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REPORT



Incoherent tilt grain boundaries stabilized by stacking faults and solute-cluster segregation: a case-study of an Mg-Gd alloy

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ABSTRACT

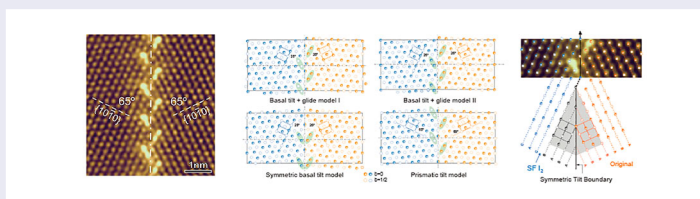
Despite their wide presence in hcp metals, incoherent tilt grain boundaries (ITGBs) are rarely studied. In this work, first-principles calculations were combined with atomic-resolution HAADF-STEM analyses to investigate the structure and formation of one special type ITGB in an Mg-Gd alloy featured with a unique Gd-rich cluster segregation pattern. Our results suggested this ITGB as a mirror-glide boundary formed by gliding the atoms along $[20\bar{2}1]$ of a $\{10\bar{1}4\} <20\bar{2}1>$ coherent twin boundary due to its interaction with stacking faults. The ITGB can be further stabilized by partial-column Gd substitution, leading to the observed unique segregation pattern.

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KEYWORDS

Mg; grain boundary; stacking fault; segregation; density functional theory



IMPACT STATEMENT

A strategy of combining first-principles calculations with atomic-resolution HAADF-STEM has been developed and showed great promises for interpreting complex ITGB structures with solute-cluster segregation in hcp crystals.

Introduction

Grain boundaries (GBs), as a major microstructure feature, play important roles in the functions and performances of polycrystalline metals [1]. Twin boundaries (TBs), as a special type of GBs, have attracted the most attention, especially for metals with low or medium stacking-fault energies. Twins can be induced through the nucleation of faulted layers during vapor deposition [2], solidification [3], or annealing recrystallization [4]. For metals with insufficient independent slip systems, such as hcp Mg, Zr, and Ti, twinning can also occur as a deformation mode, and even turn grains to a slip favored orientation [5]. Experiment evidence also exists indicating that pinning coherent twin boundaries (CTBs) with solutes may cause additional strengthening and toughening in Mg-Gd and Mg-Zn alloys after deformation

and subsequent annealing [6]. In contrast to the considerable attention on CTBs [7–11] where the twin lattice is a mirror reflection of the parent lattice, incoherent tilt grain boundaries (ITGBs) in hcp twin variants have received little attention. Previous studies of ITGBs have been mostly limited to theoretical approaches and to *fcc* metals such as Cu and Al [12, 13] and some specific oxides including SrTiO₃ [14] and α -Al₂O₃ [15]. Only very a few studies have been reported for ITGBs in *hcp* metals, and nevertheless, have been largely restricted to $<1\bar{1}00>$ twin variants using molecular dynamics. One of them suggested that $\{11\bar{2}1\}$ and $\{11\bar{2}3\}$ ITGBs could form more preferentially than their counterpart CTBs in *hcp* Mg and Ti [16]. This is seemingly surprising and anti-intuitive, owing to the obviously lower symmetry of ITGBs than CTBs. The relative stability between ITGBs

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and CTBs thus becomes both intricate and fascinating in its origin and function. It is also doubted if segregated solutes could influence the stability of ITGBs, as much as previously manifested for CTBs in Ref. [6,17]. The biggest challenge to these puzzles is the experimental analytical difficulty to solve accurately the low-symmetry ITGB structures. Atomic-level understanding of ITGB structures and the relevant behaviors and mechanisms is highly desired in this respect.

