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First principles calculations of 18R Mg alloys

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Long periodic stacking ordered (LPSO) Mg alloys show excellent mechanical properties, and the 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 inter-layer interactions are short and good estimations of linear combination between hexagonal and cubic stacking energies. Fig. 2 shows the energy differences between cubic and hexagonal structures of the different sizes with the Zn and Y additives. The energies are almost linearly dependent on the system size, which are expected from the linear dependency among 2H and 3C. The exceptions are observed in 24 atoms models with Y and Y+Zn, which indicate that these structures are relatively more stable than the simple averages. The other detailed discussions will be given on the poster. We will also report the results of Monte Carlo simulation of atomistic level LPSO formations.

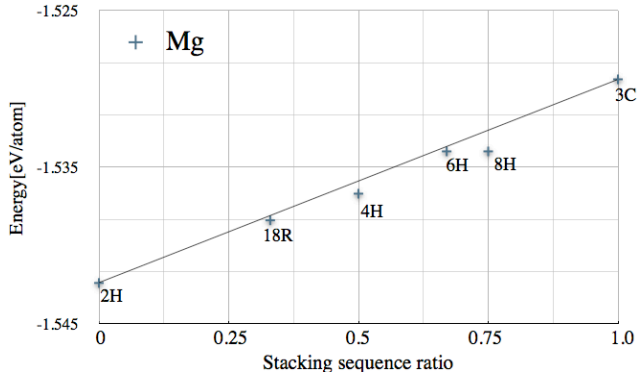

Fig1. Stacking sequence ratio between pure cubic and pure hexagonal dependency on the structure energies.

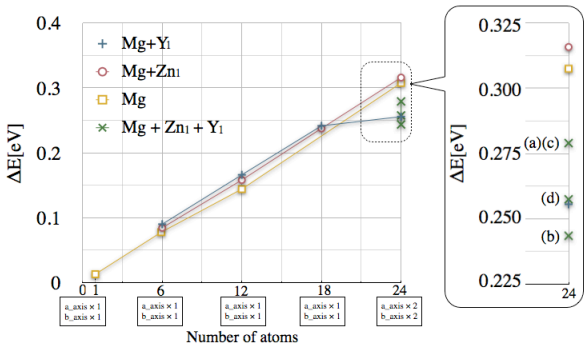

Fig2. Additions effects of the structure energy on the long stacking sequence structures.