First-Principles Analysis on Stability of Interstitial H Atom in Si and Ge crystals

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1 Introduction

Large Scale Integrations (LSIs) have been developed with downsizing in recent years. In this technical trend, the impurities such as O, H and metals should be controlled as they interact with intrinsic point defects in Si. Furthermore, Ge thin film on Si substrate attracts attentions as the carrier mobility is higher compared to Si [1-3]. Therefore, it becomes necessary to understand the behaviour of the impurities and their interactions with point defects in Ge and Ge/Si structure. In this study, the stability of interstitial H atom in Si, Ge, and SiGe was analysed by first principles calculation. It was found that H atom is most stable at T-site in Si, Ge and SiGe. Furthermore, H atom is stable at T-site in tensile strained Si when the strain is up to +1%. However, when the strain is +2 ~ +4%, H atom is most stable at B-site in Si. In compressive strained Ge, H atom is most stable at T-site when the strain is up to -4%.

2 Calculation Details

In the calculation cell of 64 atoms, one H atom has been arranged to B-, S-, T- or H-site as shown in Fig. 1. Geometry optimization was carried out by first principles calculation.

The formation energy (E_f) of H atom in Si was obtained by eq. (1) with the three-dimensional periodic boundary condition. For Ge, E_f was obtained by eq. (2).

$$E_f = E(\mathrm{Si}_{64}\mathrm{H}_1) - \{E(\mathrm{Si}_{64}) + E(\mathrm{H}_2)/2\} \quad (1)$$

$$E_f = E(\mathrm{Ge}_{64}\mathrm{H}_1) - \{E(\mathrm{Ge}_{64}) + E(\mathrm{H}_2)/2\} \quad (2)$$

Furthermore, the calculation cell of Si crystal was deformed with isotropic strain from +1 to +4%. One H atom has been arranged to B-, S-, T- or H-site. Geometry optimization was carried out by first-principles calculation, and the formation energy was obtained. For Ge crystal, the compressive strain in -1 to -4% was imposed to the calculation cell, and the similar calculations were performed.

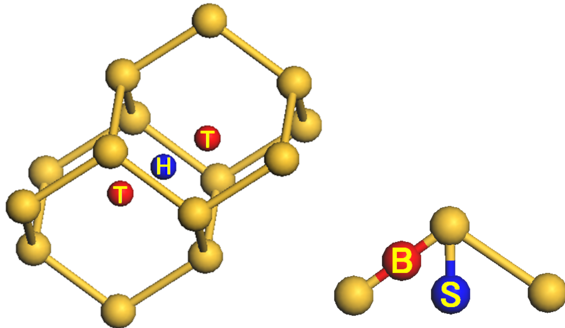

Fig. 1 B-, S-, T- and H-site in diamond structure.

In this study, first-principles calculation was performed within the generalized gradient approximation (GGA) using the CASTEP code [4]. The wave functions were expanded with the plane waves, and the ultra-soft pseudo-potential method was used to reduce the number of plane waves. The cut off energy was 310eV. The expression proposed by Perdew et al, was used for the exchange-correlation energy in the GGA [5]. Periodic boundary conditions were used with cubic super cells of 64 atoms, k-points ampling was performed at 1×1×1 special points in a Monkhorst-pack grid [6].

3 Results and discussion

The formation energy of H atom in Si crystal is shown in Fig. 2. It was found that H atom in Si has an almost equal E_f among S-, T- and H-site, and lower than that at B-site. Similar result was obtained for Ge crystal as shown in Fig. 3.

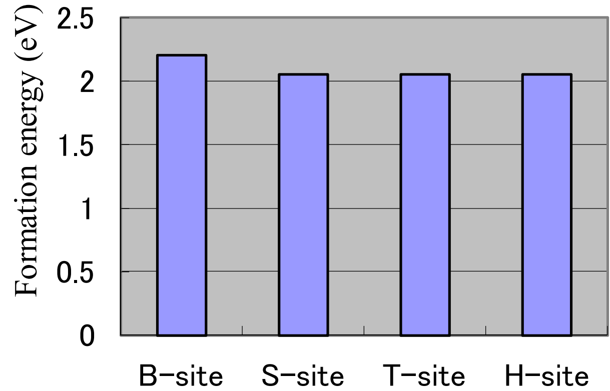

Fig. 2 Calculated E_f of H atom in Si crystal.

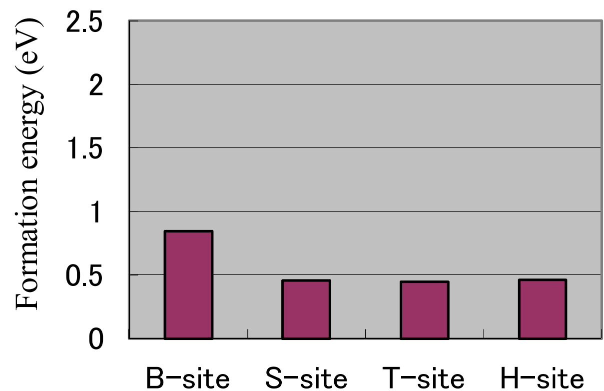

Fig. 3 Calculated E_f of H atom in Ge crystal.