Results and discussion

Recently, we have reported a series of ITGBs around $\langle 1\bar{2}10 \rangle$ in a Mg-0.2 at.%Gd alloy. Fabrication and heat treatment history of this alloy shall be referred to one our pervious study [18]. Unique segregation patterns of Gd atoms were often associated with these ITGBs. As a representative example, segregated Gd atoms form leaf-like clusters that are alternately distributed on both sides of the ITGB, with a periodic spacing of ~ 1.2 nm (see Figure 1(a)). Each cluster consists of two neighboring Gd-rich columns aligning exactly along the $\langle 20\bar{2}3 \rangle$. The edge-on state of the ITGB in Figure 1(a) has been confirmed [18]. Using the O-lattice theory analysis [19, 20], the ITGB was suggested to be a prismatic-plane tilt boundary with a tilt angle of $\theta = 65^\circ$ around the

$\langle 1\bar{2}10 \rangle$ axis [19]. To better describe this ITGB structure, the smallest repeatable stacking unit of Mg lattice along the $\langle 1\bar{2}10 \rangle$ is highlighted in green in Figure 1(b). Clearly, the smallest repeatable unit has a bi-layer structure with a total of four atoms (labeled as A, B, C, and D). All these atoms are periodically located on the two different neighboring layers of $b = 0$ and $1/2$, along the $\vec{b} = \langle 1\bar{2}10 \rangle$ perspective view in Figure 1(b). In this work, we focus on exploring the formation mechanism of this type ITGB and the associated segregation clusters from first-principles. Theoretical studies to date have been all limited to a single column of solute atom segregation to twin boundaries or symmetric tilt boundaries [6,8–10,21].

Figure 1(c) shows the atomic arrangement of the ITGB along $\langle 1\bar{2}10 \rangle$ by simply duplicating the HAADF-STEM image in Figure 1(a). Please note that, two alternative sets of lattices could be possibly assigned to the $\langle 1\bar{2}10 \rangle$ perspective view in Figure 1(c), i.e. one in solid red and the other one in dashed green. The ITGB can be thus seen as a prismatic-plane tilt boundary or a basal-plane tilt boundary, by rotating the prismatic-planes $\{10\bar{1}0\}$ about the $\langle 1\bar{2}10 \rangle$ by 2θ ($\theta = 65^\circ$) from the solid-red or the basal planes $\{0001\}$ by 2θ ($\theta = 25^\circ$) from the dashed-green half lattice on the left side of the boundary, to align with the same solid-blue half lattice on the right. These operations result in four possible

