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First principles calculations of stacking fault energy of P doped Si crystal

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Very recently, the authors have reported that the variation in stacking fault energy with annealing at 1173 K in Czochralski-grown silicon crystals heavily doped with n- or p-type dopant atoms[1]. In n-type crystals, the stacking fault energy decreased with increasing annealing time. As the concentration of dopant atoms increases, the stacking fault energy decreases. On the other hand, the energy was unchanged during annealing in p-type and non-doped crystals. These results imply that n-type dopant atoms segregate nearby a stacking fault, via their thermal migration. In this research, we investigated that the dopant effect of phosphorus is confirmed by the first principles calculations. The slab model including a stacking fault has been constructed, and been calculated by the VASP(Vienna Ab-initio Simulation Package) code with the cut-off energy of 1000eV and PAW potentials. One P atom is putted in the model and compare the energies and interatomic distances.

Fig. 1 shows the site dependency of the energy. The left pannel shows the schematic model of the slab, where the c and h represent the cubic and hexagonal stacking sequences, respectively. Thus the stacking fault are located at the site numbers of 9-10 and 11-12. In this case, because of the small unit size of slab, the replacement of one atom means that the atoms in a whole layer are replaced. The structure energies of P added Si slab show the relative stable when the P atoms are located around the sacking fault. This result strongly suggests that the lowering of the stacking fault energy is due to the P enrichment nearby the stacking fault during the annealing.

[1] Y. Ohno, T. Taishi, Y. Tokumoto, and I. Yonenaga, J. Appl. Phys. 108(2010), 073514.

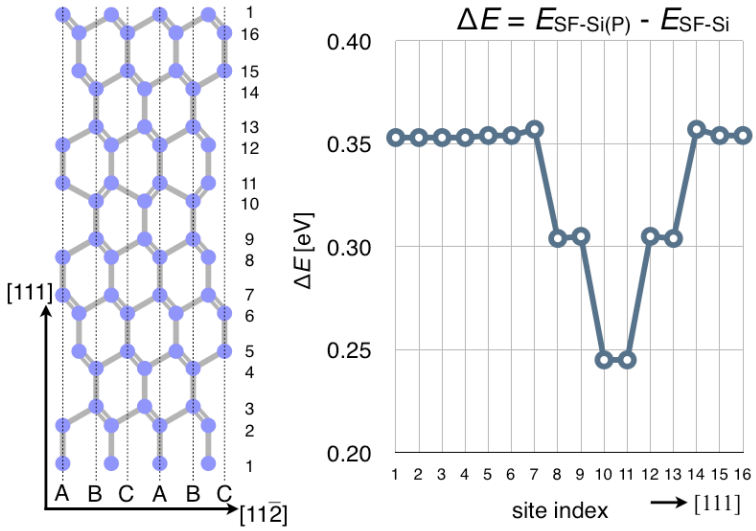

Fig.1 Schematic slab model and the energy dependency on site.