

First Principles Calculations for LPSO formation scenarios

Shigeto R. Nishitani, Yosuke Yamamoto, Yuichi Sakamoto, and Yoshihiro Masaki

Department of Informatics, Kwansai Gakuin University, Gakuen 2-1, Sanda, 669-1337, Japan, nishitani@kwansai.ac.jp

The formation mechanism of the long period stacking ordered (LPSO) structure is still under discussion. The players on the stage are two: the stacking faults (SF) and the solute atoms. Two simple scenarios are immediately derived: 1) periodic stacking faults are first induced and then the solute atoms are concentrated around each SF layer, or 2) middle range solute ordering is first occurred and then the stacking faults are induced. The aim of this research is checking the scenario by the energy assessments using the first principles calculations.

The first principles calculations have been performed with VASP(Vienna Ab initio Simulation package) for the Mg-Zn-Y system. For investigating the solute orderings, many configurations have been checked. For the interactions of solute-solute atoms, pair-pair solutes, or SF-solute atoms, the energy changes are very small or attracting the solute atoms each other. The large energy contribution is only observed in the model for the interaction between clusters and solute atoms. When we changed the distance between the $L1_2$ cluster and the Zn atoms, the energy decreased monotonously in the range of 0.2 eV as shown in Fig.1.

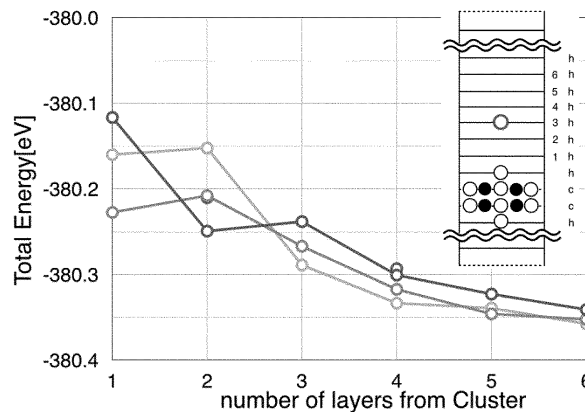


Fig.1 Energy changes on the inter-distance between $L1_2$ cluster and Zn atom. Schematic configuration of them is shown in the inset. Note that four lines represent the different equivalent sites but deviations are small.

The other critical change is observed in the solute atoms effect on the SF energies. Two blocks below and above the SF were sliding each other as schematically drawn in the inset of Fig.2. The energy changes during the sliding with and without Zn and Y atom pair are compared. The activation energy of the stacking fault formation with Zn and Y added model shows the one third of that without Zn and Y as shown in Fig.2.

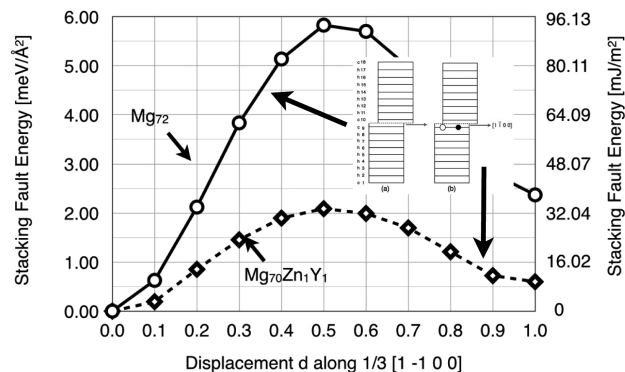


Fig.2 Energy changes on the displacement along $[1 -1 0 0]$, where solid and dotted lines represent with and without solute pair respectively. Note that the energies at $x=1.0$ mean the SF energy, and at around $x=0.5$ mean the activation energy of SF.

After the first principles energy assessment, we have a new scenario for the LPSO formation: 1) a SF attract the solute atoms and make $L1_2$ clusters, 2) additional solute atoms are swept out and condensing at a few layers off from the SF, and 3) this condensation makes other SFs induced easily.