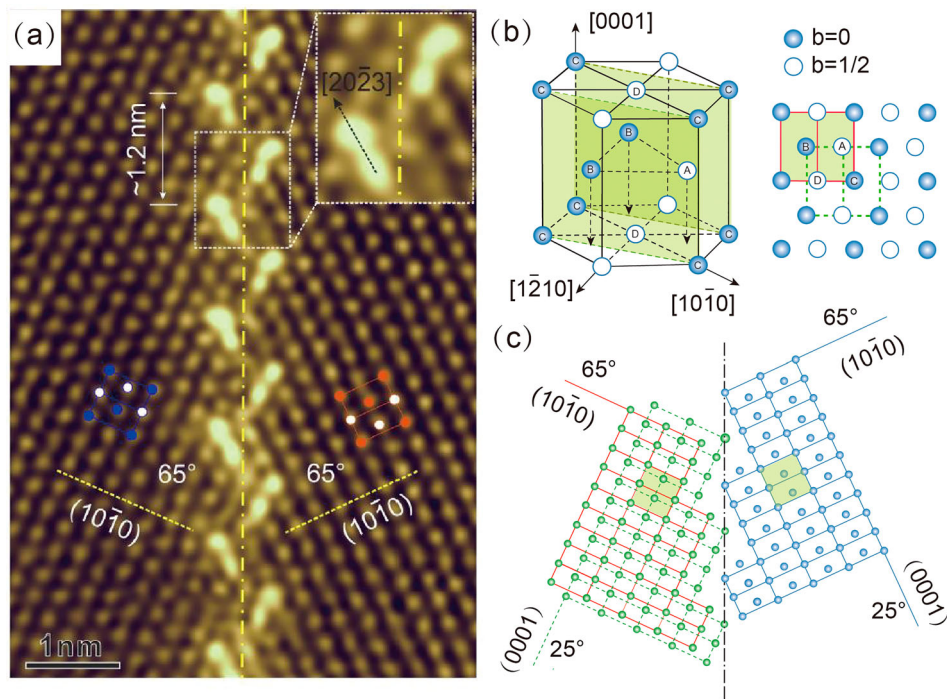


Figure 1. (a) Atomic-resolution $\langle 1\bar{2}10 \rangle$ HAADF-STEM image of one typical ITGB in an Mg-Gd alloy, featured with a unique Gd-rich segregation cluster pattern. (b) Schematic diagram showing the convention cell of hcp Mg bulk and its $\langle 1\bar{2}10 \rangle$ perspective view. (c) Atomic arrangement of the ITGB along $\vec{b} = \langle 1\bar{2}10 \rangle$ as duplicated from the contrast image in (a). (Reprinted with permission from Ref. [18]).

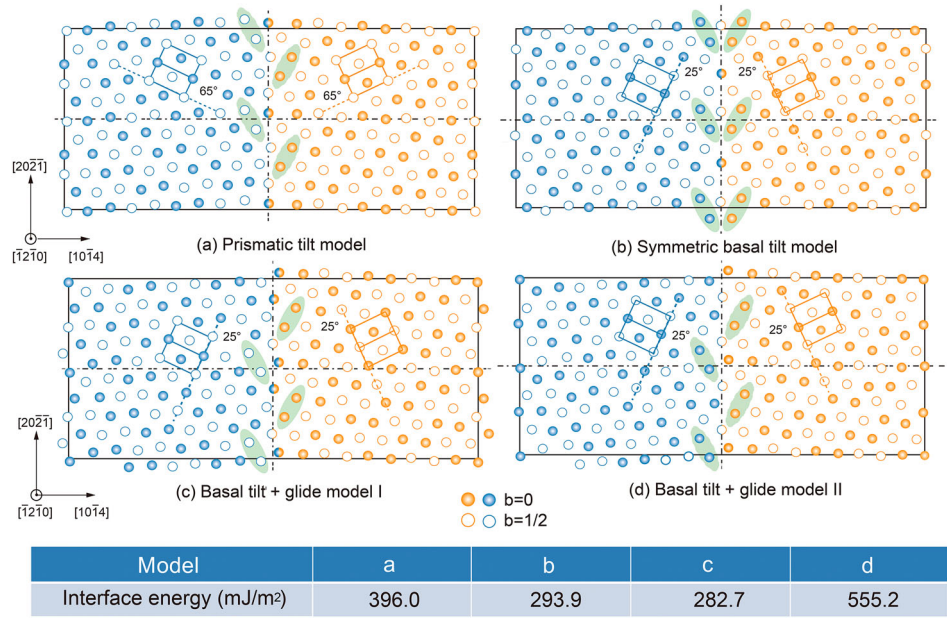


Figure 2. Four model supercells constructed for the $\{10\bar{1}4\} < 20\bar{2}\bar{1} >$ tilt boundary as viewed from the $< \bar{1}2\bar{1}0 >$: (a) the incoherent prismatic-tilt model, (b) the symmetric basal-tilt TB model, (c) the incoherent basal-tilt model I by gliding along $[20\bar{2}\bar{1}]$ from (b), and (d) the incoherent basal-tilt model II by further gliding along $[\bar{1}2\bar{1}0]$ from (c).

atomic structures of the boundary in Figure 2, which can be classified into two different categories, namely the prismatic-tilt model (model a) and the basal-tilt model (models b–d). These model structures are all constructed with periodic boundary conditions, and each contains 92 atoms with two repeatable unit cells along the c -axis (i.e. $[20\bar{2}\bar{1}]$). The green leaf-like impressions in Figure 2 help in comparing with the experimental image in Figure 1(a). Notably, the model b in Figure 2(b) yields a symmetrical basal-tilt boundary which can be regarded as a $\{10\bar{1}4\} < 20\bar{2}\bar{1} >$ CTB with the mirror symmetry. The model c in Figure 2(c), i.e. the basal tilt + glide model I, was built by shifting the right half lattice of model b by one-half period along $[20\bar{2}\bar{1}]$. The model d in Figure 2(d), i.e. the basal tilt + glide model II, was built by further shifting the right half lattice of model c by one-half period along $[\bar{1}2\bar{1}0]$. Apparently, both models c and d, together with the prismatic-tilt model (model a), can yield a structure consistent with the experimental image in Figure 1(a), but the stacking information of atoms remains uncertain and cannot be resolved by transmission electron microscopy.