The movement of H atom during geometry optimization from H- and S- to T-site in Si crystal is shown in Fig. 4. This movement indicates that there is no energy barrier among S-, T- and H-site. This is the reason why the formation energies of H atom at H atom at H-, S- and T-site are almost equal in Si. For Ge crystal similar movement was confirmed.

These results indicate that H atom in Si and Ge crystals is most stable near T-site.

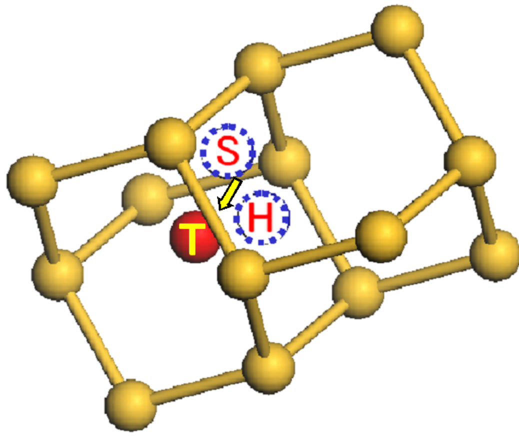

Fig.4 Movement of H atom during geometry optimisation.

Next, the formation energy of H atom in the isotropic tensile strained Si crystal is shown in Fig. 5. It was found that the formation energy of S-, T- and H-site is lower than B-site up to 1% as well as no strained Si. In this case, each H atom moved near T-site.

Furthermore, when tensile strain is larger than 2%, B-site is more stable than the other sites.

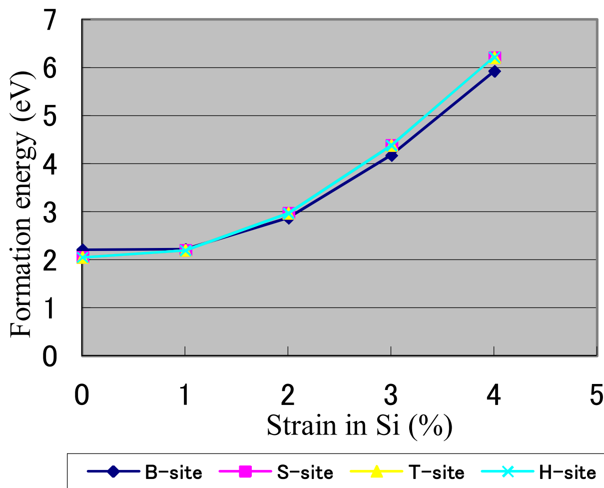

Fig.5 Calculated E_f of H atom in tensile strained Si.

The formation energy of H atom in the isotropic compressive strained Ge crystal is shown in Fig. 6. It was found that the formation energy of S-, T- and H-site is lower than B-site up to -4% as well as no strained Ge. In this case, each H atom moved near T-site.

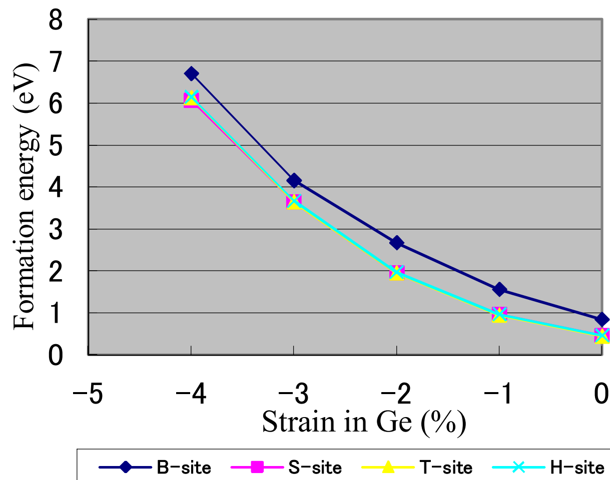

Fig.6 Calculated E_f of H atom in compressive strained Ge

4 Conclusion

First-principles analysis was performed to the stability of interstitial H atom in Si and Ge crystal. Following results were obtained.

(1) H atom is most stable near T-site in both Si and Ge crystals.

(2) B-site is metastable in both Si and Ge crystals.

(3) When the isotropic tensile strain is 1% in Si crystal, H atom is most stable near T-site. On the other hand, when strain is 2 to 4%, B-site is most stable.

(4) For Ge crystal, H atom is most stable near T-site with the compressive strain up to -4%.

References

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