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Predicting the formation of <c + a> dislocations in magnesium alloys from multiple stacking fault energies

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ABSTRACT

The presence of alloying elements in magnesium (Mg) can activate pyramidal <c + a> slip systems and thereby improve the plasticity of Mg at room temperature. In this study, we predict the effect of alloying elements on the formation of <c + a> dislocations based on a synergistic effect stemming from both leading and trailing partial dislocations. Our calculations demonstrate that the addition of rare earths, Li, Ca, and Sn significantly lowers at least one energy barrier in pure Mg, and ultimately promotes the formation of the pyramidal I and/or pyramidal II slip systems. The reduced energy barriers are mainly attributed to the local lattice distortions and charge redistribution induced by alloying atoms. These findings provide important insight into the influence of alloying on the formation of <c + a> dislocations, and may ultimately facilitate the development of a framework to design high-plasticity Mg alloys.

1. Introduction

Magnesium (Mg) and its alloys are lightweight metals, which possess attractive combination of mechanical and physical properties, for example high strength to weight ratio and good electrical properties [1]. Such property combinations have prompted the application of Mg alloys in automotive, aerospace, and electronic component industries [2,3]. However, the low plasticity of Mg makes it difficult to be processed at room temperature, and thus hinder its broader applications in modern industry [4]. The poor plasticity of Mg is associated with the inability of hexagonal-close-packed (HCP) Mg to deform plastically in <c> direction, which is accomplished primarily by dislocation glide on the pyramidal plane along <c + a> direction. Activation of non-basal slip, especially <c + a> dislocations on the pyramidal plane, is the key factor to increase the plasticity of Mg alloys. Numerous experimental [5–7] and theoretical [8–10] studies have been devoted to activating pyramidal <c + a> dislocations in Mg and its alloys; a consensus has been reached that adding specific alloying elements can improve plasticity by activating <c + a> dislocation on pyramidal planes [4,11–15]. However, an in-depth understanding on how alloying solutes affect dislocation structures and macroscopic plasticity is far from complete [2,16].

To evaluate the influence of alloying elements on the activation of <c + a> dislocations, two widely used method, termed as "Improve I_2" and "Reduce I_1" have been developed [4,17–19]. Here, I_1 and I_2 indicate two intrinsic stacking fault structures in the basal plane. The I_1 stacking fault, is formed by removal of a basal plane, followed by slipping of the crystal above this fault of 1/3 <10-10>. The I_2 stacking fault, is formed from slip of 1/3 <10-10> in a perfect crystal [20]. The "Improve I_2" method states that improving the basal I_2-type stacking fault energy (SFE) can promote the activation of <c + a> dislocations. It was proposed due to the fact that higher I_2 SFE narrows the distance between partial dislocations, promotes cross-slip between the basal and non-basal planes, and ultimately activates non-basal slip systems. The other method is named "Reduce I_1", addressing that the lower basal I_1-type SFE can promote the activation of <c + a> dislocations [4]. This method is applicable to Mg-RE alloys, because the computed I_1 SFEs of all such alloys are reduced, and at the same time large amount of <c + a> dislocations were observed in experiments [19,21]. A recent study explored the possible relationship between I_1 stacking faults and <c + a> dislocations, but did not elaborate on the non-conservative formation mechanisms of I_1 stacking faults [22].

For the study of the formation of new dislocations, the generalized stacking fault energy (GSFE) curves are often determined theoretically, by sliding one half of a crystal over the other half across a given slip plane [23]. Based on the GSFE curves, addition of alloying element may decrease the global unstable stacking fault energy (USFE) and promote

