin volume fraction. Conversely, if the pseudo-TB moves into the twin by the reverse gliding of the twinning dislocations, it decreases the twin volume fraction.[33] Very recently, a new twin nucleation, propagation, and growth (TNPG) model for hexagonal materials has been developed.[38] This TNPG model explicitly takes into account the stress relaxation associated with twin initiation and propagation. It has been rationalized that the stress relaxation drives a just-nucleated twin to propagate, while work hardening makes the twin grow after its propagation.

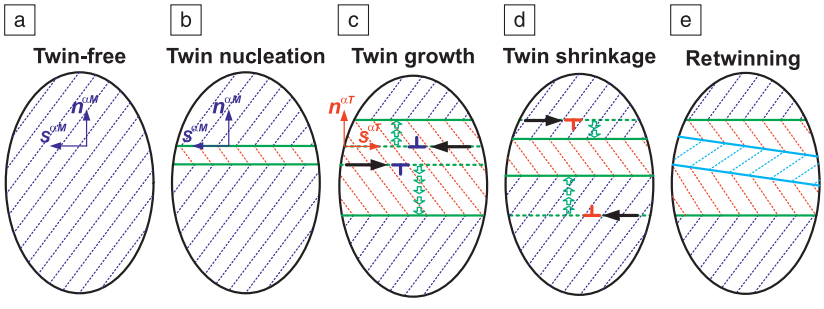


Figure 2. Schematic representation of twinning and detwinning in a grain. (a) The twin-free grain (matrix). (b) Twin nucleation. Solid green lines represent twin boundaries (TBs). Lattices in the matrix and twin are represented by dotted blue lines and dotted red lines, respectively. (c) Twin growth through the nucleation and glide of twinning dislocations on the TBs in the matrix. (d) Twin shrinkage through the nucleation and glide of twinning dislocations on the TBs within the twin. (e) Retwinning. Introduction of a twin variant in a twinned grain.[33] The symbol "⊥" represents twinning dislocation.

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Twin–twin junctions

When twin variants interact, twin–twin boundaries (TTBs) form that subsequently affect TDT processes.[39–44] Twin–twin interactions are classified as Type I for two twin variants sharing the same $\langle 11\bar{2}0 \rangle$ zone axis and as Type II for two twins with different zone axes (**Figure 3**a).[44]

Three kinds of twin–twin structures have been identified in hcp materials:[44] a quilted-looking twin structure consisting of twins arrested at other TBs (Figure 3b), an "apparent crossing" twin structure that links twins impinging independently on each side of twin lamella (Figure 3c), and a double twin structure that results from secondary twinning at twin–twin interfaces, such as T_{62} from "apparent crossing" T_6 and T_2 twin junctions (Figure 3d). For Type I twin–twin interactions, one twin does not transmit across the TB and into the other twin. For Type II twin–twin interactions, one twin can transmit into the other under some special loading conditions. In most cases, twin transmission does not occur. Instead, TTBs form that contain boundary dislocations. For Type I twin–twin interactions, the TTB is a low-angle tilt boundary with the habit plane being either the basal or a prismatic plane.[43] For Type II twin–twin interactions, the TTB is a high-index crystallographic plane.[44] TTB dislocations can be inferred by the interaction of twinning dislocations associated with the two twin variants. An "apparent crossing" twin structure is thus a consequence of TTB formation.[44]

Once TTBs have formed, twinning dislocations associated with the incoming twin are blocked at the TB and form boundary dislocations. Back stresses resulting from the pileup of these boundary dislocations hinder the motion of twinning dislocations toward the TTB, producing a strong repulsive force near the TTB. Further growth and propagation of twins requires a high stress, resulting in strain hardening during twinning. Under reversed loading, detwinning may occur as a reversal of the forming process.

