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Structure and energetics of carbon defects in SiC (0001)/SiO$_2$ systems at realistic temperatures: Defects in SiC, SiO$_2$, and at their interface

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ABSTRACT
We report systematic first-principles calculations that reveal the atomic configurations, stability, and energy levels of carbon defects in SiC (0001)/SiO$_2$ systems. We clarify the stable position (i.e., in SiC, SiO$_2$, or at SiC/SiO$_2$ interfaces) of defects depending on the oxidation environment (an oxygen-rich or -poor condition). At finite temperatures, the chemical potential of atomic species was corrected referring to thermochemical tables in order to obtain the temperature-dependent defect formation energies. Under an oxygen-rich condition, we found that the dicarbon antisite [(C$_2$)$_{fi}$] in SiC is one of the favorable defects at a typical oxidation temperature of 1600 K and it creates a localized level near the conduction band edge of SiC, being a critical defect for n-channel metal-oxide-semiconductor field-effect transistors (MOSFETs). A variety of carbon-dimer defects at a SiC/SiO$_2$ interface, such as Si—CO—CO$_2$, Si—CO—CD—Si, and Si—(CO)—CO$_2$ are stable under the oxygen-rich condition at 1600 K, and they create localized levels relatively close to the valence band edge of SiC, thus being critical defects for p-channel MOSFETs. In the viewpoint of static energetics, our results suggest that the oxidation of SiC under a high-temperature oxygen-poor condition is effective in suppressing the generation of carbon defects.

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I. INTRODUCTION
Silicon carbide (SiC) has attracted increasing attention as a suitable material for next-generation power devices, owing to its superior physical properties (e.g., wide bandgap, high critical electric field, high electron saturation velocity, and high thermal conductivity). One of the unique advantages of SiC over other compound semiconductors is that it can be thermally oxidized to form silicon dioxide (SiO$_2$). Thus, SiC metal-oxide-semiconductor field-effect transistors (MOSFETs) have been recognized as a strong candidate for power switching devices.

Despite their promising characteristics for applications, SiC MOSFETs have suffered from the unexpectedly low channel mobility, which is certainly due to the high interface state density ($D_{IT}$) of SiC/SiO$_2$ systems ($\sim$10$^{13}$ eV$^{-1}$ cm$^{-2}$). Due to this high $D_{IT}$, which is a thousandfold higher than that in typical silicon (Si)/SiO$_2$ systems ($\sim$10$^{10}$ eV$^{-1}$ cm$^{-2}$), the field-effect mobility of SiC MOSFETs is mainly limited by the carrier trapping effect of the interface states, even after proper interface nitridation.

Although the microscopic origin of the interface states is not yet identified, carbon defects have been widely believed as a possible origin. Indeed, a study based on internal photoemission (IPE) spectroscopy suggested the existence of sp$^3$-bonded and graphite-like carbon clusters near a SiC/SiO$_2$ interface. A report based on secondary ion mass spectrometry (SIMS) also provided evidence of carbon defects and discussed the correlation between the interface quality and the excess carbon density. Besides, a signal originating from carbon dangling bonds at a SiC/SiO$_2$ interface was detected by utilizing electron-spin-resonance (ESR) spectroscopy.

Theoretical calculations also suggested various candidates of carbon defects so far. As a few examples, dicarbon antisites [(C$_2$)$_{fi}$] in SiC, Si$_2$—C—O$^2$ and Si$_2$—C═C═Si$^{12−17}$ structures in SiO$_2$, and Si—(CO)—Si defects at a SiC/SiO$_2$ interface have been suggested. There is also a report that even larger carbon clusters are possible to exist near the interface. Meanwhile, it was suggested that the interface states might originate from the irregularities of SiC at the interface (i.e., not atomically smooth surface).
However, very few of the previous reports systematically deal with the defects in SiC and SiO\textsubscript{2} and at SiC/SiO\textsubscript{2} interfaces.