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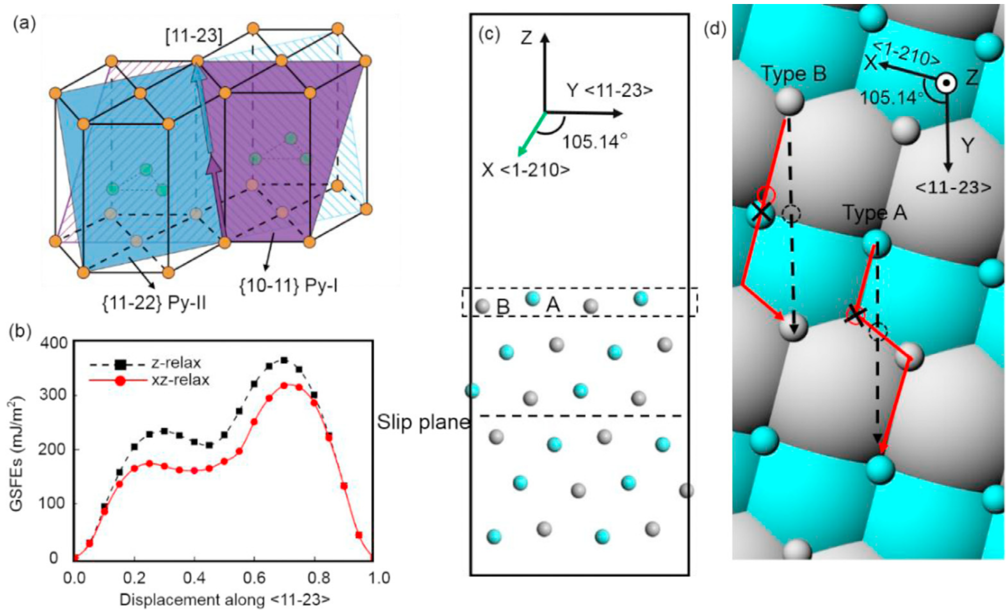

Fig. 1. (a) Schematic plot of pyramidal plane, where purple and blue plane correspond to the pyramidal I plane $\{10\bar{1}0\}$ and pyramidal II plane $\{11\bar{2}2\}$, respectively. (b) GSFE curves of $\{10\bar{1}1\} < 11\bar{2}3 >$ (Py-I) slip system of Mg calculated by z-relaxation and xz-relaxation methods. (c) Slab supercell used to calculate the GSFE curves of $\{10\bar{1}1\} < 11\bar{2}3 >$ slip system, the dotted line represents the slip plane. Cyan ball corresponds to basal type A atom, gray ball corresponds to basal B type atom. (d) Slip trace of $\{10\bar{1}1\} < 11\bar{2}3 >$ slip system of Mg calculated by z-relaxation method (black dashed line) and xz-relaxation method (red solid line); "×" symbol represents the stable position obtained by full-relaxation method.

the formation of <c + a> dislocations [14,23,24]. In fact, this method has been extensively used to rationalize the behavior of face-centered cubic (FCC) metals and <a> dislocations in HCP metals [17,25,26]. However, it is not applicable to the Mg-Y alloy since in this case the global USFE value increases but the <c + a> dislocation is observed. The above analysis indicates that evaluating the alloying effects on the formation of <c + a> dislocation by global USFE can only partially explain the available experimental observations.

In this contribution, by using density functional theory (DFT), we systematically calculate the GSFE curves of Mg and its thirteen alloys on <c + a> slip along both pyramidal I (Py-I) and pyramidal II (Py-II) slip planes. The schematic illustration of the Py-I and Py-II planes is shown in Fig. 1a. We find that the formation of <c + a> dislocation relies on the synergistic effects of the formation energy barriers of leading and trailing partial dislocations. Based on the synergistic effects, alloying elements can be divided into three categories: (1) Alloying with Zn, Al and Ag would increase the formation energies on both planes, and the formation of <c + a> dislocation would be impeded; (2) Alloying with Li and RE reduces the formation energy on Py-II and promotes the formation of the <c + a> dislocation, but increases the formation energy on Py-I and prevents the formation of <c + a> dislocation on this plane; (3) Alloying with Ca and Sn reduces the formation energies of both planes and promotes the formation of <c + a> dislocations. Our calculations also reveal that there are two possible positions to be substituted by alloying elements in Py-I slip plane, alloying elements substituting different position make the stable stacking fault exist or disappear, which explains the antipodal results for Mg and its alloys commonly exists in simulations [23,27]. Also, the formation energy of Py-II decreases with increasing atomic radius of alloying elements. This is presumably because large alloying atoms would increase the lattice distortion, which promotes the formation of stacking faults. These findings provide a physical understanding of the effects of alloying on the formation of <c + a> dislocations in Mg alloys, and provide a method to evaluate alloy elements for promoting the formation of pyramidal <c + a> dislocations.

2. Computation approach

The Vienna Ab-initio Simulation Package (VASP) code [28] was used to perform all DFT simulations. The projector augmented wave (PAW) method was employed to describe the interactions between the valence electrons and ionic cores [29]. In our computations we used the optB88-vdW [30,31] functional to include van der Waals (vdW) interactions. Using the functional, we have recently revealed the prominent role of vdW forces on mechanical properties of Mg slabs [32].

