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First-principles study of the segregation of boron dopants near the interface between crystalline Si and amorphous SiO_2

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ABSTRACT

We investigate the stability of boron dopants near the interface between crystalline Si and amorphous SiO_2 through first-principles density functional calculations. An interstitial B is found to be more stable in amorphous SiO_2 than in Si, so that B dopants tend to segregate to the interface. When defects exist in amorphous SiO_2, the stability of B is greatly enhanced, especially around Si floating bond defects, while it is not significantly affected near Si–Si dimers, which are formed by O-vacancy defects.

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1. Introduction

Among dopant impurities used in metal-oxide-semiconductor field-effect-transistor (MOSFET) devices, B dopants exhibit very peculiar behavior under thermal annealing after ion implantation, such as transient-enhanced diffusion [1], clustering [2], and segregation to the Si/SiO_2 interface [3]. Such phenomena make it difficult to control the profile of B dopants in devices. As the size of MOSFET devices is scaled down, the fabrication of short channels and shallow junctions is required. In the spatial scale of sub-0.1 μm, segregation of B dopants to the Si/SiO_2 interface significantly affects the device performance, changing the threshold voltage [4,5] and the sheet resistance [6]. In addition, simulating the profile of B dopants in nano-sized MOSFET devices is one of challenging tasks in technology computer-aided design (TCAD). To simulate and control the distribution of dopants, it is important to better understand the mechanism for dopant segregation on the atomic level.

Experiments have shown that, during the segregation, P and As dopants pile up on the Si side of the interface, while B dopants prefer to segregate to the oxide [3]. In Si with abundant Si self-interstitials, it is known that B dopants easily diffuse via the formation of a defect pair consisting of B and self-interstitial [7–9]. In previous calculations, the stability of B-related defects near the Si/α-quartz interface was studied [10]. It was suggested that diffusing B dopants segregate toward the oxide in the Si/SiO_2 interface in form of positively charged interstitials. The existence of positively charged B ions was indeed observed in recent time-dependent second harmonic generation experiments [11]. In real devices, amorphous SiO_2 is usually employed in Si/oxide interfaces, so that defects such as O-vacancy, dangling bond, and floating bond are likely to exist near the interface. However, there have been a lack of theoretical studies on the effect of defects on B segregation at the interface between Si and amorphous SiO_2.

In this work, we investigate the electronic properties and stability of B-related defects in the Si/amorphous-SiO_2 interface through first-principles calculations. We perform melt-and-quench molecular dynamics simulations to generate several atomic models for amorphous SiO_2. We examine the role of defects such as O-vacancy, Si dangling bond, and Si floating bond in the stability of B and the mechanism for B segregation.

2. Calculation method

We perform the first-principles calculations within the density functional theory framework. We use the local-density-functional approximation (LDA) in the functional form of Ceperly and Alder [12] for the exchange-correlation potential and ultrasoft pseudopotentials [13] for ionic potentials, as implemented in the VASP code [14]. The wave functions are expanded in plane waves with an energy cutoff of 400 eV. We employ 2 × 2 supercells in Si/SiO_2 interface structures and special k-points generated by the 2 × 2 × 1 Monkhorst–Pack mesh [15] for Brillouin zone integration. In the slab geometry, which consists of Si layers of 13.4 Å, SiO_2 layers of 22.0 Å, and a vacuum of 8.0 Å, the Si and O dangling bonds on both the surfaces are passivated by hydrogen.

We consider three atomic models (Fig. 1) for the interface between crystalline Si (c-Si) and amorphous SiO_2 (a-SiO_2). Using first-principles molecular dynamics (MD) simulations with a time step of 2 fs, we generate the amorphous phase of SiO_2 in the interface. For the Si/α-quartz interface structure [10], we perform