In the present study, we, therefore, perform systematic first-principles calculations that reveal the stable atomic configurations of carbon defects in SiC, SiO\textsubscript{2}, and at SiC/SiO\textsubscript{2} interfaces. We investigated 114 types of possible defect configurations and compared their formation energies under certain chemical potential conditions to discuss their stability depending on the oxidation environment (an O-rich or -poor condition). The temperature dependence of defect formation energies was also obtained by correcting the chemical potentials of atomic species at finite temperatures by referring to the NIST-JANAF thermoch\textsubscript{e}m\textsubscript{a}l tables.\textsuperscript{14} We also calculate the localized levels induced by the defects which are relatively stable at a typical oxidation temperature of SiC.

II. CALCULATION CONDITIONS

A. Computational methodologies

All the calculations in this study were carried out on the basis of density functional theory (DFT)\textsuperscript{27-29} by using the Vienna \textit{ab initio} simulation package (VASP).\textsuperscript{27-29} Both the structural optimization and the calculation of one-electron energy levels were performed by using the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional\textsuperscript{28-30} to reproduce the experimental bandgap of SiC well. The projector augmented wave (PAW) method\textsuperscript{31} as implemented in the VASP code was applied in the calculations.

B. Modeling of defects

We used a 128-atom 4H-SiC supercell (a 4 × 4 × 1 supercell), a 72-atom \textalpha\textsubscript{-quartz} SiO\textsubscript{2} supercell, and a 224-atom 4H-SiC surface slab to investigate the carbon defects in SiC, SiO\textsubscript{2}, and at their interface, respectively. We considered 114 types of defect configurations (23, 12, and 79 types of defects in SiC, SiO\textsubscript{2}, and at a SiC/SiO\textsubscript{2} interface, respectively) to investigate a variety of monon and dicarbon defects. In investigating the carbon defects in SiC, we introduced one or two additional C atoms into the 4H-SiC supercell (Fig. 1) at the positions described in Fig. 2 (i.e., a, b, a', b', 1, 2, 3, 4, 1', 2', 3', and 4') with and without removing Si atoms, and performed structural optimization to obtain the stable defect configurations. For instance, if we introduce a C atom into the position a in Fig. 2, we obtain a C-on-Si antisite (C\textsubscript{Si}). For defects in SiO\textsubscript{2}, we focused on the dicarbon defects which are reported to be stable (or metastable) from previous first-principles molecular dynamics (MD) calculations.\textsuperscript{31} In the 72-atom \textalpha\textsubscript{-quartz} SiO\textsubscript{2} supercell (Fig. 3), we reproduced the reported defect configurations shown in Fig. 4 and optimized them to obtain stable defect configurations.

In investigating the defects at a SiC (0001)/SiO\textsubscript{2} interface, we prepared a 224-atom 4H-SiC surface slab of which surface atoms were terminated by H atoms, as shown in Fig. 5. The H atoms at the (0001) face were inserted to remove the dangling bonds of surface Si atoms, which are supposed to be attached to O atoms of amorphous SiO\textsubscript{2} in SiC (0001)/SiO\textsubscript{2} systems. The surface C atoms at the (0001) face should be connected to bulk SiC, which were also terminated by H atoms. We adopted this surface-slab model instead of preparing SiC (0001)/amorphous-SiO\textsubscript{2} systems in investigating the defects, to eliminate the energy cost for the surrounding amorphous-SiO\textsubscript{2} structure which depends on each specimen (i.e., each defect configuration) and to compare the formation energies of carbon defects on equal footing. In more detail, if a defect is introduced at the SiC/amorphous-SiO\textsubscript{2} interface and then its geometry is optimized, the total energy of the system will substantially be affected by the local distortion of amorphous-SiO\textsubscript{2} structure around the defect. Since such a distortion will be released in the realistic situation, we adopted a surface-slab model to avoid this problem. We confirmed that the calculated bandgap is sufficiently accurate.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{128-atom 4H-SiC supercell (a 4 × 4 × 1 supercell) used to investigate the carbon defects in the present study. The blue and brown balls indicate the Si and C atoms, respectively.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig2.png}
\caption{Positions to introduce carbon atoms in 4H-SiC. Positions a, a', and b' are the Si-sites, and positions 1, 2, 3, 4, 1', 2', 3', and 4' are the interstitial sites. Note that sites a, a', b, b', 1, 2, 3, and 4' are equivalent to sites a, b, 1, 2, 3, and 4, respectively, but are labeled to describe the defect pair combinations. We investigated single antisites (a and b), single interstitials (1–4), antisite-antisite pairs (a, b), (a, a'), (b, b'), antisite-interstitial pairs (a, 1), (a, 2), (a, 3), (a, 4), (b, 1), (b, 2), and (b, 4), and interstitial-interstitial pairs (1, 2), (1, 3), (1, 4), (2, 3), (2, 4), (3, 4), (2, 1), and (4, 3)].}
\end{figure}
converged with respect to the slab thickness and is also close to the experimental value of 3.26 eV at 300 K. The calculated bandgap was 3.39 eV and 3.36 eV for 224- and 256-atom slabs, respectively.