We further performed the first-principles energetic assessment on these model structures. All calculations thereafter were carried out using the density functional theory code - Vienna Ab-initio Simulation Package, with the plane-wave basis sets [22]. The electron-ion interactions were described by the projector-augmented-wave method (PAW) within the frozen-core approximation [23]. The exchange–correlation functional was described

using the generalized-gradient-approximation (GGA) [24]. For pure bulk *hcp*-Mg, Brillouin-zone integrations employed a Monkhorst–Pack k -mesh of $20 \times 20 \times 12$. The plane-wave kinetic energy cutoff of 380 eV was tested as sufficient. The predicted lattice constants for bulk Mg ($a = 3.191 \text{ \AA}$ and $c/a = 1.623$) matched well with the experiment ($a = 3.209 \text{ \AA}$ and $c/a = 1.624$ [25]) and other calculations ($a = 3.189 \text{ \AA}$ and $c/a = 1.626$ [8]). Interface energies (γ) of these model structures were then calculated as

$$\gamma = (E_{TB} - N\mu_{\text{bulk}})/2A, \quad (1)$$

where E_{TB} is the total energy of each tilt boundary supercell, and N is the total number of Mg atoms in the supercell. μ_{bulk} is the chemical potential of Mg in its pure bulk phase and A the cross-sectional area of the supercell. For each supercell, a gamma-centered Monkhorst–Pack k -mesh of $8 \times 4 \times 1$ was used for Brillouin-zone integrations. Full relaxation was carefully performed on both supercell shape and volume. The self-consistence convergence criterion for electron iterations was set to 10^{-5} eV/atom, and the ground-state atomic geometries were optimized by minimizing the Hellman-Feynman force until the total force on each ion was converged to 0.02 eV/Å. Energetics evaluation over all these structures would provide valuable insights into the formation mechanism behind.

Calculated interface energies are tabulated in Figure 2. The formation energy of model a was predicted to be low

