First principles calculations of stacking fault energy of Mg-Zn-Y

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Long period stacking ordered (LPSO) structure has been very recently discovered in Mg base alloys, whose specific strength is higher than that of super duralumin, and shows good corrosion resistance [1]. One of the typical LPSO structures is 18R structure as shown in Fig.1, where the solute atoms are observed to be condensed at the stacking fault region. In this research, we aim to investigate the formation mechanism of this novel microstructure by using the first principles calculations.

The first principles calculations have been performed with VASP. The models are constructed by the 2x2x9 super cells of 2H structure for avoiding the interaction between stacking faults. Zn and Y are located on the 9th layer of 2H-Mg. The blocks below 9th and above 10th layers were sliding each other, and make the c-site as shown in Fig.1. The energy changes during the sliding with and without Zn and Y atoms are compared.

The activation energy of the stacking fault formation with Zn and Y added model shows about 4.0 meV/m^2 (65 mJ/m^2) lower than that without Zn and Y (Fig.2). These results suggest that the addition of Zn and Y makes the stacking fault formation easy.

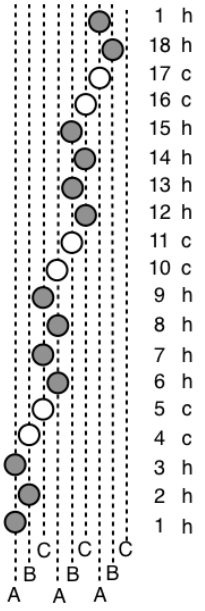

Fig.1: Illustration of atomic stacking of 18R-Mg alloy.

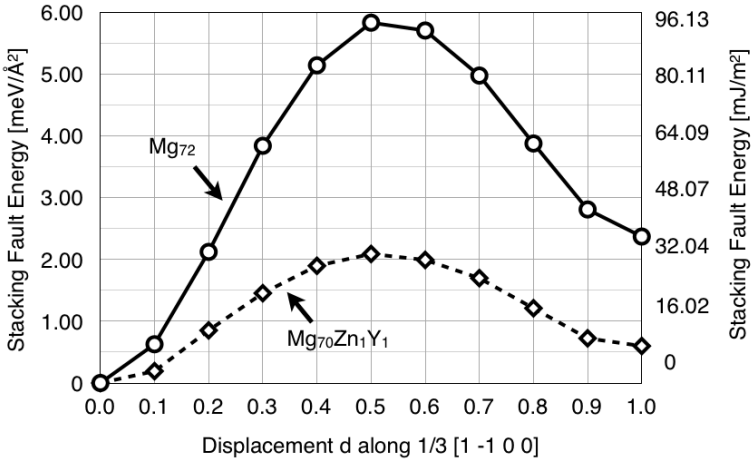

Fig.2 : The stacking fault energy of displacement along vector d = 1/3[1-100] . The solid and broken lines show the stacking fault energies of Mg_{72} and $Mg_{70}Zn_1Y_1$, respectively.

References

[1] Y. Kawamura, K. Hayashi, A. Inoue and Y. Masumoto: Mater. Trans., **42** (2001) 1172-1176.