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First principles calculations of solute pair sweeping out from stacking faults in Mg-Zn-Y alloy

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The formation mechanism of the long-period stacking-ordered (LPSO) structure of the Mg-Zn-Y alloy was investigated through energy assessments using first-principles calculations. The solute atom pairs locating at the same layer show a monotonous decrease of the energy as they get away from the precipitated $L1_2$ cluster. The swept-out solute atoms are condensed a few layers away from the stacking-fault regions and accelerate the introduction of other stacking faults. The $L1_2$ cluster in hcp lattice showed the splitting tendency of its form. A new scenario in the formation of the LPSO structure is proposed.

Keywords:*First principles calculation, long period stacking ordered (LPSO) structure, $L1_2$ cluster*

1. Introduction

Long period stacking order (LPSO) structure in Mg-Zn-Y alloy was first found by Kawamura at 2001[1)], and is characteristic with the long periodicity of stacking-faults and solute condensation at the stacking-faults. For investigating the formation mechanism of such a complex structure, the authors have made up some scenarios and assessed the possibility of each step by the first principles calculations[2, 3)].

Many assessed steps predicted from the scenarios showed the energy differences between the initial and final configurations less than 0.1eV, and such steps are hardly to be the main controlling process during the formation of LPSO. Two critical energy changes have been observed[3)]. The first one is the notable drop of the activation energy for the stacking fault introduction when Zn and Y atoms are located there. The second one is the strong repulsive interaction between the solute Y atom and the $L1_2$ cluster precipitated at stacking faults observed experimentally[4, 5)]. In this paper, the authors reported the interaction of the $L1_2$ cluster against Zn-Y solute pair and the splitting of the cluster shape in hcp lattice assessed by the first principles calculation. They also give a new scenario conducted from these possible steps.

2. Calculation method

The first principles calculations are performed by the Vienna Ab-initio Simulation Package(VASP)[6)], where GGA Perdew-Wang 91 is used for exchange-correlation interaction[7)], and Projector Augmented Wave(PAW) method is used for the pseudo-potentials[8)]. The cut-off energy was set at 300 eV, and the k-point mesh was $9 \times 9 \times 1$. The convergence criteria are 10^{-5} eV and 0.02eV/Åfor energy and force, respectively.

The used slab models are as follows. The stacking fault slab model is constructed for checking the interaction energy between the cluster and the Zn-Y solute pair. The model is shown in Fig.1, and is constructed by 18 layers of Mg with ABAB... stacking denoted by 'h', and including two stacking faults of ABC staking denoted by 'c'. The 'c' layers are located at 1-2 and 5-6 layers. One $L1_2$ cluster is located around 5-6 layers. The solution pair of Zn-Y is inserted in each layer of 8th through 12th, which indicates the 1st through 6th layer separating from the cluster or the stacking fault.

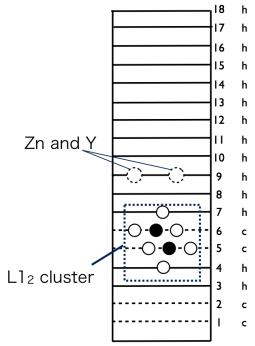

Fig. 1 Slab model include two stacking faults, one cluster and two solute atoms.

3. Results and discussions

3.1 Interaction energy between cluster and Zn-Y pair

Fig.2 shows the interaction energy change between the cluster and the Zn-Y solute pair depending on the interlayer distance of them. The fixed and full relaxed total energies are plotted in the same graph but the scales are different as in the left and right axes. The two bended lines plotted below each plots are eye guide lines for the minimum energies of each layer distance. For the fixed configurations, the interaction energy at the first layer shows most stable. The relaxed energy, however, shows the monotonous decrease against the interlayer distance, and the energy change reached to be 0.1 eV. These results indicate that the Zn-Y solute pair shows strong tendency of the sweeping out from the stacking fault or $L1_2$ cluster.

