Atomic configuration of boron pile-up at the Si/SiO$_2$ interface

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Abstract: The thermo dynamical stability of a boron atom at the Si/SiO$_2$ interface was studied by using *ab initio* calculation to investigate a mechanism of boron pile-up at the interface during thermal annealing. The B atom is stable in bulk Si site of the interface without any interface defect, which contradicts the experimental observations. By introducing an oxygen vacancy at the interface, the mechanism of B segregation into SiO$_2$ layer at the atomic scale was verified.
Keywords: boron, pile-up, Si/SiO$_2$ interface, *ab initio* calculation
Classification: Science and engineering for electronics

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1 Introduction

Excess defects in the silicon lattice, generated by ion implantation, induce both a redistribution of dopant and dopant segregation at the Si/SiO_2 interface during annealing. It is important to clarify a mechanism of B pile-up at the Si/SiO_2 interface to control B distribution in more precise manner for future CMOS technology. This is because implanted regions become closer to the interface, B pile-up affects more significantly device characteristics. A lot of studies have been made on dopant pile-up at the $Si(100)/SiO_2$ interface. P and As atoms introduced by ion implantation tend to stay in bulk Si side of the interface [1, 2], while B atoms preferentially segregate into oxide [3, 4, 5]. Although B diffusion in SiO_2 in the absence of the interface has been investigated by using first principles calculation [6], little attention has been paid to a mechanism of B pile-up near the Si/SiO_2 interface. This paper clarifies the relationship between the local defect of the SiO_2 structure and the atomic configuration of B pile-up in oxide. By changing the atomic configuration of oxygen vacancy with/without hydrogen termination, the stability of a B atom in the Si/SiO_2 interface model has been studied by using *ab initio* calculations. The aim of this work is to clarify the physical mechanism of B pile-up at the Si/SiO_2 interface and B segregation into oxide layer for a better understanding of B redistribution during thermal annealing.

2 Calculation details

In order to investigate B pile-up at the Si/SiO_2 interface, we chose tridymite [7] structure as a thin oxide layer of the interface model since it is reported that there is ~ 5 Å crystalline tridymite phase on Si (100) surface [8]. In addition, theoretical studies reveal that a tridymite phase is the most suitable for Si (100) surface whose SiO_2 layer is thinner than 7 Å [9]. Figure 1 shows the basic supercell as the perfect Si/SiO_2 interface used in this work. The unit cell of the interface model contains bulk Si, SiO_2 layer and vacuum. The periodic supercell structure consists of 48 atoms including four H atoms.

The *ab initio* total energy calculations and structural relaxations are simultaneously performed by using generalized gradient approximation. We applied Vanderbilt type ultrasoft pseudopotential code for the supercell [10]. The cutoff energy of the calculated plane-wave functions is limited under
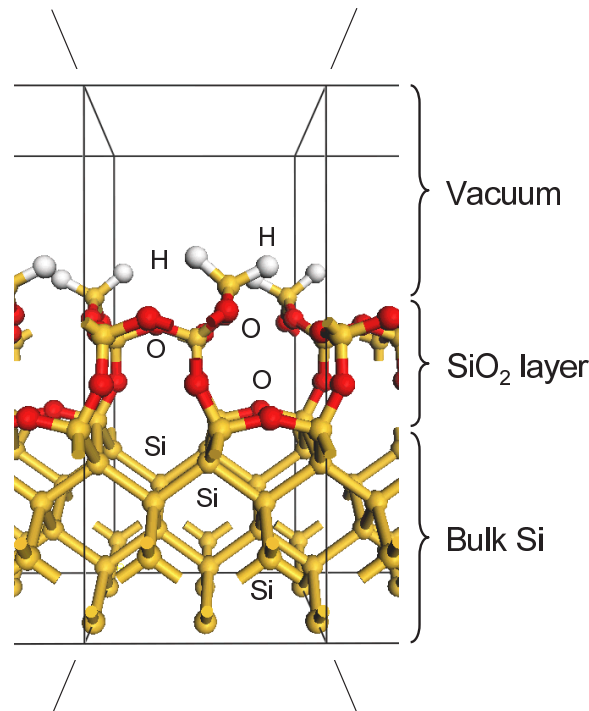
Fig. 1. The perfect Si/SiO$_2$ interface.

300 eV and $3 \times 3 \times 1$ Monkhorst-Pack **k**-point sampling are used [11].

3 Results and discussion

In order to clarify the mechanism of B pile-up at the interface, we investigated the atomic configuration of a stable B atom at the Si/SiO$_2$ interface by using *ab initio* total energy calculation. A method for this study is as follows. A Si atom replaced with a B atom and the interface structure containing a B atom was relaxed to provide the minimum total energy of the supercell. Carrying out the above operations for all Si sites in the model one after another, we could find the most stable B site at the interface.