A 12-layer slab with a (2 × 2) unit cell was established to represent the pyramidal plane stacking fault structures; the lattice constants are set to $a = 3.198$ Å and $c = 5.194$ Å [32]. We substituted one Mg atom in the sixth layer with an alloying element to model the metal alloys. A vacuums thickness of 15 Å was used to avoid the interactions between slabs. The kinetic energy cutoff was set to 400 eV and the Brillouin zone sampled used was $11 \times 7 \times 2$ k-point mesh. The total energy convergence tests showed that the total energy difference was less than 0.1 meV/atom when we used more accurate parameter settings. To study the effects of alloys on the formation of pyramidal <c + a> dislocations of Mg, we use conventional direct crystal slip technique to calculated the GSFE curves on the Py-I and Py-II planes. For structure optimization, three structure optimization methods were applied: (1) relaxation only z coordinates ("z-relaxation"); 2) relaxation both x and z coordinates ("xz-relaxation"); and 3) fully relaxation all coordinates ("full-relaxation"). For more details on the optimization methods refer to Refs. [27,33].

3. Results and discussion

3.1. Slip trace of the <c + a> dislocation on Py-I plane

We first study the stable SFE of the <c + a> dislocations on the Py-I plane, which is particularly important for understanding the core structure, formation and dissociation of <c + a> dislocations [9]. The stable SFE corresponds to the lowest point in the GSFE curves, obtained by sliding the upper half of the crystal along the $< 11\bar{2}3 >$ direction. Considering that the Py-I plane is a corrugated structure composed of both basal A and B atoms (Fig. 1c), two different structure optimization methods (z-relaxation and xz-relaxation) have been reported. As shown in Fig. 1b, using the z-relaxation method the SFE value is determined to be 213 mJ/m^2 at the position of 0.45b, while it reduces to 161 mJ/m^2 at the position of 0.4b when the xz-relaxation method was utilized. These results indicate that, allowing atoms to relax in the slip plane reduces the values of stable SFE and changes the position of stable SFE. The validity of the xz-relaxation method can be confirmed by the accurate full-relaxation method [9]. In this case, atoms at different positions move to their stable stacking faults position following relaxation with a SFE of 158 mJ/m^2, which is closer to the result obtained by the xz-relaxation method.

The validity of the xz-relaxation method is also supported by their stable stacking fault positions. Specifically, the structure of a stable stacking fault optimized by the full-relaxation method shows that both type A and B atoms are at lattice positions (cross mark in Fig. 1d). For the xz-relaxation method, type A atoms are at the lattice position, while type B atoms are close to the lattice position (red solid circle in Fig. 1d). However, as to the z-relaxation, both two types atoms are far away from the lattice position (black dashed circle in Fig. 1d). Therefore, the GSFE curves calculated by xz-relaxation method can accurately describe the slip process, which will be used in the calculations that follow.

3.2. Alloying effects on the formation of <c + a> dislocations on Py-I

Now we discuss the effect of alloying elements on Py-I slip plane. Due to the corrugated structure of Py-I, there are two possible positions that can be substituted by alloying elements (type A and B in Fig. 1c). For type A, the stable SFE appears between 0.4b and 0.5b when the atomic size of alloying elements is smaller than that of Mg (including Sn, Al, Ag, and Zn; Fig. 2a). When the atomic radii of alloying elements are larger than that of Mg (Ca and RE), the stable stacking fault shown in Fig. 2b disappears. However, the results are completely reversed when substituting atoms at type B position (Fig. 2c and 2d). In this case, the stable stacking fault exists when the atomic radii of alloying elements are larger than that of Mg (Ca and RE), but vanish when atomic radii of alloying elements are smaller than that of Mg (Sn, Al, Ag, and Zn).

Notably, stable stacking faults exist in both cases in Mg-Li alloy. This special phenomenon can be attributed to the similar atomic radius of Li (1.52 Å) and Mg (1.60 Å) [34]. However, the atomic radius of Sn (1.51 Å) [34] is also comparable with that of Li, but Sn affects Py-I dislocations completely differently from Li. To understand the different effects of these two alloying elements, we analyze the charge density distributions of Mg, Mg-Li, and Mg-Sn on Py-I slip plane. As shown in Fig. 2e, the charge density distributions of the Mg-Li are similar to the charge density distributions of Mg, while the charge density distributions of the Mg-Sn are obviously different from that of Mg, due to the different electronegativity of Li (0.98) and Sn (1.96) [34]. This makes the electrons of Mg-Li prefer to accumulate around the atom of Mg (1.31) rather than Li, while the electrons of Mg-Sn prefer to accumulate around the atom of Sn rather than Mg, resulting in different effects of Li and Sn on the formation of <c + a> dislocation on Py-I.