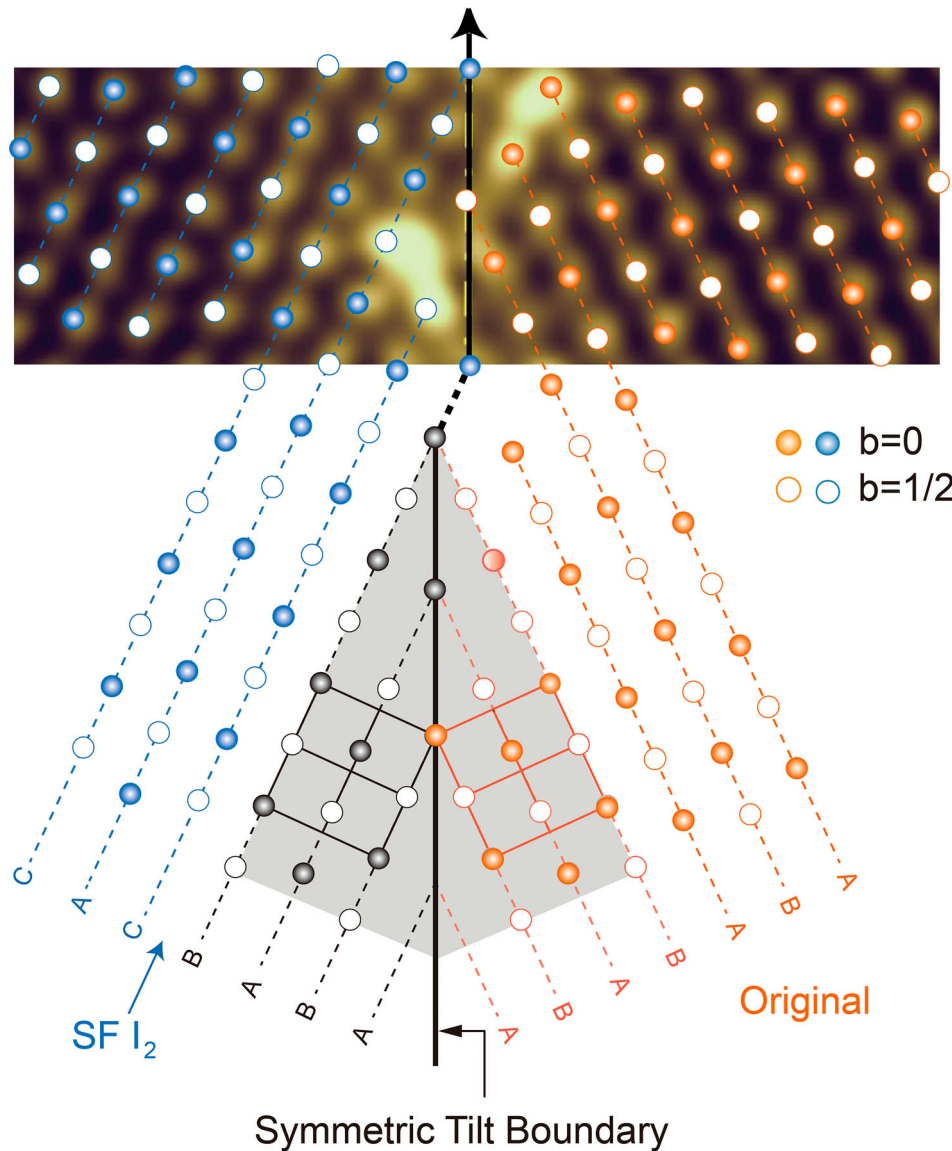


Figure 3. Schematic diagram showing how the $\{10\bar{1}4\} \langle 20\bar{2}\bar{1} \rangle$ CTB interacts with an SF I_2 , resulting in the model *c* structure in Figure 2. The orange and black atoms in basal-planes follow the perfect stacking sequence of $-[ABABAB]-$, while the blue atoms follow the SF- I_2 stacking sequence of $-[CACACA]-$.

as 0.396 J/m^2 , which is still higher than that of the symmetric basal-tilt model *b* (0.294 J/m^2). Model *b*, however, deviates obviously from the experimental contrast image of the ITGB that lacks the mirror symmetry. Gliding the right half lattice of model *b* by one-half period along $[20\bar{2}\bar{1}]$ results in the model *c* structure, and correspondingly, the formation energy is reduced to 0.283 J/m^2 . Further gliding by one-half period along $[\bar{1}2\bar{1}0]$ yields the model *d* structure which requires even higher formation energy of 0.555 J/m^2 . Interestingly, the mirror-symmetric twin boundary (model *b*) that is generally believed as a low-energy structure is not the most energy-favored version of the $\{10\bar{1}4\}$ tilt boundary. The mirror-glide model *c* is more energy-favored to form, and thus can be more suitable for describing the ITGB structure.

How to trigger gliding of the mirror-glide model *c* still remains a question. The possible role of stacking fault (SF) is worth studying. In principle, basal-plane SFs in Mg can be generally classified into four different categories, namely the intrinsic SF (I_1) with a stacking sequence of $-[ABABCBCB]-$, the intrinsic SF (I_2) of $-[ABABCACAC]-$, the extrinsic fault (EF) of $-[ABABCABAB]-$ [26], and the twin-like SF (T_2) of $-[ABABCBABA]-$ [27]. When an SF I_2 initiates on one side of the mirror-symmetric $\{10\bar{1}4\} \langle 20\bar{2}\bar{1} \rangle$ CTB (model *b* in Figure 2), the stacking sequence of basal planes changes from $-[ABABAB]-$ to $-[ABABCAC]-$. Once the SF I_2 is blocked by the TB in some ways just as a dislocation being blocked by a grain boundary [28], the mirror-glide model *c* structure can be produced.

