First principles calculations of Mg-Zn-Y alloys

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The origin of the excellent mechanical properties of Mg-TM(transition metal)-RE(rare earth) alloys is due to the query microstructures with the long periodic stacking order (LPSO). Thus the mechanism of this microstructure formation is the one of the key issues of the newly developing light-weight Mg materials. The LPSO Mg alloy, its typical composition of $Mg_{97}Zn_1Y_2$, shows 18R structure with the long period stacking sequence of the mixture of hexagonal(h) and cubic(c) layers and added elements of Zn and Y are observed to be enriched in the cubic layers.

In this research, we have investigated the energetic assessment of these structures by the first principles calculations in order to reveal the mechanism of LPSO formation. We have constructed some lattice models using MedeA and calculated the structure energies using Vienna Ab Initio Simulation Package (VASP) code. The cut-off energy was 600 eV and the k-point meshes were determined from the dimensions of models.

18R structure with pure Mg locates on the segment between pure cubic (3C) and pure hexagonal (2H) structures as shown in Fig. 1. It means that the additions of Zn and Y should stabilize the 18R structure at the ground state. Single substitution of Zn or Y with Mg in hcp and/or fcc lattice shows no clear difference. The Zn-Y pair substitution with Mg, however, shows a notable decrease of energy against the previous isolated single substitution. In 18R structure, Zn-Y pair locates near c sites. Figure 2 shows the energies of several configurations of the first nearest neighbouring Zn-Y pairs. The ch configuration, where Zn locates on c site and Y locates on h site, is the lowest energy among the several c and h configurations.

We will also show Monte Carlo simulations with two different scenarios for explaining the LPSO structure formation with the energetic speculations from those first principles calculations.

Keywords: LPSO, Monte Carlo simulation

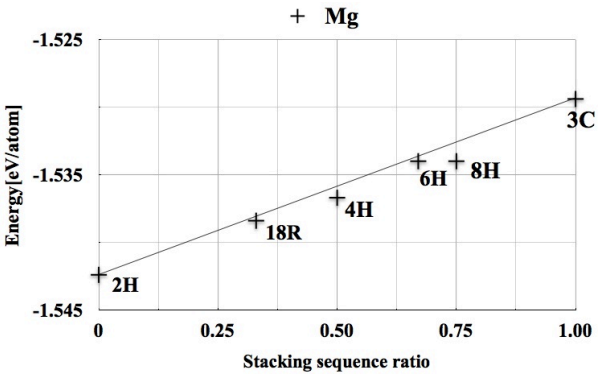

Fig. 1 Pure Mg structure energy against stacking sequence ratio of c- and h-sites.

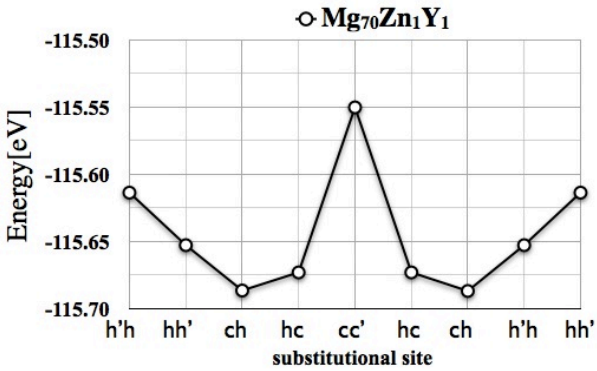

Fig. 2 Energies of 18R Mg structures with Zn and Y elements locating on c or h sites. The notifications are described in the text.