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Ab-initio study of the effect of rare-earth elements on the stacking faults of Mg solid solutions

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ABSTRACT

The effects of RE (RE = Pr, Nd, Gd, Tb, Dy) solute atoms on four basal stacking faults of Mg solid solutions have been studied using density functional theory. From the generalized stacking fault energy surface, both stable and unstable stacking fault energies are reduced obviously with the addition of RE elements, and the effect becomes weak with increase of the atomic number of RE elements. Due to the decrease of fault energies of I_2 stacking fault, the extended dislocation configuration tends to be stabilized and the ductility could also be improved by the addition of RE atoms. Then the deformation mechanisms are further studied by means of both the Rice and ZCT criterions. Finally, the electronic structure further reveals the underlying mechanisms for the effects of RE solutes on stacking faults of Mg solid solutions.

1. Introduction

Stacking faults are common two-dimensional defects and may be formed during the growth process and/or deformation process [1,2]. Mechanical properties of materials are closely related to stacking faults and dislocations. Especially stacking faults are directly associated with the dissociation of perfect dislocations into two Shockley partials and the energies of crystal twinning, which further affect strength, ductility and fracture of materials. Therefore, stacking faults are very important underlying factors for understanding and improving the mechanical properties of materials.

Unfortunately, it is difficult to accurately measure the stacking fault energies (SFEs) in experiments because the SFEs are small [3,4]. By contrast, *ab-initio* calculations have been considered to be an effective method to obtain the SFEs. Chetty et al. [1] have studied the basal stacking faults in hexagonal-close-packed (hcp) magnesium, including two intrinsic faults I_1 and I_2, an extrinsic fault E and a twin-like fault T_2. Our previous work also investigated systematically these basal stacking faults, and derived the generalized stacking fault energy surfaces and the corresponding stacking fault energies for pure magnesium [5]. However, theoretical investigations about the effect of solute atoms on stacking faults of Mg alloys are still very scarce [6,7].

In general, the addition of alloying elements has been one of the most effective ways to improve the mechanical properties of magnesium alloys owing to the solid-solution strengthening [8,9]. Recently, the rare earth (RE) metals and transition metals are widely used in the Mg alloys as the alloying elements. Especially the addition of RE elements is of major significance for improvement of the mechanical properties such as ductility, creep resistance, and casting characteristics [10–14]. To further improve the mechanical properties and understand the underlying mechanism, the investigations on stacking faults of Mg-RE solid solutions are necessary and urgent.

In this paper, the four basal stacking faults of the Mg-RE (RE = Pr, Nd, Gd, Tb, Dy) solid solutions have been studied systematically using density functional theory. After the structural optimization, the generalized stacking fault (GSF) energy surfaces (γ-surfaces) are calculated, then the stable and unstable stacking fault energies are obtained, and dislocation configuration, intrinsic ductility and deformation mechanism are further discussed through I_2 stacking fault. Finally, the electronic properties of stacking fault plane are analyzed in details.

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2. Method

The present calculations were performed using the Vienna *ab-initio* Simulation Package [15] based on density functional theory and the projector augmented wave (PAW) method [16]. The exchange-correlation energy functional was treated with the well-established Perdew–Wang (PW91) version of the generalized gradient approximation (GGA) [17]. The cut-off energy of plane wave basis set was chosen at 350 eV. In calculation of SFEs, periodic supercells of 2×2 unit cells with 12 layers were used for I_1, I_2 and T_2 stacking faults, and with 13 layers for E stacking fault. In Mg-RE solid solutions, one Mg atom at the center site of fault plane (the seventh atomic layer) was substituted with a solute atom RE (RE = Pr, Nd, Gd, Tb, Dy) [18], so the concentration of the solute atom is 2.08% for the whole system (1.92% for E stacking fault), corresponding to 25% monolayer coverage at the fault plane. A 10 Å vacuum region was added in the direction normal to the slip plane to avoid interactions with periodic images [19]. The Brillouin zone integrations were performed using k-points grids $7 \times 7 \times 1$ of γ-centered Monkhorst–Pack grids [20]. The total-energy calculation was performed using linear tetrahedron method with Blöchl correction [21]. The first order Methfessel–Paxton [22] with a temperature broadening parameter of 0.2 eV was used for structural optimization until the Hellmann–Feynman force on all atomic sites was less than 10^{-2} eV/Å. The convergence tests with respect to these parameters showed that the error bar for the total energy was less than 1 meV/atom. The γ-surfaces were calculated by displacing one part of the crystal with respect to the other along the slipping direction on the stacking fault plane. The positions of all the atoms were allowed to relax in the direction perpendicular to the stacking fault plane. The calculation details of γ-surfaces were described elsewhere [23].

3. Results and discussion

3.1. Structure parameters and stability

The structural optimization of pure Mg and Mg-RE (RE = Pr, Nd, Gd, Tb, Dy) solid solutions were firstly performed and the calculation results were listed in Table 1. The calculated lattice parameter a for pure Mg was 3.189 Å and the ratio of c/a was 1.628, showing good agreement with the experimental data [24] and the other theoretical results [2,25]. Therefore, the calculation of this work should be reasonable and reliable.

