First principles calculations of the solution energy of dopant in Si crystal with stacking fault

Yosuke Yamamoto[1], Y. Ohno[2], Y. Tokumoto[2], I. Yonenaga[2], and S. R. Nishitani[1]

[1]*Department of Informatics, Kwansei Gakuin University, Gakuen 2-1, Sanda, 669-1337 Japan*

[2]*Institute for Materials Research, Tohoku University, Katahira 2-1-1, Aoba-ku, Sendai 980-8577, Japan*

Recently, The authors have reported that the interaction between the dopant atoms and stacking faults in Si crystal [1]. When P and As are doped, the stacking fault energies decrease with increasing annealing time. On the other hand, when B is doped, the stacking fault energy remains unchanged. In this research, we have calculated that the dopant atom dependency of the stacking fault energy by the first principles calculations.

VASP(Vienna Ab-initio Simulation Package) code was used for the energy calculation, and the cut-off energy were set 350eV and PAW potential was used. Fig. 1 shows the calculation model of Si crystal with stacking fault plane locating between the 9 and 10th layers. The c and h represent the local stacking order of fcc and hcp, respectively. The p-type (B, Al, Ga, In) or n-type(N, P, As, Sb) dopant atom was substituted with a Si atom at each layer and the solution energies were calculated from the difference from the pure Si slab model with a stacking fault.

We used two slab models with 1x1 and 2x2 unit cells for the basal plane. Since the dopant atom is substituted with the one atom, the dopant concentrations in the layer are 100% and 25% for 1x1 and 2x2 units, respectively. Fig.2 shows the top views of the doping layers in those two slab models. Fig. 3 shows the site dependency of the solution energy for the case of P dopant, where solid and dotted lines represent the dopant concentration of 25% and 100%, respectively. The solution energy shows lower level when P locates around the stacking fault. Other dopant atoms except B and N also show the same tendency. These results indicate that the elements, such as P, Al, Ga, In, As, and Sb, tend to enrich around the stacking fault region and reduce the stacking fault energy, which are consistent with the experimental results[1].

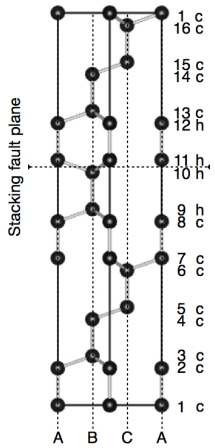

Fig.1 Schematic slab model with a stacking fault.

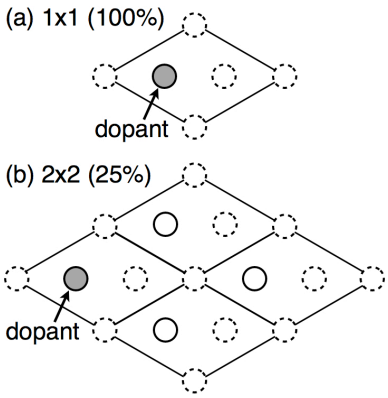

Fig.2 The top views of the doped layers in (a)1x1 and (b)2x2 slab models.

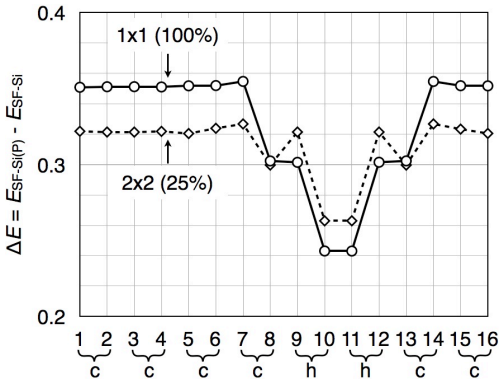

Fig.3 The solution energy dependence of substituted site.

References

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