We further calculated the cohesive energy of Mg alloys to determine the suitable substitute position of alloy elements. The cohesive energy E_{coh} is defined as [35]:

$$E_{coh} = \left(E_{total} - N_{mg}E_{Mg} - N_X E_X\right)/\left(N_{Mg} + N_X\right) \quad (1)$$

where E_{total}, E_{Mg} and E_X represent total energies of the Mg-X, the energy of single Mg atom and single X atom in an isolated state, respectively; N_{Mg} and N_X denote the number of Mg and alloying element atoms in the system, correspondingly. Our calculated results show that the cohesive energies at these two positions are almost identical, suggesting that both positions are allowed to be substituted by alloying elements. To further consider the influence of alloying elements on the GSFE curves, we build a larger 2 × 4 supercell, in which Mg atoms on both A and B positions can be substituted by alloying elements simultaneously, and the interaction between alloy elements can be neglected. We re-calculated the GSFE curves of this large supercell with the xz-relaxation method, and find that the stable stacking fault exists for all Mg alloys (see Fig. 3a), which corresponds to the position of dislocation dissociation.

Now we focus on the effects of alloying elements on the formation of <c + a> dislocations. Note that the global USFE alone cannot explain the observed <c + a> dislocations in the Mg-Y alloy, because the global USFE was increased but the <c + a> dislocation was observed in experiment [4,36]. To understand this contradiction, we now analyze the formation of <c + a> dislocations on pyramidal plane. Considering that the Burgers vectors of <c + a> dislocation is larger than that of <a> dislocation, and the <c + a> dislocation is usually dissociated into leading and trailing partial dislocations at the position of stable stacking fault [8,33,36,37]. Thus, the synergistic effect of the leading and trailing partial dislocations should be considered in the formation process. As shown in Fig. 3b, the formation of a leading partial dislocation need to overcome the local unstable SFE γ_L, which is defined as E_i^1 (i = I and II) for different slip plane; the formation of trailing dislocation depends on the energy difference of global unstable SFE and stable SFE, which is

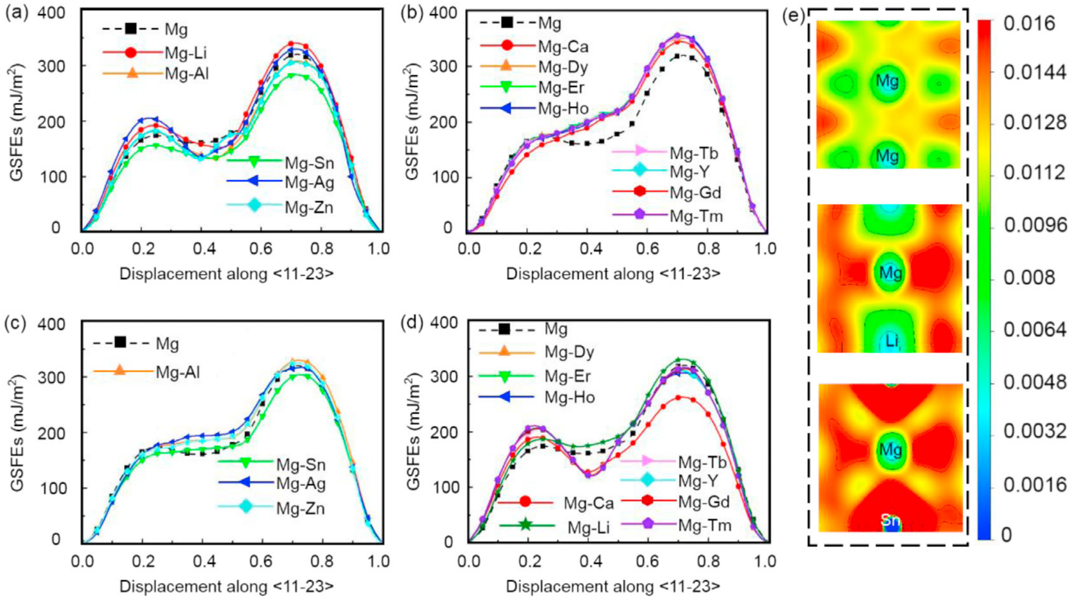

Fig. 2. (a, b) The GSFE curves of Py-I slip systems of Mg alloys calculated by xz-relaxation method when alloying elements substituting Mg atom on type A position. (c, d) The GSFE curves of Py-I slip systems of Mg alloys calculated by xz-relaxation method when alloying elements substituting Mg atom on type B position. (e) Charge density distributions of Mg and its alloys at stable SFE position. In the plots of charge density distributions, red color denotes the area with higher charge density. The charge density distributions of Mg-Li are similar to that of Mg.

