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# First principles calculations of solution energies of dopants around stacking faults in Ge crystal

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## 1 Introduction

The authors have proposed a new model which describes the dopant behavior at the stacking fault of Si crystal[1]. The previously proposed model expected that only the n-type dopants precipitate at the stacking fault due to the donor level drops[2, 3]. This model, however, failed to explain the newly obtained experimental results of the dopants precipitations in Si, where not only n-type dopants but also the p-type dopants prefer locating at stacking fault region reported by Ohno et al[4, 5].

Our new model describes not only pop-up of the acceptor level but also the drop-down of covalent band, which lead the total energy drop and prefer locating aroung stacking fault region. This model is totally consistent with the experimental results of dopants in Si crystal observed by Ohno et al. In this research, for investigating the dopant behavior in Ge crystal, we have performed the first principles calculations.

## 2 Method

The first principles calculations were performed using the Vienna ab initio simulation package (VASP)[6, 7, 8, 9]. We used the projector-augmented wave (PAW) methods[10] and the generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE) for calculating the exchange-correlation functional[11] The energy cut-off was set to 350 eV for consistency with the PAW potentials of Si and the dopants. For all calculations, the electronic energy convergence for a self-consistent loop and the force convergence for an atomic relaxation loop were set to $10^{-4}$ eV and $10^{-2}$ eV/Å, respectively. The k-point meshes of the Brillouin zone sampling in a primitive cell were based on the Monkhorst-Pack scheme[12].

Fig. 1 shows a side view of the calculated slab model of a diamond-Ge lattice with a stacking fault, which is located between layers 10 and 11. In this figure, the local stacking order of the hcp and fcc lattices is given as AaBbAaBb, indicated by "h", and AaBbCc, indicated by "c". The letters A, B, and C indicate the columnar sites in the basal plane, and "h" and "c" indicate hcp and fcc environments, respectively.

The p-type (Al, Ga, In) or n-type (P, As, Sb) dopants were substituted in place of Ge atoms at each layer. Solution energy are calculated by the following equation,

$$E_{\text{solution}} = \left(E^{\text{SF}}_{\text{Ge}_{63}\text{X}_1} - E^{\text{cubic}}_{\text{Ge}_{63}\text{X}_1}\right) - \left(E^{\text{SF}}_{\text{Ge}_{64}} - E^{\text{cubic}}_{\text{Ge}_{64}}\right) \quad (1)$$

where, $E^{\text{SF}}_{\text{Ge}_{63}\text{X}_1}$ is the total energy for a slab model with a stacking fault and an X dopant, $E^{\text{cubic}}_{\text{Ge}_{63}\text{X}_1}$ is the total energy for a pure Ge crystal with an X dopant, $E^{\text{SF}}_{\text{Ge}_{64}}$ is the total energy for a slab model with a stacking fault and without dopant, and $E^{\text{cubic}}_{\text{Ge}_{64}}$ is the total energy for a pure Ge crystal. The first term of the right hand side represents the solution energy with a stacking fault energy, and which is cancelled by the second term.

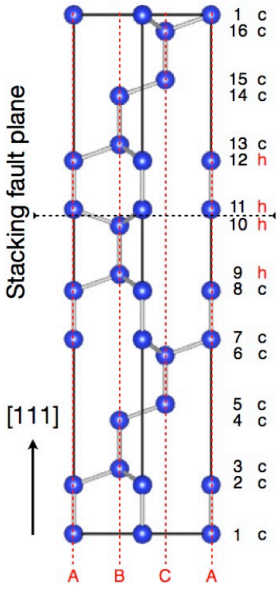


Figure 1: Schematic drawing of the unit cell of the slab model.

## 3 Results

Figures 2 show the solution energy dependency on the site where a dopant is inserted in the Ge and Si crystals. The solution energies in Si have been reported in the previous letter[1]. The top row panels show the results of n-type dopants of Al, Ga and In, and the bottom row panels show those of p-type dopants of P, As and Sb. Both n-type and p-type dopants inserted in Ge crystals show the tendency of the energy drops around stacking faults, which are located between 10th and 11th layers.

The drops of solution energy around the stacking fault in n-type dopants are smooth valley shapes, but those in p-type dopants show zigzag shapes or not smooth change, where the energies next to stacking faults are higher than those of next nearest sites. The zigzag bending in Ge crystal are weaeker than those in Si crystals.

The solution energy drops at stacking fault region of dopants for Si and Ge crystal are summarized in Table I. All the dopants in Ge crystal show smaller energy drop than