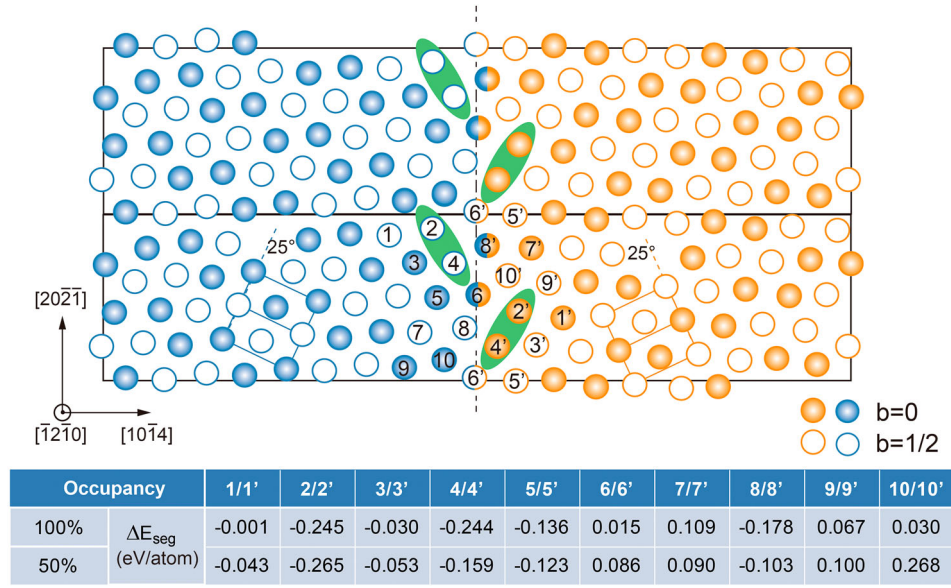


Figure 4. Possible column sites and the corresponding energies for single-column Gd segregation at the ITGB of model *c*, with the column occupancy of 50% and 100%.

A schematic diagram showing this mechanism is provided in Figure 3, which can not only well reproduce the experimental Z-contrast image but also clearly demonstrate the stacking information of all atoms. That is, the resulting model *c* structure can be regarded as an SF-I₂ stabilized ITGB. Considering that the formation energy of this ITGB is ~ 0.011 J/m² lower than the CTB (model *b*), and SF-I₂ in Mg itself has the formation energy of 0.034–0.048 J/m² [26, 29], the interaction with SF-I₂ may reduce the total energy of the CTB system by 0.045–0.059 J/m². Also expectably, a geometrically-tolerant atomic step would present between the faulted and un-faulted portions of the boundary as schematically shown in Figure 3, perhaps through the shuffling of local atoms [30]. We have neither experimental evidence of ITGBs in pure Mg, nor that of SF-I₂ and steps in our Mg-Gd alloy samples. Nevertheless, SFs in CTBs have been observed in an Mg-Nd-Ag alloy [17]. Our proposed SF-I₂ assisted formation mechanism of ITGBs awaits further experimental verification.

Based on the discussion above, the mirror-glide boundary of model *c* was then adopted to assess the Gd segregation. The segregation energy (ΔE_{seg}) that measures the total energy difference before and after Gd segregation can be evaluated as

$$\Delta E_{\text{seg}} = [(E_{\text{ITGB, nGd}} - E_{\text{ITGB}}) - n(E_{\text{bulk, Gd}} - E_{\text{bulk}})]/n, \quad (2)$$

where E_{ITGB} or $E_{\text{ITGB, nGd}}$ is the total energy of the ITGB supercell before or after segregation, respectively. n is the total number of segregated Gd atoms. E_{bulk} is the total

energy of the perfect supercell of pure Mg with the exactly same number of atoms as in the clean ITGB supercell. $E_{\text{bulk, Gd}}$ is the total energy of the same Mg bulk supercell but substituted with one single Gd atom. Apparently, ΔE_{seg} must be negative to enable Gd segregation. The comparison of ΔE_{seg} among various segregation sites reveals the formation preference of segregation patterns.