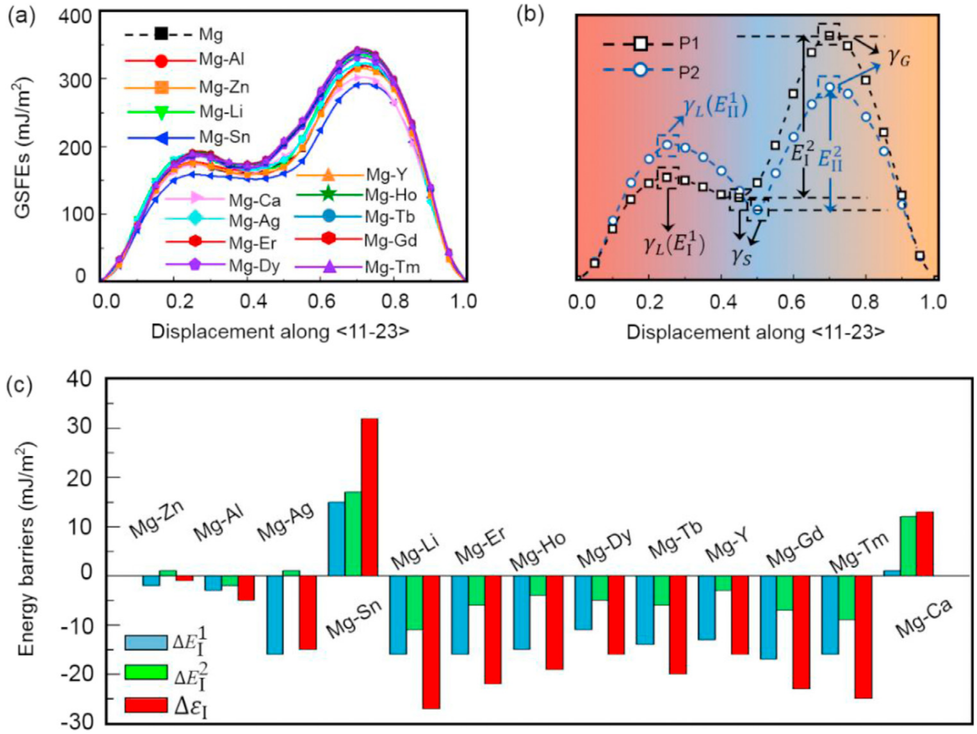

Fig. 3. (a) The GSFE curves of Py-I slip systems of Mg alloy calculated by xz-relaxation method when alloying elements substituting Mg atom on both A and B positions simultaneously. (b) The schematics of GSFE curves on two slip planes. There are two unstable SFEs and one stable SFE on the curves: the first maximum in the curves named as local unstable SFE (γ_L), the second maximum in the curves named as global unstable SFE (γ_G), and the minimum between them named as stable SFE (γ_s). The formation energy barrier of leading partial dislocation E_i^1 is equal to γ_L, the formation energy barrier of trailing partial dislocation E_i^2 is equal to the difference of γ_G and γ_s. (c) The energy barrier difference between Mg and its alloys for leading partial dislocation (ΔE_{I}^1), trailing partial dislocation (ΔE_{I}^2) and full dislocation ($\Delta\varepsilon_{\mathrm{I}}$). A positive value indicates that alloying element can promote the formation of this partial dislocation.

defined as E_i^2 ($E_i^2 = \gamma_G - \gamma_s$; $i =$ I and II); the synergistic effect of these two partial dislocations can be defined as ε_{i} ($\varepsilon_{\mathrm{i}} = E_i^1 + E_i^2$; $i =$ I and II).