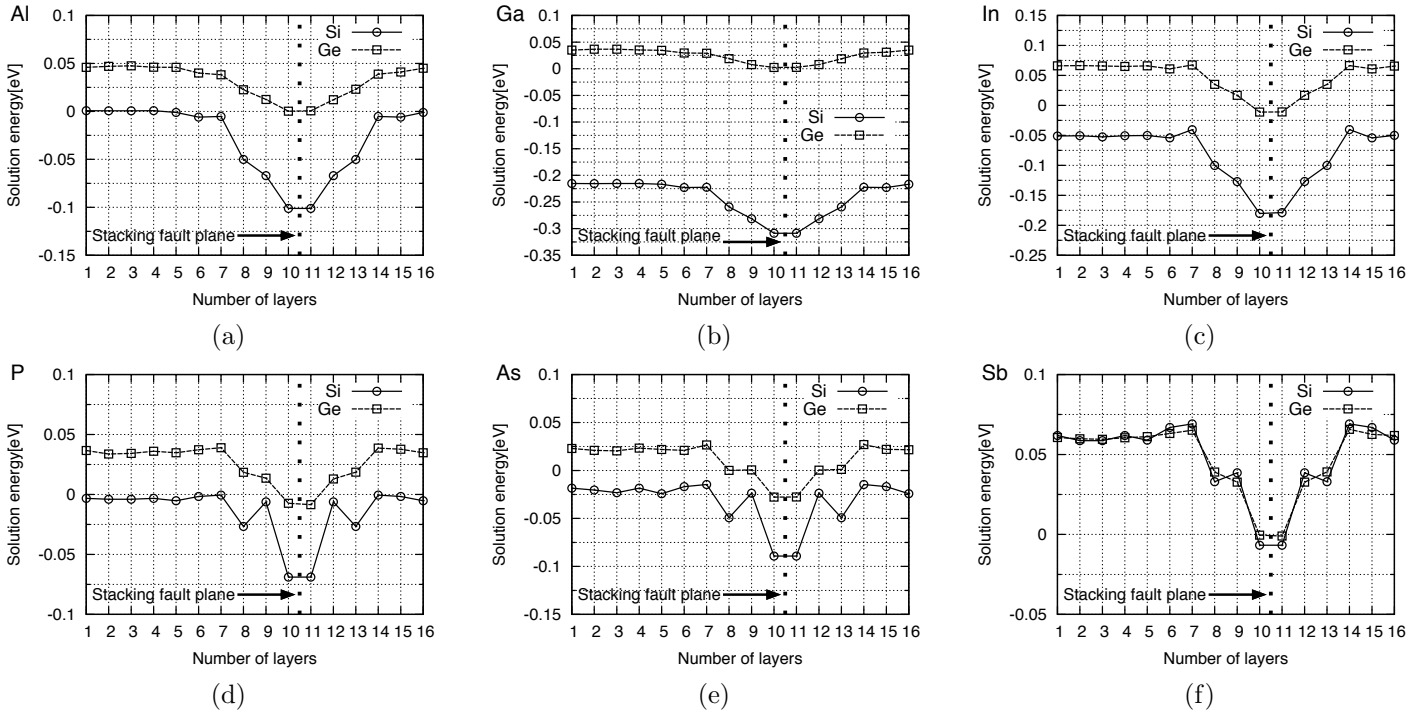


Figure 2: Solution energy dependence of the substituting site for p-type ((a) Al, (b) Ga, and (c) In) and n-type ((d) P, (e) As, and (f) Sb) dopants. The solid and dashed lines represent the results for Si and Ge crystals, respectively.

Table 1: Energy drops in eV between perfect site and stacking fault site in Si and Ge crystals.

| dopant | Al | Ga | In | P | As | Sb |
|---|---|---|---|---|---|---|
| in Si | 0.101 | 0.093 | 0.1296 | 0.0648 | 0.066 | 0.065 |
| in Ge | 0.047 | 0.034 | 0.076 | 0.041 | 0.048 | 0.0599 |

those in Si. The difference between Si and Ge is small for the dopants of In and Sb.

# 4 Conclusions

In the first principles calculations, the electron structures of Ge crystal at Γ-point have been checked, but been very complicated than those in Si, and the remarkable changes of covalent band drops around the stacking faults are not observed. At least, however, from the total energy change, the dopants in Ge crystal should prefer to locate in stacking faults regions. The tendencies of the concentrating around stacking faults are weaker than those in Si crystals.

# References


[1] Y. Yamamoto, K. Togase, Y. Ohno, I. Yonenaga, and S. R. Nishitani, J. J. Appl. Phys. 53 (2014) 061302.

[2] J. F. Justo, T. M. Schmidt, A. Fazzio, A. Antonelli: Physica B. **302** (2001) 403.

[3] T. A. Arias and J. D. Joannopoulos: Phys. Rev. Lett. **69** (1992) 3330

[4] Y. Ohno, T. Shirakawa, T. Taishi, and I. Yonenaga: Appl. Phys. Lett. **95** (2009) 091915.

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

[6] G. Kresse and J. Hafner: Phys. Rev. B **47** (1993) 558–561.

[7] G. Kresse and J. Hafner: Phys. Rev. B **49** (1994) 14251–14269.

[8] G. Kresse and J. Furthmüller: Comput. Mat. Sci. **6** (1996) 15–50.

[9] G. Kresse and J. Furthmüller: Phys. Rev. B **54** (1996) 11169–11186.

[10] G. Kresse and D. Joubert: Phys. Rev. B **59** (1999) 1758–1775.

[11] J. P. Perdew, K. Burke and M. Ernzerhof: Phys. Rev. Lett. **77** (1996) 3865–3868.

[12] H. J. Monkhorst and J. D. Pack: Phys. Rev. B **13** (1976) 5188.