3.2 Cluster energy and its splitting

The $L1_2$ clusters observed by Yokobayashi et al.[4)] and Egusa and Abe[5)] are inserted in fcc, 6H and 18H slab models. The atomic configuration of the cluster in hcp lattice has not been reported, thus we made up models by sliding up-half of $L1_2$ cluster as shown in Fig.3. Two types

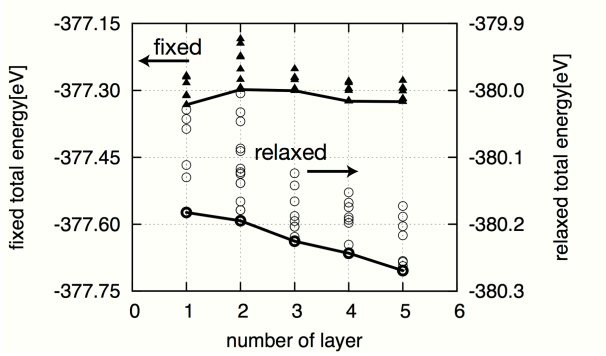

Fig. 2 Total energy dependence on the number of layers between cluster and Zn-Y pair.

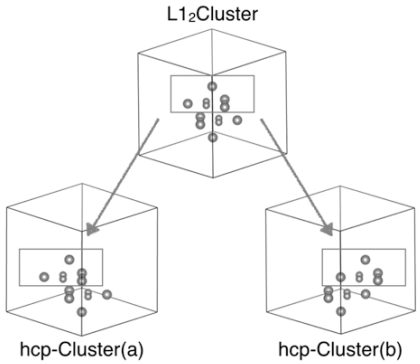

Fig. 3 Schematic illustrations of the original $L1_2$ cluster and two types of clusters in hcp lattice, where the upper half of the cluster enclosed by the square slides opposite direction.

of clusters are considered due to the different direction of the sliding, and will be called type-(a) and type-(b) respectively.

Energy change due to the insertion of the Zn-Y cluster in each slab model of hcp, fcc, 6H, or 14H lattices are shown in Table I. Energies are calculated from the segregation limit of solution. The cluster energies show that the cluster in fcc is unstable, and clusters in 6H and 14H show similar energies. In hcp lattice, type-(a) cluster is most unstable, but type-(b) cluster is most stable. Especially type-(b) cluster is more stable than that in 14H lattice.

The type-(b) cluster in hcp lattice shows very unique configuration as shown in Fig.4(b), after the relaxation. This cluster is almost split to two smaller clusters. The size of this smaller cluster is close to those observed experimentally by Okuda et al.[9)]

Table 1 Energy of Zn-Y cluster inserted in hcp, fcc, 6H, and 14H lattices.

	hcp(a)	hcp(b)	fcc	6H	14H
E_{cluster}[eV]	-3.04	-4.42	-3.78	-4.04	-4.05

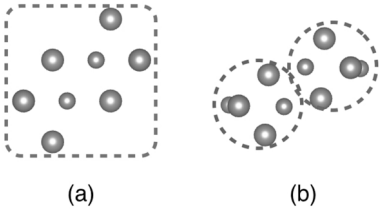

Fig. 4 Close views of (a) fixed and (b) relaxed configurations of the cluster type-(b) in hcp lattice.

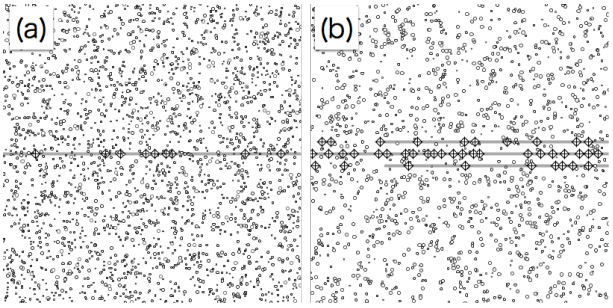

Fig. 5 Newly proposed scenario, where the marks are described on text in detail.

4. Conclusion and newly proposed scenario

Now the authors propose a new scenario of the LPSO structure formation as shown in Fig.5. The stacking fault marked as an horizontal line in the center aggregates solute atoms, which form many clusters marked by diamond symbol. After clusters are formed, the other solute atoms are swept out from the stacking fault, and stayed a little away from it. The solute atoms accelerate the introduction of the other stacking faults as reported by Sakamoto et al.[3)] as shown in Fig.5(b). These steps are repeated, and the LPSO structures grow vertically. The small clusters observed in hcp lattice in Fig.4(b) are candidates of moving unit of the solute atoms, instead of the vacancy mechanism of usual isolated atoms.

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