First principles calculations on Mg Alloys with Long-Period Stacking Ordered Structure

Y. **Masaki**[1], Y. Yamamoto[1], and S. R. Nishitani[1]

1 Department of Information, Kwansei Gakuin University, Gakuen 2-1, Sanda, 669-1337 Japan. (masaki@kwansei.ac.jp)

Long periodic stacking ordered (LPSO) Mg alloys show excellent mechanical properties, and the mechanism of such a query microstructure formation is the one of the key issues of the newly developing light-weight Mg materials. The LPSO Mg alloys, its typical composition of $Mg_{97}Zn_1Y_2$, show 18R structure with the long period stacking sequence of the mixture of hexagonal and cubic layers and added Zn and Y atoms are enriched in 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 in Mg alloys. We have performed the atomistic model constructions using MedeA and the structure energy calculations using Vienna Ab Initio Simulation Package (VASP) code. The cut-off energy was 600 eV and the k-point meshes were determined from the shapes of models. Fig. 1 shows the energies of the stacking sequence ratios between pure hexagonal(2H) to pure cubic(3C) stacking sequences. The 18R structure locates on the line between 2H and 3C, and either do the other structures, which indicates that the 18R structure is not uniquely stable comparing from those with the other stacking sequences. The additives of Zn and Y, however, affect on the stability of 18R structure. Fig. 2 shows the energy dependency on the special site selections of Zn and Y atoms, which locate both or either on the cubic layers(No.5 and No.6) with the second and first nearest neighbor sites. Those results indicate that the ordering of the additives makes 18R structure more stable. The other detailed discussions will be given on the poster.

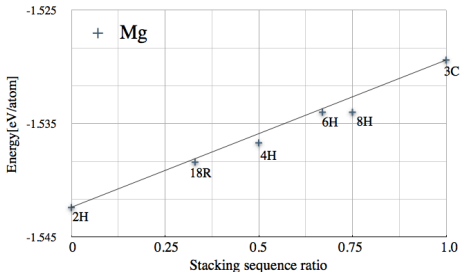

Fig1. Structure energy dependency on the stacking sequence ratio between pure cubic and pure hexagonal sequences.

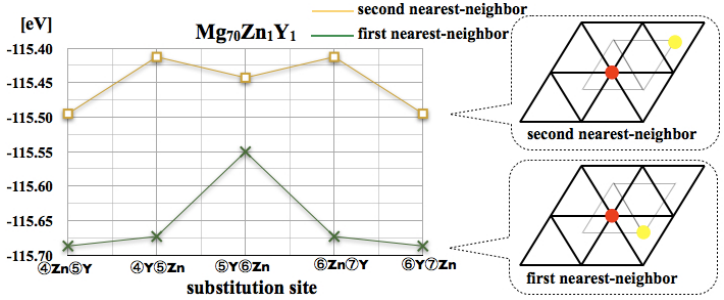

Fig2. Additions effects of the structure energy on the long stacking sequence structures.