Comparing the formation energy difference of two partial dislocations of Mg and its alloys ($\Delta E_{\mathrm{I}}^{\mathrm{i}} = E_{\mathrm{I}}^{\mathrm{i}}(\mathrm{Mg}) - E_{\mathrm{I}}^{\mathrm{i}}(\mathrm{Mg\text{-}X})$) reveals that (1) alloying with Sn and Ca results in positive ΔE_{I}^1 and ΔE_{I}^2, and promotes the formation of both leading and trailing partial dislocation on Py-I; (2) alloying with Al, Li and RE produces negative ΔE_{I}^1 and ΔE_{I}^2, and impedes the formation of both leading and trailing partial dislocations on Py-I; (3) alloying with Zn and Ag promotes the formation of the leading partial dislocation and prevents the formation of the trailing partial dislocation, due to the positive ΔE_{I}^1 and negative ΔE_{I}^2 of these alloys (see Fig. 3c). Alloying with Zn and Ag reduces E_{I}^2, but increases E_{I}^1, which would promote the formation of leading partial dislocation and prevent the formation of trailing partial dislocation. Comparing the total energy difference of Mg and its alloys ($\Delta\varepsilon_{\mathrm{I}} = \Delta E_{\mathrm{I}}^1 + \Delta E_{\mathrm{I}}^2$), alloying with Ca and Sn (Li, Ag, Al, Zn, and RE) would promote or impede the formation of <c + a> dislocation on Py-I.

3.3. Alloying effects on the formation of <c + a> dislocations on Py-II

Now we turn to the effects of alloying on the formation of <c + a> dislocations on the Py-II slip plane. We first calculate the GSFE curves of Mg and Mg-Y alloy using the xz-relaxation method. As shown in Fig. 4c, the stable SFE locates at 0.5b, which is consistent with pervious DFT [38,39] and experimental results [33] that Py-II <c + a> dislocation would dissociate into two equal $1/6 < 11\bar{2}3 >$ partials. Contrast to the corrugated stacking structure of atoms on Py-I plane, the atoms on Py-II are arranged in a planar structure, along with only one type of atom on the Py-II plane, as shown in Fig. 4a. In our recent work [27], we reported that there exists a flat potential-energy surface (PES) in Py-II around the position of stable stacking fault. The existence of this PES would lead to the stacking fault cooperative movement (SFCM) and induce Py-II <c + a> dislocation dissociates into two symmetrical partial dislocations (Fig. 4b). This phenomenon decreases the global unstable SFE of the trailing partial dislocation significantly (Fig. 4c). Importantly, both the magnitudes of unstable SFE and the stable SFE decrease upon the alloying of Y, which facilitates the formation of <c + a> dislocations on Py-II plane.

Fig. 4d shows the GSFE curves of Py-II plane of other alloys. Similar stable SFE position and SFCM phenomenon can be seen in all Mg alloys. To consider the alloying effect on the formation of <c + a> dislocation on Py-II slip plane, the energy barrier difference of two partial dislocations of Mg and its alloys (($\Delta E_{\mathrm{II}}^{\mathrm{i}} = E_{\mathrm{II}}^{\mathrm{i}}(\mathrm{Mg}) - E_{\mathrm{II}}^{\mathrm{i}}(\mathrm{Mg\text{-}X})$) are shown in Fig. 4e. We find that alloying with Li can produce negative ΔE_{II}^1 and positive ΔE_{II}^2, and prevent the formation of the leading partial dislocation and promote the formation of the trailing partial dislocation; alloying with Sn and Ca can produce positive $\Delta E_{\mathrm{II}}^{\mathrm{i}}$, promote the formation of both leading and trailing partial dislocation on Py-II; alloying with RE can produce positiveΔE_{II}^1 and negative ΔE_{II}^2, promote the formation of leading partial dislocations on Py-II. Comparing the total energy difference of Mg and its alloys ($\Delta\varepsilon_{\mathrm{II}} = \Delta E_{\mathrm{II}}^1 + \Delta E_{\mathrm{II}}^2$), alloying with Li, Sn, Ca and RE would promote the formation of <c + a> dislocation on Py-II, whilst alloying with Al, Ag, and Zn would impede their formation.