For interacting twins, TTB dislocations can dissociate into twinning dislocations that glide on the twinning plane, resulting in a decrease in the twin thickness. However, the dissociation is an energetically unfavorable process, therefore, detwinning becomes more difficult with increasing loading cycles because more TTBs form that hinder detwinning.[44] This is consistent with experimental measurements.[9] More interestingly, secondary twins can propagate from TTBs through two mechanisms:[44] (1) secondary twins leading to "detwinning from inside"; and (2) secondary twins where the secondary twin plane intersects with the primary twin plane along the same intersection line, as observed in Figure 3d.

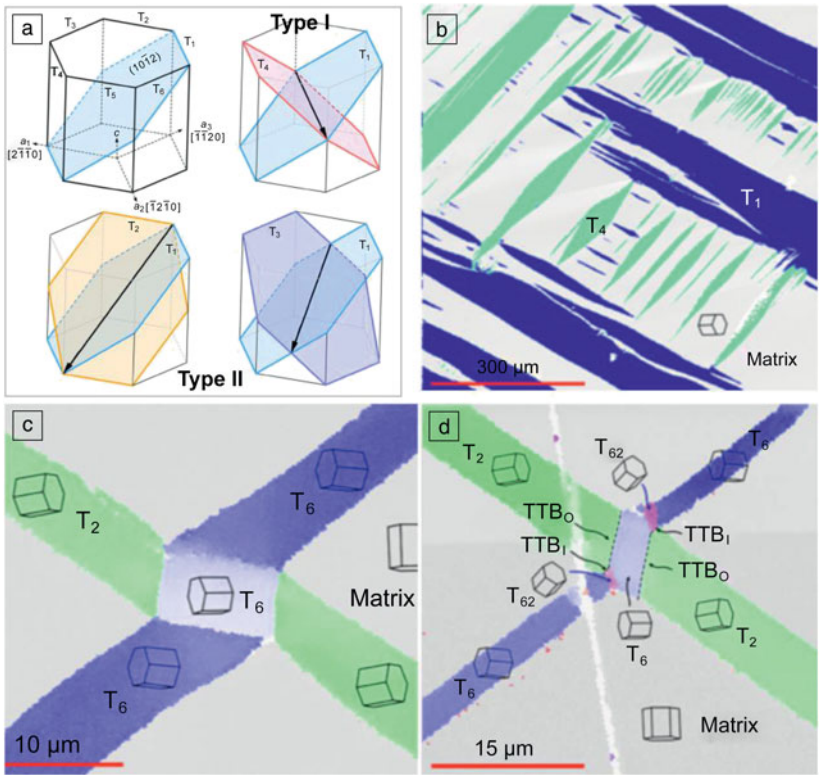


Figure 3. (a) Six $\{10\bar{1}2\}\langle\bar{1}011\rangle$ twin variants T_i (i = 1 to 6) in a hexagonal close-packed structure can form three crystallographically different types of twin–twin interactions: Type I twin–twin pair $T_4 \longleftrightarrow T_1$ with the intersection line along $[\bar{1}2\bar{1}0]$, and Type II twin–twin interaction $T_2 \longleftrightarrow T_1$ with the intersection along $[\bar{2}\bar{2}43]$ and twin–twin interaction $T_3 \longleftrightarrow T_1$ with the intersection line along $[0\bar{2}21]$. (b) Quilted-looking twin–twin junctions, (c) "apparent crossing" twin–twin junctions $T_6 \longleftrightarrow T_2$, and (d) formation of secondary twins T_{62} from "apparent crossing" T_6 and T_2 twin junctions.[44] Note: TTB, twin–twin boundary.

Solute segregation in fully CTBs and annealing strengthening

Over the past decade, considerable efforts have been made to impede the growth of deformation twins by changing the orientation and dimensions of Mg grains or by introducing secondary phase particles. Rare-earth elements are found to be effective in weakening the basal texture of Mg alloys after extrusion to make deformation twinning more difficult to occur upon compression loading along the extrusion direction.

