

Research Article

Zigzag Dissociation Mode of $\langle c+a \rangle$ **Dislocations on the** $\{10\overline{1}1\}$ **Plane in Magnesium Alloys**

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Fundamental understanding of the dissociation mode of $\langle c+a \rangle$ dislocations on the $\{10\overline{1}1\}$ plane is required before the goal of improving the ductility of Mg alloys attained. In this study, our density-functional theory calculations reveal that the atoms in the $\{10\overline{1}1\}$ plane slip along a zigzag trace through a low-energy pathway. We thus propose a novel zigzag dissociation mode based on this slip trace. In particular, the shuffling motion of atoms is observed at the position of stable stacking fault, which is closely related to the *c/a* ratio of the hexagonal closed-packed lattices.

1. Introduction

Alloying rare Earth elements is an effective approach to improve the room temperature plasticity of Mg, by activating the pyramidal $\langle c+a \rangle$ dislocations [1–3]. The activation of pyramidal $\langle c+a \rangle$ dislocation can fulfill the von Mises' criterion for a general plastic deformation (requirements for five independent slip systems). The $\langle c+a \rangle$ dislocation usually dissociates at a stable stacking fault due to the large Burgers vectors [4], and thus, it is critical to understand the dissociation modes of $\langle c+a \rangle$ dislocations [5]. Unfortunately, it is a tremendous task to completely understand the dissociation process of $\langle c+a \rangle$ dislocations solely on the basis of experiments [6].

On the basis of theoretical simulations, several dissociation modes of $\langle c+a \rangle$ dislocation on the {1011} plane have been proposed. For instance, molecular dynamics (MD) simulations revealed that a $\langle c+a \rangle$ dislocation on the {1011} plane dissociates into two equivalent 1/6[2023] and 1/ 6[0223] partial dislocations [7]. In this mode, however, atoms at a stable stacking fault position are deviated from their stable positions (so-called "off-lattice" position), and thus, atoms move along a high-energy pathway [8]. An alternative dissociation mode was proposed based on density-functional theory (DFT) computations, addressing that $\langle c+a \rangle$ dislocation on the {1011} plane dissociates into two collinear 1/ 6[1123] partial dislocations [5]. However, in this collinear disassociation mode, atoms are also deviated from their stable positions because the stable stacking fault position on the {1011} plane is not located at the [1123] direction [9]. In light of the aforementioned discussion, it is evident that no consensus has yet been reached on the precise dissociation mode for $\langle c+a \rangle$ dislocations of Mg alloys on the {1011} plane.

In this article, by using DFT calculations, we propose a zigzag mode to describe the dissociation of $\langle c+a \rangle$ dislocations on the $\{10\overline{1}1\}$ plane. Our mode has two prominent features that are different from previous ones: (1) the atoms on the $\{10\overline{1}1\}$ plane are located at (or adjacent to) a stable site and thus move along a low-energy pathway; and (2) in contrast to the collinear dissociation mode, the atoms slip along a zigzag trace that is more suitable to the corrugated $\{10\overline{1}1\}$ plane.

Using the lattice constant of a = 3.198 Å and c = 5.194 Å [10] of Mg, we established a 12-layer slab (2 × 2 unit cell) for the {1011} planes (Figure 1(a)). One Mg atom in the sixth layer was substituted by a Y atom to model the Mg-Y alloys. All DFT calculations were performed using the VASP code [11]. The interaction between the valence electrons and ionic cores was described by the projector augmented wave method [12]. The dispersion-inclusive optB88-vdW functional was employed [13]. A vacuum region of 15 Å was used to eliminate artificial interactions between slabs. The residual force threshold of 1 meV/Å, a cutoff energy of 400 eV, a k-point mesh of $11 \times 7 \times 2$, and the pressure of the sample set to zero were utilized for geometry optimization. We relaxed both *x* and *z* coordinates of the corrugated {1011} plane (Figure 1(a)) [14].