3.4. Comprehensive effect of alloying element on the formation of pyramidal dislocations

Finally, we focus on the effect of alloy elements on the formation of <c + a> dislocations on the pyramidal plane. The difference of total energy barriers between Mg and its alloys $\Delta\varepsilon_i$ ($i =$ I and II) determines the contribution of alloying elements to the formation of pyramidal dislocations. According to the different influences of alloying elements on the formation energies of two pathways, we divide these alloying elements into three categories (Fig. 5). When alloying with Zn, Al and Ag, the formation energies of both two pathways are larger than those of Mg, so the formation of <c + a> dislocation would be impeded. This is consistent with early simulation results that alloying with Ag, Zn and Al do not contribute to the plasticity of materials [2]. When alloying with Li and RE elements, the formation energy of <c + a> dislocations on Py-II is lower than that of Mg, which suggests that <c + a> dislocations on Py-II are more likely to be formed. This is consistent with available experimental reports that alloying with Li and RE can increase their plasticity by promoting the formation of pyramidal <c + a> dislocations [2,4,12,13]. When alloying with Ca and Sn, the formation energies of both Py-I and Py-II are lower than those of Mg, and thus both Py-I and Py-II <c + a> dislocation on these two alloys are more likely to be formed. This is

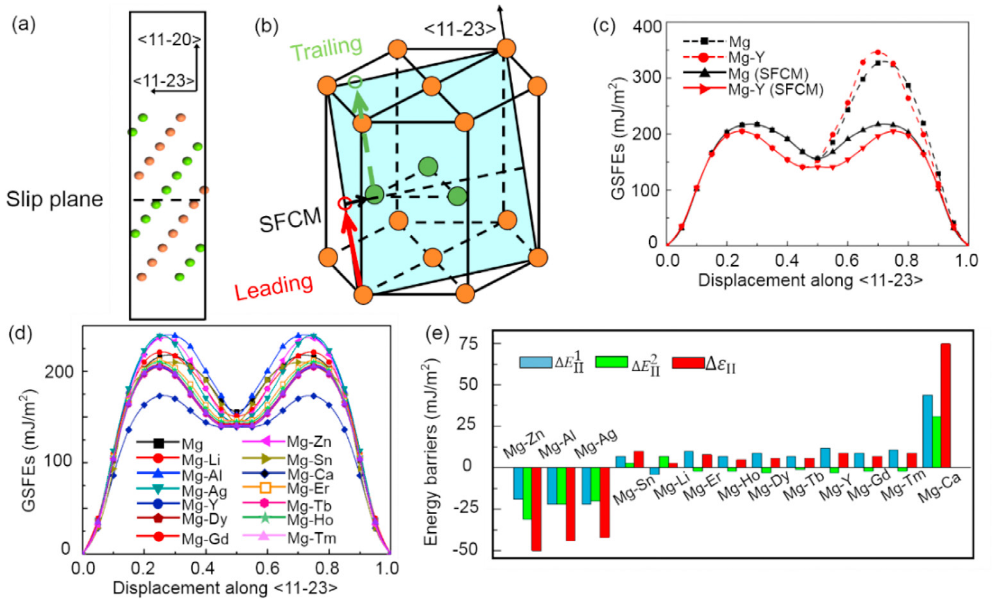

Fig. 4. (a) The slab supercells used to calculate the GSFE curves of $\{11\bar{2}2\} < 11\bar{2}3 >$ (Py-II) slip system, the dotted line represents the slip plane. (b) The schematics of sliding pathway of Py-II <c + a> dislocation involve the SFCM. The red solid arrow, green dashed arrow, and black solid arrow correspond to the leading partial dislocation, trailing partial dislocation, and the stacking fault cooperative movement, respectively. (c) The GSFE curve of $\{11\bar{2}2\} < 11\bar{2}3 >$ slip system of Mg and Mg-Y and the GSFE curves of Mg and Mg-Y involve the SFCM. (d) The symmetric GSFE curves for Mg and its alloys that involve the stacking fault cooperative movement. (e) The difference value between the energy barriers of leading and trailing partial dislocations of Mg and its alloys involve the stacking fault cooperative movement.