Figure 4 shows the possible ten column sites (numbered from 1 to 10) for Gd segregation at the ITGB. Due to the unique mirror-glide symmetry and bi-layer structure of model *c*, ten equivalent sites can be labeled out (from 1' to 10') on the other side of the boundary. The corresponding segregation energies for single-column Gd substitution were first calculated for a comparison. It was predicted that with the column occupancy of 50%, site 2 (or 2') is the most preferred, followed by site 4 (or 4'). While at the 100% occupancy, Gd prefers both sites 2 (or 2') and 4 (or 4') almost equally. Some column sites such as 5 (or 5') and 8 (or 8') are less likely but still possible. All the other sites are very unlikely or even forbidden. This prediction seems consistent with the experimental observation of Gd-rich leaf-like clusters on the HAADF-STEM image (Figure 1(a)), but the above calculations have been restricted to single-column segregation only.

Segregated Gd atoms do not have to fill up one single column before they start to cluster at the ITGB as observed in Figure 1(a). Further calculations were thus carried out to assess the pair-column segregation of Gd. Based on the single-column results, we focused on the column pairs about site 2 or 4. Given that this ITGB has a bi-layer structure along $[\bar{1}2\bar{1}0]$, our calculations were,

Table 1. Calculated energies for pair-column Gd segregation at the ITGB.

Column pair	ΔE_{seg} (eV/atom)		
	100% occupancy	50% Occupancy	
		Pair on the same layer	Pair on alternative layers
(2 + 1)	−0.115	−0.203	−0.202
(2 + 3)	−0.051	–	−0.108
(2 + 4)	−0.023	−0.129	−0.276
(2 + 6')	0.071	−0.045	−0.151
(2 + 8')	−0.153	–	−0.189
(2 + 9)	−0.044	–	−0.026
(2 + 10)	−0.093	–	0.004
(4 + 3)	−0.071	–	−0.064
(4 + 5)	−0.083	–	−0.098
(4 + 6)	−0.063	–	−0.038
(4 + 8')	−0.033	–	−0.132

thus again, focused on the 50% and 100% column substitutions. For the case of 50% substitution, we considered two extreme scenarios, i.e. segregated Gd atoms being paired on the same layer (if allowable), or alternately located on the two different layers ($b = 0$ or $1/2$). We targeted to predict a general trend, thus other scenarios of random occupancies were tentatively ignored. The corresponding segregation energies are compared in Table 1. The following important implications can be suggested. With the 100% substitution, the preferred ordering of pair-column segregation was predicted as $(2 + 8') > (2 + 1) > (2 + 10) > (4 + 5)$, which, however, obviously deviates from the experimental observation. While at the 50% substitution, the preference for Gd in two alternate layers becomes the most obvious in the $(2 + 4)$ pair-column, followed by the $(2 + 1)$ pair-column. The total energy of the system can be thus reduced by 0.2–0.3 eV per Gd atom, being comparable to those of single-column segregation. It can be thus deduced that the experimentally observed leaf-like Gd clusters are very possibly resulted from the partial substitution of Gd in some specific atom-columns at the ITGB. The real occupancy of Gd is unknown but such segregation is likely to be a self-restraint process. Increasing continuously to a full substitution is not favored by energy, as suggested in Table 1.

Conclusion

The unique segregation pattern along a $\{10\bar{1}4\}$ ITGB in an Mg-Gd alloy has been thoroughly studied using first-principles calculations. Our results suggested that this ITGB structure can be more energy-favored than its CTB counterpart even without Gd segregation. Two stabilization mechanisms, i.e. stacking faults and solute segregation, jointly contribute to the formation of the ITGB with Gd segregation. Specifically, the ITGB can form

preferentially from the gliding along $[20\bar{2}1]$ of a symmetric basal-tilt twin boundary, i.e. a $\{10\bar{1}4\} < 20\bar{2}1 >$ CTB, through its interaction with intrinsic stacking fault SF- I_2 . Gd tends to segregate to some specific atom-columns at the boundary, to further stabilize the ITGB. Partial substitution of Gd in these columns leads to the leaf-like Gd-rich cluster patterns along the ITGB. This shall also offer a reasonable explanation for the scarce observation of $\{10\bar{1}4\}$ CTBs in Mg and its alloys. The methodology developed in this study shows great promises for interpreting many other complex ITGB structures with solute-cluster segregation in Mg alloys.

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Disclosure statement

No potential conflict of interest was reported by the author(s).

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