In investigating the defects, carbon atoms were inserted on the top of the surface Si atoms at a SiC (0001) surface with removing several H atoms from the surface. The investigated defect configurations are depicted in Fig. 6. In preparing the c1d1 defects in Fig. 6, for instance, we put a single C atom above the center of gravity of three topmost Si atoms, together with removing three surface H atoms. Then, three C—Si bonds are generated. A dangling bond is left on the inserted C atom, which is treated by four different ways, as depicted in Fig. 7: a dangling bond (d), O—(o), OH— (h), and SiH3— (s) terminations. Finally, structural optimization is performed to obtain stable defect configurations.

C. Defect formation energy

The formation energy, $E_f$, of a neutral defect was calculated by

$$E_f = E_D - E_0 - \sum_i N_i \mu_i,$$

where $E_D$ and $E_0$ are the total energies of the simulation cell with and without the defect, respectively. $N_i$ and $\mu_i$ are the number of the removed ($N_i < 0$) or added ($N_i > 0$) $i$-type atoms and its chemical potential, respectively. We supposed four extreme situations, where the chemical potentials of the atomic species were calculated as

$$\mu_{\text{Si}} = \frac{E(\text{SiO}_2)}{2} - 2\mu_{\text{O}}, \quad \mu_{\text{C}} = \frac{E(\text{SiC})}{2} - \mu_{\text{Si}},$$

$$\mu_{\text{O}} = \frac{E(\text{O}_2)}{2}$$

(C-rich, O-rich); (2)

$$\mu_{\text{Si}} = E(\text{Si}), \quad \mu_{\text{C}} = E(\text{CO}_2) - 2\mu_{\text{O}},$$

$$\mu_{\text{O}} = \frac{E(\text{SiO}_2)}{2} - \mu_{\text{Si}}$$

(C-rich, O-rich); (3)
and \( \mu_0 \) were calculated as \( \mu_0 = E(SiO_2) - 2\mu_O \) and \( \mu_O = E(O)/2 \) (O-rich) or \( \mu_O = E(Si) \) and \( \mu_0 = (E(SiO_2) - \mu_O)/2 \) (O-poor). Then, \( \mu_C \) was calculated either by \( \mu_C = E(SiC) - \mu_S \), or \( \mu_C = E(CO_2) - 2\mu_O \), depending on the condition (O-rich or O-poor). Since the chemical potential of Si is low (−15.19 eV) and that of O is high (−6.98 eV) under the O-rich condition, \( \mu_C = E(SiC) - \mu_S \) (−2.23 eV) and \( \mu_C = E(CO_2) - 2\mu_O \) (−14.37 eV) correspond to the C-rich and -poor limits, respectively. Conversely, under the O-poor condition, since the chemical potential of Si is high (−6.28 eV) and that of O is low (−11.44 eV), \( \mu_C = E(SiC) - \mu_S \) (−11.15 eV) and \( \mu_C = E(CO_2) - 2\mu_O \) (−5.45 eV) correspond to the C-poor and -rich limits, respectively. As we focused on the carbon defects, we considered the C-rich limits [Eqs. (2) and (3)] in the present study. Note that, in these extreme carbon-rich conditions [Eq. (2) and (3)], \( \mu_C \) takes even higher values than that in diamond (i.e., \( \mu_C = E(C) = −10.52 \) eV). As we approximated the SiC/SiO\(_2\) interface with an H-terminated SiC slab (Fig. 5), the chemical potential of an H atom is also needed to calculate the formation energy [Eq. (1)], which was calculated as

