Energetic assessment between $L1_2$ and small clusters in Mg-Zn-Y alloy

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The authors have performed the energetic assessments on the formation mechanism of Mg-LPSO structure. The interacation energy between the isolated or pair formed solute atoms of Zn and Y and the $L1_2$ cluster located at the stacking faults shows the monotonous decrease on the interlayer distance, which have done by the first principles calculations. The most reliable scinario on our results is "After the initial $L1_2$ clusters are formed at the stacking faults, the additional solute atoms are swept out and induces the other stacking fault formation[1]." The monotonous decrease shows no characteristic feature on the middle range ordering expected by the long periodicity of LPSO structure. In this research, we have performed the similar calculations on the interactions between the $L1_2$ cluster and the cluster which is smaller than the $L1_2$ cluster but larger than the Zn-Y pair.

Kiyohara *et al.* have reported that a $L1_2$ like cluster embedded in hcp lattice shows the unique relaxed structure which is almost split in two smaller clusters[2]. The size of these clusters are close to those observed in the initial stage of the formation of the LPSO structure from the amorphous phase detected by the small angle scattering reported by Okuda *et al.*[3] In this research, these smaller clusters were embedded in the slab model with 18 stacking layers as shown in Fig.1. The relaxed structures and energies are obtained by the first principle calculation of VASP.

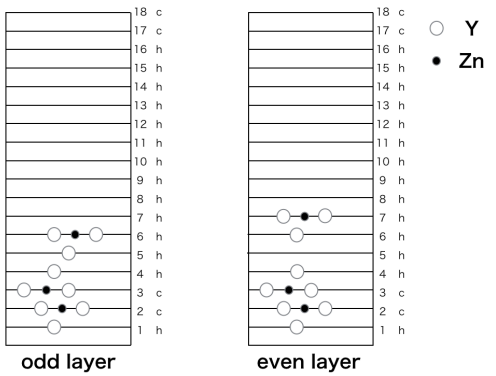

Figure 1: Schematic drawings of the side view of models.

At first, we have checked the smaller cluster energy change for the splitting, whose directions are vertical and horizontal. The vertically splitted cluster shows the lower formation energy and stable structure. This cluster is embedded in each layer apart from a $L1_2$ cluster located at the stacking fault, as shown in Fig.1. The total energy change calculated by VASP shows the tendency as shown in Fig.2. The relaxation of the fourth layer is failed. The energy change is not a monotounous tendency but the slight minimum at the middle range of 4-5 layers. We are now performing the same calculations with a size larger model for checking the further distance interactions.

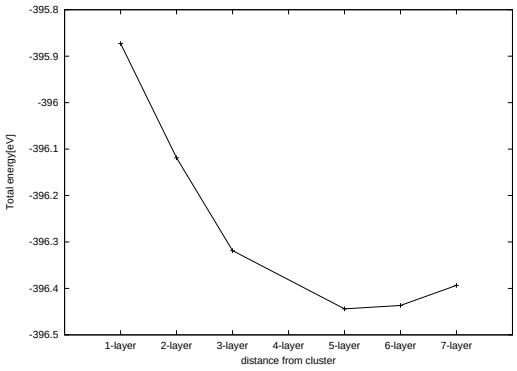

Figure 2: Interlayer distance dependency of interaction energy between $L1_2$ and smaller clusters.

References

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