3. Results and Discussion

Our recent work has reported that there are two positions (types A and B in Figure 1(a)) on the $\{10\overline{1}1\}$ plane that can be substituted by alloy elements [15]. The types A and B are different in the $\{10\overline{1}1\}$ plane; the $\{10\overline{1}1\}$ plane is composed of planes of the basal type A and B atoms, and the surrounding environments of the type A and B atoms are different. Interestingly, we found that the stable stacking fault energy (SFE) disappears when type A atoms are substituted by Y atoms (red curve in Figure 1(b)); while when type B atoms are substituted, the stable SFE exists at 0.4 b and the $\langle c+a \rangle$ dislocation dissociates at the position of the stable SFE [15]. To understand this phenomenon, we plot out the charge density distribution at the 0.4 b positions. As shown in Figure 1(b), when the Mg atoms were substituted at A position, there are high charge density areas surrounding Mg atoms (labeled $I_{\rm A}$ and $I_{\rm B}$ in Figure 1(b)). In contrast, when the Mg atoms were substituted at B position, almost all the charges are concentrated around the Y atom. Additionally, the contour lines of Y atom in type B is larger than that of type A, which also implies that there are more charges around Y atom in type B than those in type A. Furthermore, when the Mg atoms were substituted at A position, the charges almost spread at the slipping plane, leading to the gentle changes in structures, which means the close energies near 0.4 b in the GSFE curves. When the alloying elements are substituted at position B, the charges gather around the atom Y, indicating that the position is stable, and thus, the lowest energy occurs at 0.4 b in the GSFE curves. Therefore, the lower energy SFE and stable structure of type B are mainly due to the more concentrated charge distribution around Y atom located on the slip plane. It is notable that the alloying element cannot be substituted on a specific position in a real material. To determine the suitable substitute position of alloy elements, we calculated the cohesive energy of Mg-Y alloys. 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 Y on

the Mg-Y alloy, we build a larger 2×4 supercell, in which Mg atoms on both A and B positions can be substituted by alloying elements simultaneously. We recalculated the GSFE curves of this large supercell (AB type in Figure 1(b)) and found that the stable stacking fault exists in the Mg-Y alloy.

Now we focus on the dissociation of $\langle c+a \rangle$ dislocations on the $\{10\overline{1}1\}$ plane. We found that type B atoms slip along the $[02\overline{2}3]$ direction (Figure 2(a)), which is consistent with the so-called "equivalent dissociation mode" [7]. However, in this case, type A atoms are far from the stable position (the lattice position or the junction of atoms), which would be unstable in structure and energetically unfavorable. Meanwhile, compared with the gamma surface of $\{10\overline{1}1\}$ plane in [9], there are two stable stacking fault positions along different directions. This phenomenon suggests that there are two possible dissociation pathways in the $\{10\overline{1}1\}$ plane. Besides, two types of atoms slip along different directions to arrive at stable stacking fault positions, which cannot be explained by the equivalent dissociation mode.

Two types of atoms slip along different directions, suggesting that the atoms in the $\{10\overline{1}1\}$ plane slip along a zigzag trace. Specifically, type A atoms slip along $[20\overline{2}3]$ and [0223] directions for leading and trailing partial dislocations; type B atoms slip along [0223] and [2023] directions for leading and trailing partial dislocations. In this zigzag dissociation mode, both type A and B atoms on the $\{10\overline{1}1\}$ plane are located at (or adjacent to) a stable site and thus move along a low-energy pathway; and in contrast to the equivalent dissociation mode, the atoms slip along a zigzag trace that is more suitable to the corrugated $\{10\overline{1}1\}$ plane. Meanwhile, we find distinct length of leading partial dislocation of two types of atoms. For type A (B) atoms, the length of leading partial dislocation is smaller (larger) than that of $1/6[20\overline{2}3]$ ($1/6[02\overline{2}3]$). This deviation from the ideal $1/6[20\overline{2}3]$ is similar to the "shuffling motion;" *i.e.*, atoms on a pyramidal plane first move to their stable positions, end up at off-lattice positions, and then move back to their lattice position [6].

Based on the shuffling motion, the $\langle c+a \rangle$ dislocation on the $\{10\overline{1}1\}$ plane can be formed via different modes. As shown in Figure 3(a), for type A (B) atoms, first the leading partial dislocation having Burgers vectors $\mathbf{b}_{\mathbf{I}} = (1-\lambda)/6[20\overline{2}3]$ $(\lambda = 0.03$ is the length of the leading partial dislocation ought to be 3.12 Å, which is 3% lower than the value 3.21 Å in our calculations) ($\mathbf{b}_{\mathbf{I}} = (1 + \lambda)/6[02\overline{2}3]$) arrives at the off-lattice position; second, atoms move $\mathbf{b}_{s} = \lambda/6[20\overline{2}3]$ (\mathbf{b}_{s} $=-\lambda/6[02\overline{2}3])$ from the off-lattice position to the lattice position by shuffling motion, considering the movement exists on a flat potential-energy surface, which allows atoms to move freely in this potential-energy surface and finally moves from off-lattice position to on-lattice position. This shuffling motion process would occur spontaneously and does not require more energy; third, the trailing partial dislocation starting from the lattice position has Burgers vectors $\mathbf{b}_{t} = 1/6[02\overline{2}3]$ ($\mathbf{b}_{t} = 1/6[20\overline{2}3]$). Thus, $\langle c+a \rangle$ dislocation on the $\{10\overline{1}1\}$ plane can be dissociated with a zigzag mode described as



