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24R-type LPSO microstructure of the novel Mg-Y-Zn alloy

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Abstract. The microstructue of the novel long period stacking ordered(LPSO) structure in Mg-Y-Zn alloy has been systematically studied based on the density functional theory. The lattice positions of the Y and Zn atoms are determined theoretically, it is shown that the additive atoms are firstly enriched in the stacking fault layers at the two ends, a small amount are distributed in the interior stacking fault layers of the structure. And the arrangement of these Y and Zn atoms trends to be along the diagonal line of the unit cell.

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Key words: Mg-Y-Zn alloy, LPSO, additive atoms, density functional theory, microstructure

1 Introduction

Mg-based alloys have become more and more important nowdays, because of its low density, high specific strength and elastic modulus and high recycling efficiency [1]. Mg-based alloys with excellent properties have been applied in many fields such as microelectronics, automobile and aerospace industries. To further improve the mechanical properties of Mg-based alloys, great endeavor has been made through adding rare-earth (RE) elements and transition metal elements. Recently, superior performance of Mg-Y-Zn alloy with extremely high tensile yield strength of 610MPa and elongation of 5% has been recently developed by rapidly solidified (RS) powder metallurgy [2-5]. Furthermore, the Mg-Y-Zn alloy still shows high corrosion resistance at room temperature [6].

The excellent properties of Mg-Y-Zn alloy are due to the hcp (2H)-Mg fine grain matrix of 100-200 nm with a novel long-period stacking ordered (LPSO) phase and homogeneously dispersed $Mg_{24}Y_5$ fine particles of less than 10 nm [7-9]. The morphological, crystallographic and chemical characterizations of the LPSO phase have been performed

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by conventional transmission electron microscope (CTEM) [7], high-angle annular dark-field scanning TEM with Z-contrast [8], high-resolution transmission electron microscope (HRTEM) observations [10], and three-dimensional atom probe [11]. So far, five kinds of LPSO structures (6H, 10H, 14H, 18R, and 24R) are observed in these Mg-based alloys [7]. The 6H, 14H and 18R structures are dominantly observed while the 10H and 24R are relatively rare. The novel LPSO structures have also been observed in other Mg-RE-Zn alloys and Mg-RE-Cu alloys [11-14]. Due to its importance in improving the mechanical properties of the Mg-based alloys, investigation of the structure and properties of the novel LPSO is crucial for design and application of the alloy materials.

2 Computation details

The present work is based on density functional theory at the level of the generalized gradient approximation (GGA) (using the PW-91 exchange-correlation functional). The method was implemented in the Vienna Ab initio Simulation Package (VASP) program, which used a plane-wave basis set with a kinetic energy cutoff at 300 eV and ultra-soft pseudopotentials for the election-ion interaction, the valence electron configurations considered are 3*s*, 2*p* for Mg, 3*d*, 4*s* for Zn and 4*s*, 4*p*, 5*s*, 4*d* for Y. For the 24R-type (ABABABABCACACACABCBCBCBC) LPSO structure in Mg-Y-Zn alloy, the supercell with 96 atoms (2×2 unit cell of 24 layers) is adopted. The Brillouin zone (BZ) is sampled with a mesh of $8\times8\times1$ k-points of Monkhorst-Pack scheme for 2×2 unit cell of 24 layers as supercell of 24R-type LPSO structure. And $10\times10\times1$ is chose for the electronic density of states. The convergence tests with respect to these parameters show that the error bar for the total energy is less than 1meV/atom ($\approx$0.1kJ/mol) [15]. These parameters have been tested to be sufficient for convergence. Structural optimization is performed using the first-order Methfessel-Paxton method with a temperature broadening parameter of 0.2 eV, and the positions of atoms are fully relaxed until the total forces on each ion are less than 0.02 eV/Å. Ionic relaxation and electronic energy minimization were performed using the conjugate gradient (CG) algorithm. For the calculation for density of states (DOS), the tetrahedron method with Bloch corrections were used as implemented in VASP.

3 Results and discussion

3.1 The microstructure

The lattice constants of pure Mg, Y and Zn are calculated to test the calculation parameters and pseudopotentials. The obtained results for pure Mg is $a=0.320$ nm and $c=0.513$ nm, for Y $a=0.365$ nm and $c=0.567$ nm, for Zn $a=2.67$ nm and $c=0.484$ nm, respectively. These results are agreement well with experimental values and other theoretical calculations [16]. So the present calculation results are reasonable and reliable.