\[
\mu_H = \frac{E(SiH_4) - \mu_H}{4},
\]

irrespective of the conditions [Eq. (2) or (3)]. Here, \( E(SiH_4) \) is the total energy of a silane (SiH\(_4\)) molecule per formula unit; the calculated value of \( E(SiH_4) \) was −21.95 eV at 0 K. Since most of the H atoms were used to terminate the Si-dangling bonds, we here adopted \( E(SiH_4) \) in calculating \( \mu_H \). At finite temperatures, we obtained the temperature dependence of enthalpy, \( H(T) \) and entropy, \( S(T) \) of gaseous molecules, O\(_2\), CO, CO\(_2\), and SiH\(_4\) at the standard state pressure \( (p^0 = 0.1 \) MPa) from the NIST-JANAF thermochromical tables\(^{24} \) to correct their energies.

III. RESULTS AND DISCUSSION

A. Defect formation energy

Figures 8(a) and 8(b) show the temperature dependence of formation energies for the carbon defects in SiC (0001)/SiO\(_2\) systems. Here, the energies of gaseous CO and CO\(_2\) molecules are also shown for comparison. The structure of the carbon defects is depicted in Fig. 9. Since a C-rich situation is considered, dicarbon defects tend to be more favorable than the monocarbon ones at either condition (O-rich or -poor), as shown in Fig. 9. At the O-rich limit [Fig. 8(a)], the formation energies of defects #1–#5 are quite low at 1600 K, which is about the typical experimental temperature of SiC oxidation, and the energies are even comparable with those of gaseous CO and CO\(_2\) molecules. Such a result suggests that, during the oxidation of SiC under a condition close to the O-rich limit, a significant portion of C atoms will favor staying around the interface to create defects than to be ejected from the system as CO or CO\(_2\) molecules. We also see that the defects with O atoms tend to appear as stable forms in the O-rich condition (Fig. 9). At the O-poor limit [Fig. 8(b)], the formation energies of the defects are relatively high compared to the energies of CO and CO\(_2\) molecules. Therefore, in the viewpoint of static energetics, oxidation under an O-poor condition is more favorable than under
an O-rich condition in reducing the carbon defects at a SiC/SiO\textsubscript{2} interface. When looking at the temperature dependences, CO and CO\textsubscript{2} molecules become more favorable compared to the carbon defects at higher temperatures, suggesting that oxidation at higher temperatures is also favorable. In fact, a recent experimental study proved that high-temperature oxidation over 1400 °C (∼1670 K) combined with rapid cooling reduces the defects at a SiC (0001)/SiO\textsubscript{2} interface.

Also, post-oxidation annealing in argon (Ar) ambient with a very low oxygen partial pressure at 1500 °C (∼1770 K), of which condition is considered to be close to the O-poor limit [Fig. 8(b)], reduces defects at SiC (0001)/SiO\textsubscript{2} interfaces.\textsuperscript{34} Such results can be qualitatively understood by our calculation results.