First, we calculated the total energy as a function of B sites near the perfect Si/SiO$_2$ interface. An energy minimum is found at B atom replaced with a Si atom adjacent to the interface layer. The total energy is 0.48 eV lower than the B atom replaced with a Si atom in deep bulk Si. The total energy steeply increases up to 2.2 eV in SiO$_2$ layer than that of replaced B in deep bulk Si site. These calculated results indicate that B atom is the most stable in Si side of the interface. This is, however, contrary to the experimental observations where B atoms segregate into oxide side at the interface [3, 4, 5].

Next, we introduced an O vacancy to the perfect interface which may account for the experimental observations. B atom could be stable at a defect site in defective SiO$_2$ rather than in the crystalline SiO$_2$. In fact, there are lots of point defects in SiO$_2$ such as O and Si vacancies with dangling bonds since thermal SiO$_2$ is grown into amorphous phase. Figure 2 (a) $\sim$ (c) shows three types of the Si/SiO$_2$ interfaces including an O vacancy, from

(a) No H termination   (b) One H termination   (c) Two H terminations
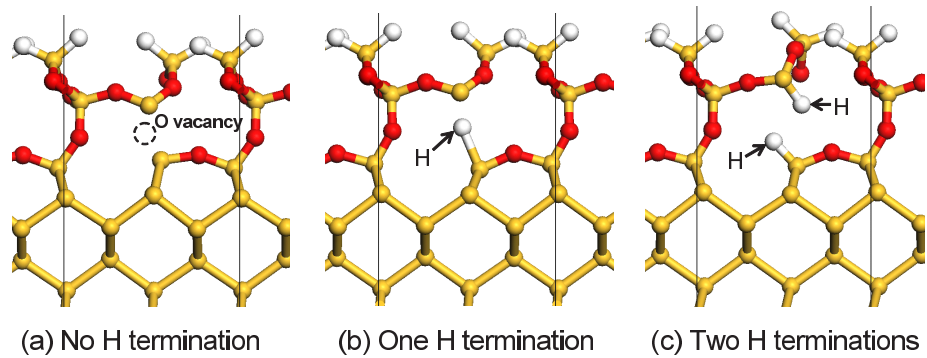
Fig. 2. Optimized $Si(100)/SiO_2$ interfaces including an O vacancy. From the left, the interfaces (a) without H termination, (b) with one H termination and (c) with two H terminations at an O vacancy.

the left, the interface without H termination, with one H termination and with two H terminations at an O vacancy. We calculated the total energies of these supercells in which a B atom is replaced with each Si atom. For the interface including an O vacancy without H termination or with two H terminations, the total energies of supercells with B atom being in Si site of SiO_2 layer are lower than that of the perfect interface. However, note that B atom is still the most stable in Si side of the interface. For the case of the Si/SiO_2 interface including an O vacancy with one H termination, the total energy becomes minimum at Si site in SiO_2 side of the interface, where the O vacancy neighbors. It is approximately $1.2\,eV$ lower than the energy in deep bulk Si site. The H atom terminates the dangling bond of the O vacancy, the B atom takes a threefold-coordinate configuration at the interface as shown in figure 3 (b). The B atom is the most stable in SiO_2 side of the interface, which supports the experimental observations.

The total energy calculations of the perfect interface and the supercells including an O vacancy reveal that B atom is trapped by the O vacancy during thermal annealing and becomes stable in oxide side at the interface.
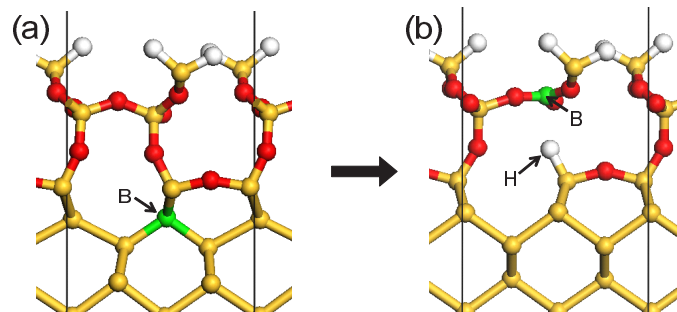
Fig. 3. The energy minimum configuration for a B atom in (a) the perfect interface and (b) the interface including an O vacancy. When an O vacancy generates at the interface, a B atom is trapped in SiO_2 side by the O vacancy terminated with a H atom.

Then, B atoms may diffuse into oxide via this configuration. This result seems contradictory to a report that B in SiO_2 forms the most stable configuration with an O interstitial [6]. However, a lattice mismatch between bulk Si and SiO_2 layer induces significant number of dangling bonds and O vacancies terminated with H atoms. A combination of a H atom and an O vacancy is the important factor to trap B atoms at the Si/SiO_2 interface.

4 Conclusion

We investigated the mechanism of B pile-up at the Si/SiO_2 interface by using *ab initio* total energy calculation. In the perfect interface without any defects, B atom is stable near the interface in bulk Si. While B atom is stable in oxide layer of the interface which includes an O vacancy as a point defect. We found that the B atom is trapped by O vacancy and segregates in oxide side of the interface.

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