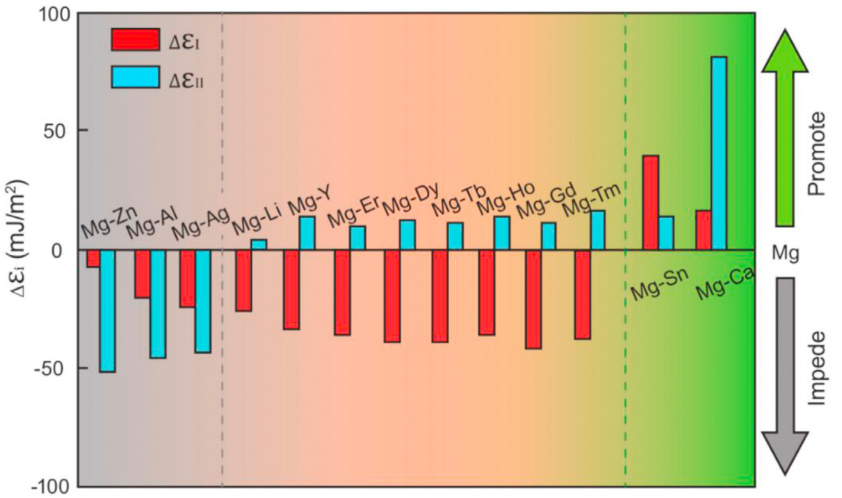

Fig. 5. The formation energy of Mg alloys for determining whether the alloying elements promote the formation of pyramidal <c + a> dislocation. $\Delta\varepsilon_i$ (i = I and II) is the difference value of formation energies between Mg and its alloys, a positive value implies promoting the formation of dislocations. The red bar represents the different value of Mg and its alloys on Py-I; the cyan bar represents the different value on Py-II.

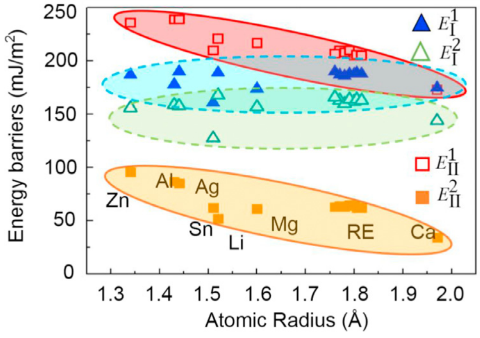

Fig. 6. The relationship between formation energies of partial dislocations and atomic radius of alloying elements. The formation energies of partial dislocations on Py-II are negatively related to the atomic radius.

consistent with experimental results that <c + a> dislocation can be observed in Mg-Ca and Mg-Sn alloys [40,41].

To further understand the effects of alloying elements on the formation energies of the four partial dislocations on the Py-I and Py-II planes, we established a relationship between atomic radius and formation energies. As shown in Fig. 6, the most important feature is that the behavior of Py-II is different from Py-I. For Py-I plane, the formation energies of different alloys are close to those of Mg, and no obvious relationship can be found between formation energies and atomic radius of alloying elements. This phenomenon is presumably because of the corrugated structure of Py-I plane, which introduces limited lattice distortion, and thus leads to similar formation energies for Mg and its alloys. As for the Py-II plane, a negative relationship between $E_{\rm II}^i$ (i = 1 and 2) and atomic radius of alloying elements can be observed, suggesting that the alloying elements with larger atomic radius is more likely to promote the formation of Py-II <c + a> dislocations. This finding is attributed to the planar structure of Py-II, adding alloying element with larger atomic radius would increase the lattice distortion and promote the formation of stacking faults [24,42]. On the basis of the above analysis, one can conclude that the atomic size of the alloying elements is strongly related to the plasticity of the Mg alloys.

4. Conclusions

We have carried out density-functional theory calculations to systematically study the effect of alloying elements on the formation of pyramidal <c + a> dislocations. Our calculations suggest that the formation of <c + a> dislocation is based on the synergistic effect of partial dislocations. It is predicted that alloying with RE and Li promotes the formation of pyramidal II (Py-II) plane; alloying with Zn, Al and Ag does not improve the formation of pyramidal <c + a> dislocations; alloying with Ca and Sn can promotes the formation of pyramidal I (Py-I) and Py-II <c + a> dislocations, and these results are all in good agreement with experimental observations. Furthermore, we find that alloying elements substituting two different positions on Py-I can make the stable stacking fault form or disappear, which explains the contradictory simulation results reported in the literature. Meanwhile, the energy barriers of <c + a> dislocations on Py-II is inversely proportional to the atomic radius of alloying elements. It is noted that, the atomic radius of alloying elements usually dominates in the formation of <c + a> dislocations, while electronegativity of the alloying elements also play an important role on the plasticity of the Mg alloy, when the atomic radius of alloying elements is similar. These findings provide novel insight into the effects of alloying on the formation of <c + a> dislocations in Mg alloys, and may ultimately facilitate the development to design high-plasticity Mg alloys.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary material

Supplementary material associated with this article can be found, in the online version, at doi:https://doi.org/10.1016/j.mtla.2019.100352.

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