The lattice parameters and volume of Mg-RE (RE = Pr, Nd, Gd, Tb, Dy) solid solution systems were also shown in Table 1. It can be seen that in comparison with pure Mg, the lattice parameter a and volume V_0 of Mg-RE solid solutions are larger, while c/a values of Mg-RE solid solutions become smaller, due to the larger atomic radius of RE elements. With the increase of atomic number of RE elements, the lattice parameter a and volume V_0 of Mg-RE solid solutions exhibit a slightly decrease, while c/a values demonstrate a tendency of increase. It is expected that the reduction of the c/a ratios with the addition of RE elements play an important role in increasing the room temperature formability of Mg solid solution [26].

Table 1
The lattice parameters a (in Å), equilibrium volume V_0 (in Å^3), formation enthalpy H_f (in meV/atom) of Mg-RE (RE = Pr, Nd, Gd, Tb, Dy) solid solutions.

Material	This work		Experimental data		V_0	H_f
	a	c/a	a	c/a		
Mg	3.189	1.628	3.209	1.624	1097.59	0
Mg-Pr	3.223	1.608	–	–	1118.76	−1.341
Mg-Nd	3.222	1.609	–	–	1118.69	−1.402
Mg-Gd	3.215	1.613	–	–	1114.05	−1.581
Mg-Tb	3.213	1.613	–	–	1111.91	−1.641
Mg-Dy	3.211	1.614	–	–	1111.03	−1.684

The stability of Mg-RE solid solutions was also studied from formation enthalpy, which was calculated as $H_f = (E_{tot} - N_{Mg}E^{Mg}_{solid} - N_{RE}E^{RE}_{solid})/(N_{Mg} + N_{RE})$, where E_{tot} is the total energy of the supercell used in the present calculation, N_{Mg} and N_{RE} are the total number of Mg and RE atoms in supercell, respectively, E^{Mg}_{solid} and E^{RE}_{solid} are the total electronic energies per atom in the ground state of pure element solid of Mg and RE atoms. The negative formation enthalpy showed that Mg-RE solid solutions were thermodynamically stable. With increase of the atomic number of RE elements, the formation enthalpy was more negative, so the stability of Mg-RE solid solutions was stronger.

3.2. The effect of RE elements on stacking faults

For hcp Mg crystal, the typical slip plane is basal plane because it is the densest atomic plane. The sketch of the (0001) plane and the configurations of I_1, I_2, E and T_2 stacking faults are shown in Fig. 1(a and b), respectively. To study the effect of solutes on the stacking faults of Mg-RE solid solutions, four basal stacking faults of pure magnesium have been firstly studied. The calculated stable stacking fault energies of I_1, I_2, E and T_2 for pure Mg are 17.1 mJ/m^2, 33.8 mJ/m^2, 53.8 mJ/m^2 and 40.2 mJ/m^2, and the calculated unstable stacking fault energies of I_1, I_2, E and T_2 for pure Mg are 86.2 mJ/m^2, 87.6 mJ/m^2, 438.9 mJ/m^2 and 154.3 mJ/m^2, respectively, which are in general agreement with the previous theoretical values [1,2,5] and available experimental data [3,4].

The generalized stacking fault (GSF) energy surface (γ-surface) can provide a comprehensive description of stacking faults, so it is also very important for analyzing the dislocation core and revealing essential deformation mechanism [27–29]. Therefore, it is necessary to study the GSF energy surfaces (γ-surfaces) of Mg-RE (RE = Pr, Nd, Gd, Tb, Dy) solid solutions. Due to the similarity of the obtained γ-surfaces of basal stacking faults for Mg-RE solid solutions considered, only the γ-surfaces of Mg-Dy solid solution are shown in Fig. 2 as a representative example. From Fig. 2, it can be seen that similar to the γ-surfaces of pure Mg [5], in Mg-RE solid solutions the $[10\bar{1}0]$ direction is still the lowest energy path for I_1, I_2 and T_2 stacking faults because the unstable stacking fault energy along $[10\bar{1}0]$ slip direction is lower than that along $[11\bar{2}0]$ slip direction. Furthermore, the positions of stable stacking fault energies of Mg-RE solid solutions are still located at the $b/3[10\bar{1}0]$ ($b = \sqrt{3}a$), while the positions of unstable stacking fault energies are located at the $b/6[10\bar{1}0]$ for I_2 and T_2 stacking faults and $b/2[10\bar{1}0]$ for I_1 stacking fault, respectively. It is worthy of mentioning that for extrinsic stacking fault E, the unstable stacking fault energy along $[10\bar{1}0]$ direction is just the same as that along $[11\bar{2}0]$ direction due to the same initial configuration of inserting an atomic plane into the pure Mg. However, the GSF energies along $[10\bar{1}0]$ direction go down more quickly than that along $[11\bar{2}0]$ direction, and the stable stacking fault energy is also located at the $b/3[10\bar{1}0]$ displacement, so $[10\bar{1}0]$ slip direction of E stacking fault is still the lowest energy path. On the other hands, in comparison with the previous work about the γ-surfaces of pure Mg [5], all the GSF energies in the γ-surfaces for the four stacking faults become smaller by doping the RE elements.

To further reveal the effect of RE elements on the four basal stacking faults, the γ-curves of pure Mg and Mg-RE (RE = Pr, Nd, Gd, Tb, Dy) solid solutions along the $[10\bar{1}0]$ direction have been further plotted, as shown in Fig. 3, and the computed values of stable and unstable stacking fault energies are listed in Table 3. It is noted that