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# An amorphous $SiO_2$/4H-SiC(0001) interface: Band offsets and accurate charge transition levels of typical defects

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ABSTRACT

A defect-free structural model of the amorphous $SiO_2$/4H-SiC(0001) interface is presented through first-principle calculations. Following the potential lineup method, we first calculate the valence- and conduction-band offsets of this interface, which are in good agreement with the experimental values. Based on this interface model, we create several typical interface defects and estimate the accurate charge transition levels of these defects within the HSE06 hybrid functional scheme. The results indicate that the silicon interstitial in $SiO_2$ and carbon dimers in both SiC and $SiO_2$ are the possible candidates for the large interface states experimentally observed near the conduction band of 4H-SiC.

## 1. Introduction

Silicon carbide (SiC) has been demonstrated to outperform silicon in high temperature, high frequency, and high power applications, due to its excellent physical properties [1–5]. Compared with other desirable semiconductor materials, SiC has the ability to grow the gate oxide ($SiO_2$) through thermal oxidation techniques, which makes it possible to manufacture SiC-based metal-oxide-semiconductor (MOS) devices using traditional Si-MOS processes [3]. However, the high density of interface traps at the $SiO_2$/SiC interface hinders the development of the SiC-based MOS power devices [4,5].

For further progress, it is therefore important to understand the origin of the experimentally observed interface states [4–12]. Photo-stimulated tunneling (PST) measurements on SiC devices revealed that the negatively charged defects near the interface led to the interface states located approximately 0.1 eV below the conduction band of 4H-SiC, called near interface traps (NIT) [4–7]. These defects are considered to be responsible for the observed mobility degradation [4–7]. To identify the origin of these interface states, a real amorphous $SiO_2$/SiC interface model with good structural and electronic properties needs to be constructed. Knaup et al. presented a simple $SiO_2$/SiC interface model to account for the origin of interface states [13–15]. However, the oxide density of this interface model is approximately 3.2 g/cm$^3$, higher than the experimental value of amorphous $SiO_2$. Recently, Devynck et al. generated a $SiO_2$/SiC interface slab model through a sequence of classical and *ab initio* simulation methods [16,17]. Using this slab model, they calculated the charge transition levels of several defects at the $SiO_2$/SiC interface [18,19]. Nevertheless, this slab model has a surface polarization effect, which may affect the calculated defect levels.

In this work, we construct a new amorphous $SiO_2$/SiC superlattice model to avoid the surface polarization effect. Based on this model, we create several typical defect configurations at the $SiO_2$/SiC interface and examine the charge transition levels of these defects.

## 2. Calculation methods and models

Structural relaxations were performed based on the generalized gradient approximation exchange-correlation functional proposed by Perdew, Burke, and Ernzerhof (PBE) [20]. The electronic structures of bulk SiC and $SiO_2$ were determined through the Heyd–Scuseria–Ernzerhof (HSE06) hybrid functional [21]. Core–valence interactions for all atoms were described using the projector augmented wave method [22,23]. The cutoff energy for the wave functions of the valence electrons was set to 500 eV. The Monkhorst–Pack $k$-point mesh was sampled with a constant separation of 0.025 Å$^{-1}$ in the Brillouin zone [24].

The amorphous $SiO_2$/SiC interface model was constructed by a 222-atom superlattice that contains 60 carbon atoms, 72 oxygen atoms, and 90 silicon atoms. The surface size of the amorphous $SiO_2$ was chosen to match that of the $(3 \times 4)$ 4H-SiC (0001) surface. The structure model was simulated using *ab initio* molecular dynamics

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(AIMD) and carried out with the Vienna *ab initio* simulation package (VASP) [25,26]. The interface structures were quenched from 2000 K in successive steps of 200 K. At each temperature, a well-equilibrated configuration was established after running for 2 ps. During the annealing process, the atomic positions of the 4H-SiC substrate were kept fixed up to 1000 K, and below this temperature, all atoms were allowed to move. The final structure was further relaxed using the VASP scheme, and the optimized interface structure is illustrated in Fig. 1(a). This model is an ideal defect-free superlattice structure, which is of great significance to the accurate determination of defect levels at the interface. Using similar AIMD simulations, we also constructed an amorphous $SiO_2$ structure with 90 atoms, as shown in Fig. 1(b). In our interface model, the average density of the amorphous $SiO_2$ component is approximately 2.4 g/cm$^3$, slightly larger than the density of vitreous $SiO_2$ (2.2 g/cm$^3$).

