First-Principles Analysis on Stability of Interstitial O Atom in Si and Ge Crystals

Tatsunori Yamato, Hiroaki Kariyazaki and Koji Sueoka

Dept. of Communication Eng., Okayama Prefectural University, Japan

1 Introduction

In recent years, Large Scale Integration (LSI) devices have been developed with downsizing. In this technology trend, high quality and large diameter Si wafers are used as substrates with controlling the impurities. It is well known that O atoms are incorporated in Si crystals during Czochralski crystal growth [1]. O atoms have an advantage for increasing the strength of Si wafers [2].

Furthermore, Ge film/Si substrate is under consideration for the channel material as the carrier mobility in Ge is higher than that in Si [3]. Therefore, Ge film/Si substrate structure is considered for the next generation LSI materials. In this structure, O atoms diffuse into Ge thin film from the Si substrate during the thenmal treatments. The purpose of this study is to clarify the properties of O atoms in Si and Ge crystals. Furthermore, the influence of lattice strain in Ge/Si structure on the stability of O atoms was considered.

2 Calculation Details

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 $1 \times 1 \times 1$ special points in a Monkhorst-Pack grid [6].

In the 64-atom calculation cell, one O atom was arranged at four sites as shown in Fig. 1. Geometry optimization was performed, and total energies E_{tot} were calculated for each calculation cell. Furthermore, the formation energy E_f of O atom was calculated by the following equations, and the stability of O atom at each site was estimated.

$$\text{Si}: E_f = E_{tot}(\text{Si}_{64}\text{O}_1) - \{E_{tot}(\text{Si}_{64}) + \frac{1}{2}E_{tot}(\text{O}_2)\} \quad (1)$$

$$\text{Ge}: E_f = E_{tot}(\text{Ge}_{64}\text{O}_1) - \{E_{tot}(\text{Ge}_{64}) + \frac{1}{2}E_{tot}(\text{O}_2)\} \quad (2)$$

Isotropic tensile-strain of 1%~4% was imposed to Si cell, and isotropic compressive-strain of 1%~4% was imposed to Ge cell. Similar analysis to the unstrained cell was performed.

3 Results and discussion

The calculated formation energy of O atom in Si crystal is shown in Fig. 2. It was found that E_f of O atom at B-, S- and H-site was almost equal, and became lower than that at T-site. Moreover, O atom arranged at S- and H-site moves to near B-site during geometry optimization, as shown in Fig. 3. Therefore, the most stable position of O atom in Si crystal is considered to be near B-site.

The calculated formation energy of O atom in Ge crystal is shown in Fig. 4. The formation energy of O atom arranged at B- and S-site was almost equal, and became lower than that at T- and H-site. Moreover, O atom arranged at S-site moved to near B-site during geometry optimization, as shown in Fig. 5. Therefore, the most stable position of O atom in Ge crystal is considered to be near B-site.

The strain dependence of formation energy of O atom is shown in Figs. 6 and 7. For Si crystal. B-site was the most stable independent of tensile-strain.

On the other hand, for Ge crystals, the formation energy of O atom at B-site with 4 % compressive-strain became higher than that at T-site.

4 Conclusion

In this study, first-principles analysis on stability of interstitial O atom in Si and Ge crystals was performed with considering the stain. The main results can be summarized as follows.

(1) In non-strained Si and Ge crystals, the most stable position of O atom is near B-site.

(2) In the tensile-strained Si crystal, the most stable position of O atom is near B-site independent of the strain.

(3) In the compressive-strained Ge crystal, the formation energy of O atom at B-site with 4% compressive strain became higher than T site.

References

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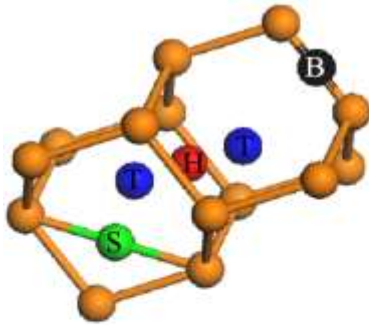

Fig.1 B-,S-,T- and H-site in diamond structure.

