Energetic assessment on formation of Mg-LPSO structure

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LPSO(Long Period Stacking Order) structure in the Mg-Zn-Y alloy was first found by Kawamura in 2001[1]. It's superior mechanical properties and lightness attract attention as the next generation structural materials for the flight vehicle. The authors have performed the energetic assessments of the first principles calculations on each step of the formation mechanism of LPSO[2,3]. We've found that the $L1_2$ clusters locating at the stacking faults shows repulsive energy against the solution atoms of Zn and Y. We will report the calculation details and the induced scenario of the LPSO formation at this conference.

We use VASP for the first principles calculations. We made slab models including two stacking faults and a $L1_2$ cluster, which is observed by Yokobayashi *et al*.[4] and Egusa and Abe[5]. Zn and Y pair is locating in the same layer separating from the cluster. The atomic configurations are fully relaxed. As shown in Fig.1, the total system energy shows monotonous decrease with increasing the distance between the cluster and the solution pair. The energy difference reached about 0.2 eV, which means the Zn-Y pair is swept out from the cluster locating at the stacking fault.

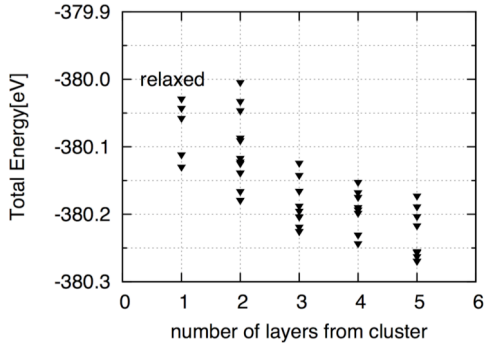

Fig.1: Interaction energy change between solute pair and $L1_2$ cluster.

We now adapt a scenario illustrated in Fig.2. A stacking fault, which is at first introduced by the thermal stress, collect solute atoms, which forms clusters marked as 'キ' in the left panel of Fig.2. The additional solute atoms are swept out from the stacking faults and concentrated on the few layers away from the first stacking fault. The condensed solute atoms lead the other stacking faults occurrence, as illustrated in the right panel of Fig.2. The repeated loop of these steps makes the stacking faults periodically.

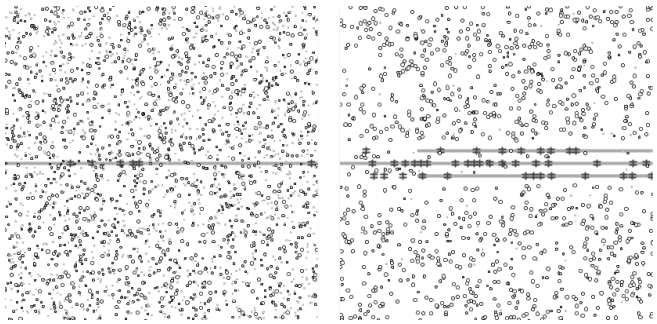

Fig.2: Schematic drawings of new scenario for LPSO formation.

[1] Y. Kawamura, K. Hayashi, A. Inoue, T. Masumoto, Mater. Trans., **42**, (2001) 1172.
[2] Y. Yamamoto, Y. akamoto, Y. Masaki and S. R. Nishitani , Mater. Trans., **54**, (2013), 656.
[3] Y. Sakamoto, C. Shirayama, Y. Yamamoto, R. Kubo, M. Kiyohara, and S. R. Nishitani, Mater. Trans., **56**, (2015), 933.
[4] H. Yokobayashi, K. Kishida, H. Inui, M. Yamasaki, Y. Kawamura, Acta Mater., **59**, (2011), 7287.
[5] D. Egusa, E. Abe, Acta Mater., **60**, (2012), 166.