A large number of studies have been conducted to understand the interaction between solute atoms and the motion of dislocations at the atomic level.[45,46] In addition, the pinning effect of solute atoms on TBs has recently attracted considerable attention.[5,8]

Two types of TBs have been recently recognized for $\{10\bar{1}2\}$ twins: CTBs, and the BP and PB boundaries.[15,16] It has been suggested that the CTBs are responsible for twin propagation and growth, which involve gliding of twinning dislocations. BP and PB boundaries, on the other hand, are involved in twin nucleation via a pure-shuffle nucleation mechanism and in twin growth via the migration of the BP and PB boundaries. These TBs have distinctive

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structures that may lead to different solubility of solute atoms. The CTB shares atoms at regular intervals wherein A and B sites have different excess volumes (negative in A site and positive in B site),[5] as shown in **Figure 4**a. In addition, due to their crystallography, a BP or PB boundary experiences a normal stress (compression or tension) when a CTB is subjected to a shear stress associated with twinning.[5] This difference in stress state may further change solubility of solute atoms among TBs and, in turn, change the distribution of solute atoms at TBs.[5]

Nie et al. discovered periodic segregation of solute atoms at CTBs (Figure 4b) using scanning TEM (STEM).[8] DFT calculations provided further insights into understanding solubility of 24 solute atoms along CTB (Figure 4c).[5] The solute atoms with the greater radius than Mg atom are preferred at the B site, while solute atoms with the smaller radius than Mg atom are preferred at the A site, corresponding to the excess volume at A and B sites.[5] The distributed solute atoms along TBs have been demonstrated experimentally to suppress twin growth and strengthen the materials.[8] These phenomena are anomalous and intriguing, because it is commonly accepted in the field of physical metallurgy that solute atoms do not segregate to fully CTBs, and annealing makes alloys softer. The segregation of solute atoms in TBs provide vital clues to the development of Mg extrusion alloys with further increased compression yield strength by suppressing/retarding twin growth.

Future directions

Twins are sheared domains in a matrix. Naturally, they have a three-dimensional shape. However, twins are generally viewed as two-dimensional (2D) domains that propagate along the twin shear direction and grow perpendicular to the twin plane. Most of the substantial work performed in recent decades on twins have regarded twins as 2D entities, and have concentrated on the motion and structure of the twin profile along the twinning direction as if twins were straight infinite entities in the third dimension. Clearly, the mobility of the lateral twin–parent interface has to play a role in the lateral propagation of the twin, and has to depend strongly on the configuration of the interface.

Understanding the crystallographic character of the lateral twin–parent interface of deformation twins will advance our understanding of physical mechanisms of twinning and promote further studies on twin propagation/growth.

Regarding the pinning effect of solute atoms on TBs, STEM images show periodic segregation of solute atoms in CTBs in Mg alloys. The pinning effect of solute atoms on TBs was demonstrated during mechanical loading. However, it is not clear how solute atoms affect the motion of CTBs, PBs, and BPs. For example, because the motion of CTBs is accomplished through the glide of twinning dislocations, the pinning effect could be ascribed to the increase in the friction force associated with the gliding of twinning dislocations, or to the increase in the energy barrier to the nucleation of twinning dislocations along the CTBs. In addition, twin–twin junctions form when multiple twins interact with each other.