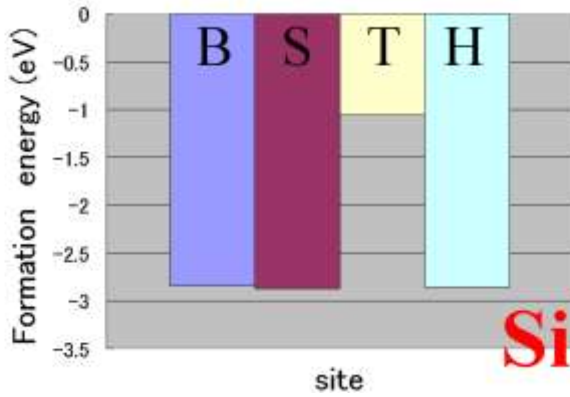

Fig.2 Calculated E_f of O atom in non-strained Si.

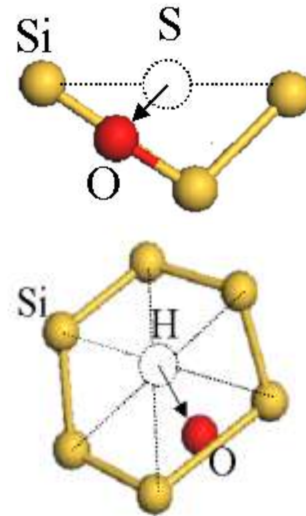

Fig.3 Movement of O atom in Si during geometry optimization.

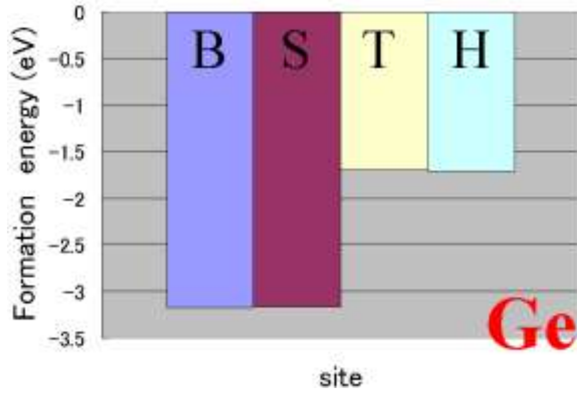

Fig.4 Calculated E_f of O atom in non-strained Ge.

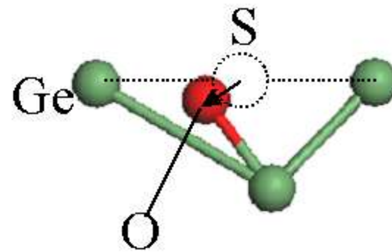

Fig.5Movement of O atom in Ge during geometry optimization.

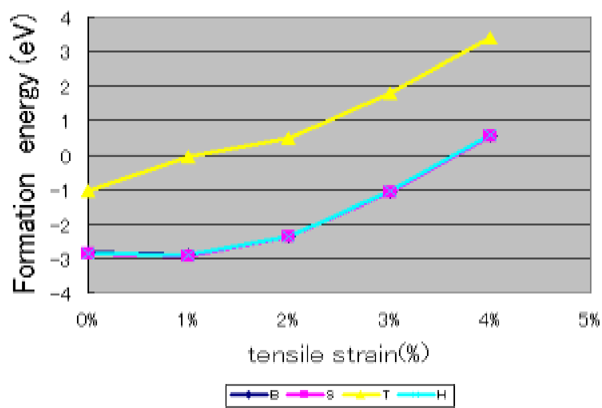

Fig.6 Calculated E_f of O atom in tensile-stained Si.

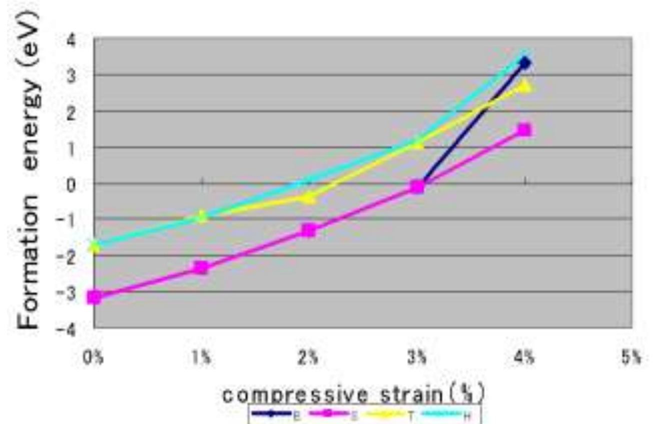

Fig.7 Calculated E_f of O atom in compressive stained Ge.