B. Defect energy levels

Figure 10 shows the energy levels of the carbon defects stable at 1600 K under either the O-rich or -poor condition. Under the O-rich condition, the dicarbon antisite in the SiC side [(C\textsubscript{2})\textsubscript{Si}(#2)] is stable (Fig. 9), and it creates a defect level near the conduction band edge (E\textsubscript{C}) of SiC (about E\textsubscript{C}−0.1 eV for the h-site and E\textsubscript{C}−0.4 eV for the k-site defect: Fig. 10),\textsuperscript{35} thus being a critical defect for n-channel MOSFETs. Under the O-rich condition [Eq. (2)], the chemical potential of Si is low (Si-poor) and that of C is high (C-rich), which facilitates the creation of (C\textsubscript{2})\textsubscript{Si} by lowering the formation energies of silicon vacancies and carbon clusters at the same time. The existence of (C\textsubscript{2})\textsubscript{Si} near the SiC/SiO\textsubscript{2} interface is also predicted in Refs. 12 and 13, where models with top-SiO\textsubscript{2} layers were employed. Many types of interface carbon-dimer defects, such as Si—CO—CO\textsubscript{2} (##1), Si—CO—CO—Si (##4), and Si—CO—CO\textsubscript{2} (##5), are stable under the O-rich condition and they create defect levels relatively close to the valence band edge (E\textsubscript{V}) of SiC (Fig. 10). Thus, they are critical defects for n-channel MOSFETs. For the O-poor condition, the interface carbon-dimer defect (Si—C—C—Si, #6) is the most stable and it will affect the performance of n-channel MOSFETs, since it creates a defect level near E\textsubscript{V} (about E\textsubscript{V}−0.1 eV: Fig. 10). We see that the carbon-dimer defect in the SiO\textsubscript{2} side (Si—C—C—Si, #9) appears as one of the metastable defects, which is also discussed in previous literature.\textsuperscript{14,15} For p-channel MOSFETs, the O-poor condition seems to
FIG. 8. Temperature dependence of defect formation energies in comparison with the energies of gaseous CO and CO$_2$ molecules at the (a) C-rich, O-rich and (b) C-rich, O-poor limits. The zeros of the formation energies are set at the energy of a CO molecule. The structure of the defects (#1–#10) is depicted in Fig. 9. The temperature dependence of defect formation energies was calculated by correcting the chemical potentials of atomic species at finite temperatures by referring to thermochemical tables as described in Sec. II C. Lines in dark contrast (red, blue, and black) indicate the defects stable at 1600 K, which is about the typical experimental temperature of SiC oxidation. The red, blue, and black solid lines correspond to the energies of defects in SiC, SiO$_2$, and at SiC/SiO$_2$ interfaces, respectively. Green lines represent the energies of gaseous CO and CO$_2$ molecules.

FIG. 9. Structure of the defects stable at 1600 K, which is about the typical experimental temperature of SiC oxidation. The structures are listed in order of stability in either oxidation environment (the C-rich, O-rich or C-rich, O-poor limit). The blue, brown, red, and small white balls are the Si, C, O, and H atoms, respectively. Note that the structures were attached to H atoms instead of Si or O atoms of amorphous SiO$_2$. 

more stable

| Interface | Structure | Stability |
|-----------|-----------|-----------|
| #1 Si-CO-CO$_2$ | C-rich, O-rich (1600 K) | more stable |
| #2 (C$_2$)$_{Si}$ | SiC-side |
| #3 Si-(CO)-(CO)O | interface |
| #4 Si-CO-CO-Si | interface |
| #5 Si-(CO)-CO$_2$ | interface |
| #6 Si-C-C-Si | interface |
| #7 Si-C-C-O-Si | interface |
| #8 Si$_2$-C-C-O | interface |
| #9 Si$_2$-C-C-Si$_2$ | SiO$_2$-side |
| #10 Si$_3$-C | interface |
be quite favorable, and there are few stable defects which create defect levels near $E_v$ inside the bandgap (Figs. 9 and 10).

IV. SUMMARY

We investigated the stable atomic configurations and energy levels of carbon defects in SiC and SiO$_2$, and at SiC (0001)/SiO$_2$ interfaces. The temperature-dependent defect formation energies were obtained by correcting the chemical potentials of atomic species at finite temperatures by referring to thermochromical tables. Our results indicate that the oxidation of SiC under an O-rich condition, especially at low temperatures, results in the creation of critical defects for both $n$- and $p$-channel MOSFETs. For instance, the dicarbon antisite in the SiC side [(C$_{2}$)$_{Si}$] is stable under the O-rich condition, and it creates a defect level near $E_v$, being crucial for $n$-channel MOSFETs. As critical defects for $p$-channel MOSFETs, many types of interface carbon-defect, such as Si—CO—CO$_2$ (1), Si—CO—CO—Si (4), and Si—(CO)—CO$_2$ (5), are stable under the O-rich condition and they create defect levels relatively close to $E_v$. Thus, in the viewpoint of static energetics, we suggest the oxidation of SiC at a high-temperature O-poor condition in order to suppress the generation of the carbon defects.

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