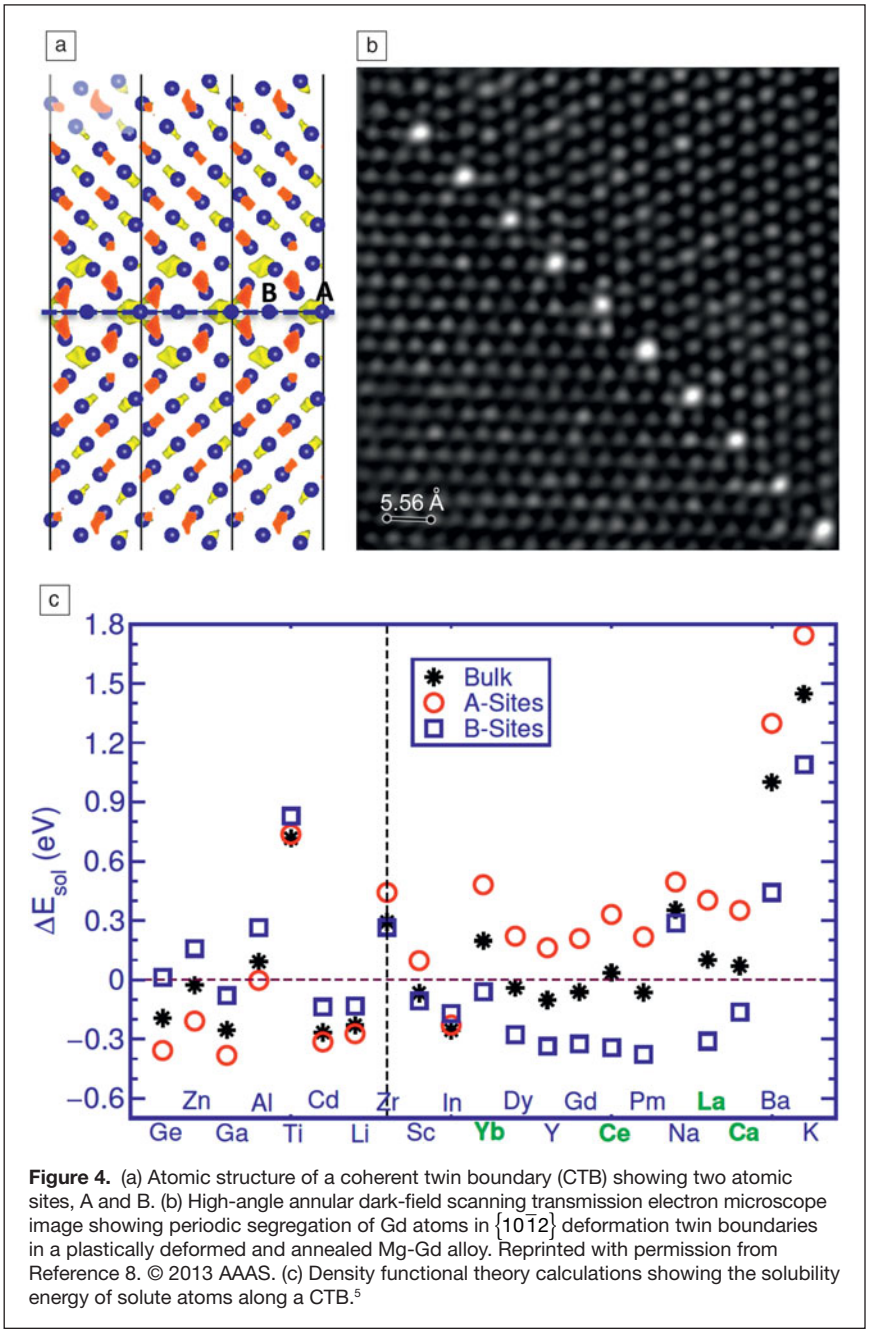


Figure 4. (a) Atomic structure of a coherent twin boundary (CTB) showing two atomic sites, A and B. (b) High-angle annular dark-field scanning transmission electron microscope image showing periodic segregation of Gd atoms in $\{10\bar{1}2\}$ deformation twin boundaries in a plastically deformed and annealed Mg-Gd alloy. Reprinted with permission from Reference 8. © 2013 AAAS. (c) Density functional theory calculations showing the solubility energy of solute atoms along a CTB.[5]

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Solute atoms can segregate to these junctions, strengthening the pinning effect on detwinning. However, atomic structures of twin–twin junctions have not been characterized yet, and the pinning strength of twin–twin junctions has not been experimentally accessed.

Finally, crystal plasticity-based approaches have been developed and demonstrated to be capable of modeling the constitutive behavior of textured hexagonal alloys under monotonic loading, strain path changes, or repeated loading for only a few cycles. With increasing loading cycles, twin–twin junctions form, and they have been shown to play a crucial role in increasing strain hardening and controlling microstructural evolution. A quantitative description of twin–twin interactions and twin–twin junctions is still a challenge in developing meso-/macroscale materials modeling tools.

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