To obtain the defect levels amenable to comparison with experimental results, we focus on the charge-state transition levels associated with interface defects. The key quantity that determines the charge transition levels is the defect formation energy. For a given defect D with charge state $q$, the formation energy [27,28] as a functional of the electron chemical potential (*i.e.*, Fermi energy) $\mu_F$ is computed by

$$E_f^{D,q}(\mu_F) = E_{\mathrm{tot}}^{D,q} - E_{\mathrm{tot}}^{0} - \sum_i n_i \mu_i + q(\mu_F + E_V) \tag{1}$$

In this expression, $E_{\mathrm{tot}}^{D,q}$ and $E_{\mathrm{tot}}^{0}$ are the total energy with and without the defect D. The integer $n_i$ represents the number of added ($n_i > 0$) or deleted ($n_i < 0$) atoms of type $i$ when creating a defect, and $\mu_i$ refers to the corresponding chemical potential. The valence-band maximum (VBM) of bulk material $E_V$ is used as the reference scale of the electron chemical potential. The charge transition level is defined as the Fermi-level position where the charge states $q$ and $q'$ have equal formation energy [29–32], *i.e.*,

$$\varepsilon(q/q') = \frac{E_{\mathrm{tot}}^{D,q} - E_{\mathrm{tot}}^{D,q'}}{q' - q} - E_V. \tag{2}$$

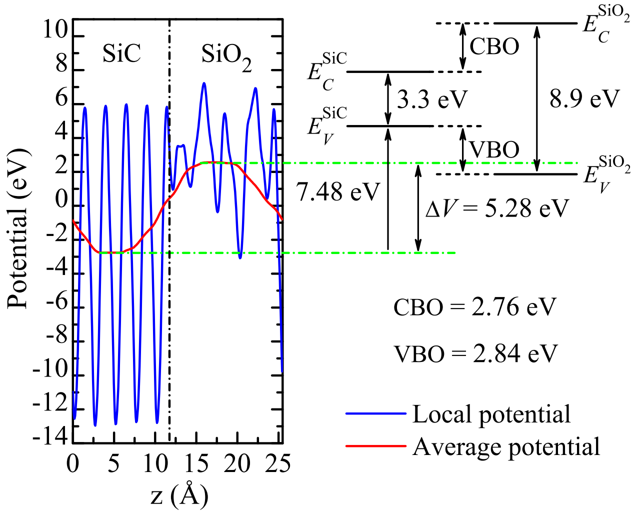

**Fig. 2.** (Color online) Schematic illustration of band offsets at the $SiO_2$/SiC interface. The left panel shows the local (blue curve) and macroscopic average (red curve) electrostatic potentials of this interface along the SiC (0001) direction. The values of the VBM $E_V$ are aligned with respect to the macroscopic average electrostatic potential in each material.

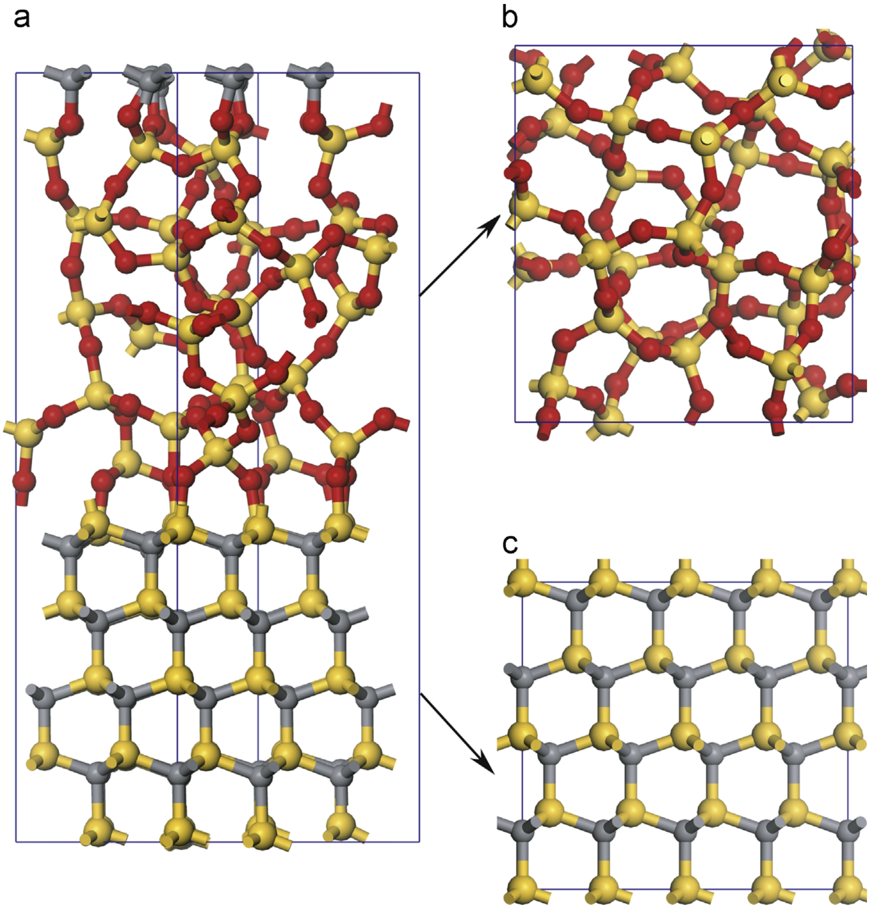

**Fig. 1.** (Color online) (a) The atomic structures of the amorphous $SiO_2$/4H-SiC (0001) interface model. (b) An amorphous $SiO_2$ structure. (c) Bulk 4H-SiC structure. Si, C, and O atoms are depicted by the orange, gray, and red spheres, respectively.