First principles calculastions of structure energy difference of semiconductor compounds

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The stacking fault energies control the dissociation widths of the dislocations and thus important parameters of the mechanical or electronic properties of materials. These energies are precisely estimated by the direct observations of week beam or high resolution images of transmission electron microscopy. The stacking fault region in zincblende or wurtzite crystals has the wurtzite or zincblende structure, respectively, and therefore, the stacking fault energy of a tetrahedrally coordinated crystal is closely related to the free energy difference between the zincblende and the wurtzite structures. The energy difference of these structures, however, are hardly determined experimentally.

In this paper, we have performed the ab-initio electronic structure calculations on the zincblende-wurtzite energy differences. The plane wave basis calculations have been performed using the Vienna Ab Initio Simulation Package (VASP) with the GGA Perdew-Wang 91 exchange-correlation functional, a projector augmented-wave (PAW) ion-core orbital description, 0.1[1/Å] of the k-point mesh, and a cut-off energy of 1000 eV.

The relations between the experimentally determined stacking fault energies (γ') [1] and the calculated structural energy differences (ΔE) are shown in Fig. 1. γ' shows positive correlation with ΔE except CdSe. The lineality of the relation, however, shows not so strong. We are under consideration about these disagreements.

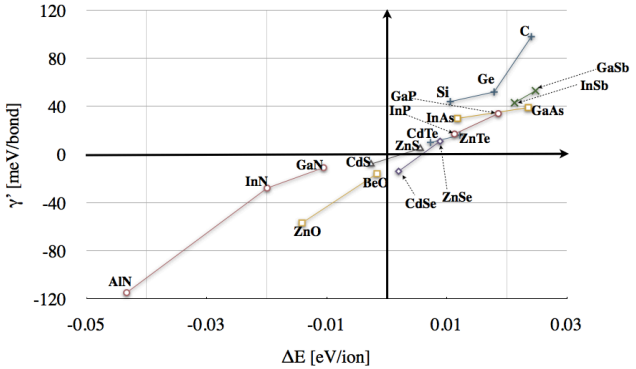

Fig.1 Stacking fault energy(γ') and the structural energy difference between zincblende and wurtzite(ΔE).

[1] S. Takeuchi, and K. Suzuki, "Stacking Fault Energies of Tetrahedrally Coordinated Crystals," Phys. Stat. Sol., (a) **171** (1999), 99-103.