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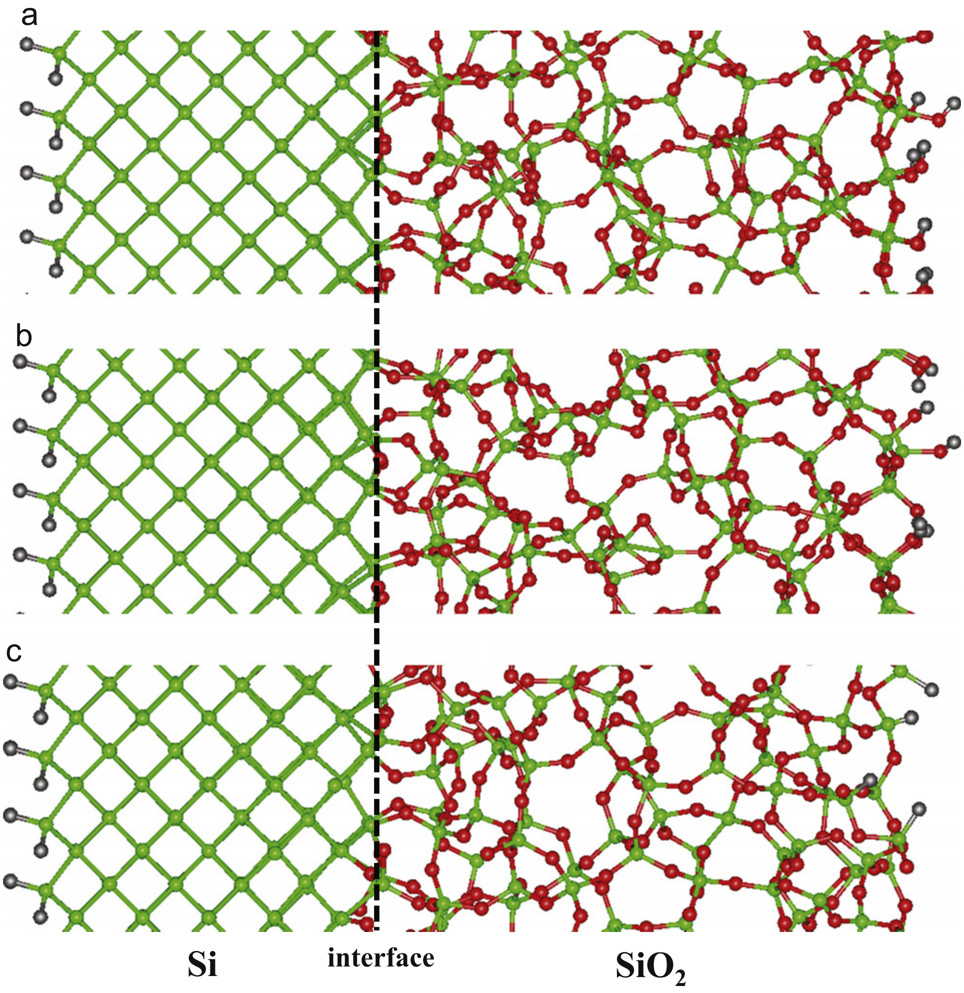

Fig. 1. Slab geometries of three atomic models for the Si(100)/a-SiO_2 interface. Green, red, and dark gray balls denote the Si, O, and H atoms, respectively. (a) Interface #1, (b) Interface #2, (c) Interface #3. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1
The densities (ρ), the O:Si ratios, and the numbers of defects are compared for three amorphous models for SiO_2. The densities and the O:Si ratios are obtained by excluding atoms within the distance of 5 Å from the surface and interface of amorphous SiO_2.

Interface	ρ (g/cm^3)	O:Si	Si floating bond	Si dangling bond	Si–Si dimer
# 1	2.22	1.97	3	1	1
# 2	2.33	1.95	3	0	0
# 3	2.30	2.00	3	0	2

melt-and-quench MD simulations [16], in which only crystalline SiO_2 is melted at 4000 K for 4 ps, while the crystalline phase of Si is maintained during the melting process. Then, liquid SiO_2 is rapidly quenched from 1500 to 0 K with the cooling rate of 500 K/ps. We obtain two additional interface structures by performing successively the melt-and-quench MD simulations for the first interface model, with the same cooling rate. After the interface is generated, the ionic coordinates are fully optimized until the residual forces are less than 0.05 eV/Å.

3. Results and discussion

The densities of amorphous SiO_2 in the interface structures are in the range of 2.22–2.33 g/cm^3 (Table 1), in good agreement with the measured value of 2.2 g/cm^3 [17]. We find that several point defects exist in amorphous SiO_2, such as Si–Si dimer, fivefold-coordinated Si (floating bond) [18], and threefold-coordinated Si (dangling bond). The bonding states of the fivefold-coordinated Si are dispersed within the valence bands of SiO_2, without defect levels in the Si band gap. Due to an extra electron, the Si floating bond remains in the -1 charge state if the Fermi level lies within the Si band gap. On the other hand, the threefold-coordinated Si atom generates a defect level in the oxide band gap. Actually, our calculations show that this defect level is pinned near the valence band maximum (VBM) of Si.

In α-quartz, the stability of an interstitial B (B_I) was well studied [19]. In the neutral state, B forms a split-interstitial complex with a Si atom, whereas it intervenes between the Si and O atoms in the $+1$ charge state. However, in a-SiO_2, an interstitial B can exist in various forms due to the flexible network and the existence of point defects. We examine various B interstitial configurations in the oxide region of the interface structure and find that the stability of B depends on whether B is placed right next to point defects or not. To examine the stability of various B-related defects, we compare the total energies of B defects in SiO_2 with that of a B–self-interstitial (B–I) complex in the bulk region of Si. It is known that the B–I complex, in which a Si self-interstitial (I) is located at the adjacent tetrahedral site of a substitutional B, is the most stable defect in p-type Si. The B–I complex is easily formed upon thermal annealing after ion implantation [1], and this complex was suggested to play a role for the diffusion of B dopants [7].

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