

## Solute configuration energies of Mg-Zn-Y alloy

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The excellent mechanical properties of Mg-TM(transition metal)-RE(rare earth) alloys have been reported to be due to the query microstructures with the long periodic stacking order (LPSO). 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. The added elements of Zn and Y are observed to be enriched in the cubic layers. The mechanism of this microstructure formation is one of the key issues of the newly developing light-weight Mg materials.

In this research, we have explored the energetic investigation on the LPSO structure by the first principles calculations in order to reveal the mechanism of LPSO formation. Monte Carlo simulations show two possible scenarios for explaining the LPSO structure formation; one is the periodic stacking fault induced and the other is the ordering of solute atoms induced. We have constructed a few 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.

As shown in Fig. 1, 18R structure with pure Mg locates on the segment between pure cubic (3C) and pure hexagonal (2H) structures, which 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 from the isolated single substitution. In 18R structure, the nearest neighboring Zn-Y pair with Zn locating on c site and Y locating on h site, is the lowest energy among the several c and h configurations. Fig.3 shows the energy dependence on the periodicity of solute ordering. Number on x-axis shows the ordering period. The atomic configurations named (a) parallel and (b) reverse for period of four shows on the right panel. In hcp-Mg, 6 or 7 periodic structures show the relatively low energies, which indicate the solute ordering in hcp-Mg occurs before the stacking ordering of 18R Mg. The energy difference, however, is relatively small and the other possibility will be discussed on the symposium.

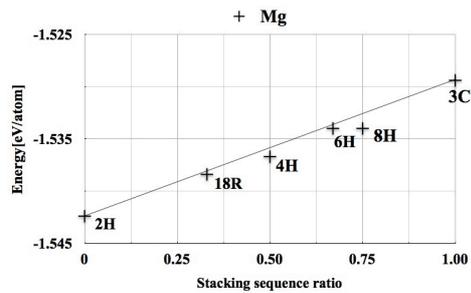


Fig. 1 Pure Mg structure energy against stacking sequence ratio of c- and h-sites.

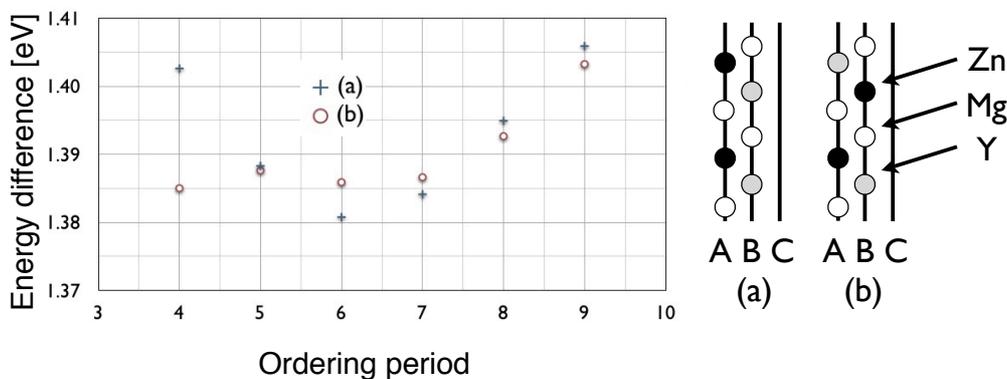


Fig. 2 Energy dependence on solute ordering periodicity. Number on x-axis shows the ordering period. The atomic configurations named (a) parallel and (b) reverse are schematically drawn for the period of four shows on the right panel.