FIGURE 1: (a) Slab supercell of $\{10\overline{1}1\}11\overline{2}3$ slip system of Mg. Orange and green spheres indicate basal type A and type B atoms, respectively. (b) The distributions of charge densities on the 0.4 b positions in the generalized stacking fault energy (GSFE) curves on the $\{10\overline{1}1\}$ planes of Mg-Y alloys. Red (blue) region denotes the area with high (low) charge density. Contour lines are drawn at a constant interval. Note that the GSFE curves are taken from our recent work [15], wherein the stable stacking fault energy is denoted as γ_5 , which is related to the dissociation of $\langle c + a \rangle$ dislocation.



FIGURE 2: (a, b) The equivalent (corrugated) dissociation modes of $\{10\overline{1}1\}11\overline{2}3$ slip system. Orange and green spheres indicate type A and B atoms, respectively. Blue dashed line and white (black) solid line denote the full $\langle c+a \rangle$ dislocation and the partial dislocations, respectively; black dash circle denotes the stable stacking fault position of type A and B atoms. (a) Equivalent dissociation. (b) Corrugated dissociation.

type A:
$$\langle c + a \rangle = \frac{1}{3} [11\overline{2}3] = \mathbf{b_l} + \mathbf{b_s} + \mathbf{b_t} = \frac{(1-\lambda)}{6} [20\overline{2}3] + \frac{\lambda}{6} [20\overline{2}3] + \frac{1}{6} [02\overline{2}3],$$
(1)

type B:
$$\langle c + a \rangle = \frac{1}{3} [11\overline{2}3] = \mathbf{b_l} + \mathbf{b_s} + \mathbf{b_t} = \frac{(1-\lambda)}{6} [02\overline{2}3] - \frac{\lambda}{6} [02\overline{2}3] + \frac{1}{6} [20\overline{2}3].$$
 (2)

Recent experimental findings report that alloying Y, Er, and Li can reduce the *c/a* ratio and promote the activation of $\langle c+a \rangle$ dislocations [16, 17]. We thus assume that the shuffling motion may origin from the deviation of *c/a* value from its ideal value. As shown in Figure 3(b), when *c/* a = 1.624, the length of leading partial dislocation for type B atom is larger than that of 1/6[20–23] (3.12 Å). Notably, when *c/a* is the ideal value of 1.633 (a = 3.198 Å and c = 5.222 Å), the length of leading partial dislocations for both type A and B atoms is equal to the ideal length of 1/6[2023] (3.14 Å). As shown in Figure 3(*c*), alloying Y can reduce the *c/a* ratio to 1.616, which causes a larger range of shuffling motion of Mg-Y than that of Mg, suggesting that alloying Y can promote the



FIGURE 3: (a) Sliding pathway of $\langle c+a \rangle$ dislocation by the zigzag dissociation mode involved shuffling motion. The length of leading partial dislocations when the *c/a* ratio is equal to (b) 1.624 and 1.633. (c) The zigzag dissociation modes of Mg-Y alloy. Orange, green, and cyan spheres indicate type A Mg atoms, type B Mg atoms, and Y atom, respectively.

formation of $\langle c+a \rangle$ dislocation on the $\{10\overline{1}1\}$ plane. On the basis of above analysis, we conclude that the presence of an alloying element which reduces the c/a ratio can help increase the range of shuffling motion and promote the formation of $\langle c+a \rangle$ dislocation on the $\{10\overline{1}1\}$ plane.

4. Conclusion

We propose, for the first time, a zigzag dissociation mode combined shuffling motion on the $\{10\overline{1}1\}$ plane. We found that the shuffling motion around the stable stacking fault position originates from the fact that the c/a ratio of Mg deviates from the ideal value. Our computational results provide novel insights into the dissociation mode on $\langle c+a \rangle$ dislocations in Mg and thereby represent a novel approach to identify alloying elements that can effectively enhance the plasticity of Mg alloys.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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