

First Principles Study of N Incorporation Effect during SiC Oxidation

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Abstract

We investigated the atomistic mechanism of N incorporation during SiC oxidation by the first principles calculation. We found that N atoms tend to form three-fold coordinated covalent bonds on a SiC(0001) surface, which enable termination of the odd number of dangling bonds. These results indicate that N incorporation is effective to suppress defect state generation at SiO₂/SiC interfaces during SiC oxidation.

1. Introduction

Silicon Carbide (SiC) is expected as a promising material for the next generation's high power and high frequency electronic devices because SiC has superior physical properties to Si such as high breakdown field, high thermal conductivity and high saturation electron drift velocity. Adding to physical properties, one of advantages of SiC for practical application is the formation of insulating silicon oxide (SiO₂) layers on SiC by thermal oxidation process, being important for the fabrication of SiC-based metal oxide semiconductor field effect transistors (MOSFETs).

However, it is known that quality of SiC/SiO₂ interfaces is much worse than that of conventional Si/SiO₂ interfaces. SiC MOSFETs have still suffered from low channel mobility and low drain current due to the high interface state density of SiC/SiO₂ [1]. One of the most well-known recipes to suppress its large interface state density is N incorporation into SiC/SiO₂ interfaces. Experimentally, it has been reported that N incorporation is effective to improve interface properties [2]. However, the physical origin of N effect is still unclear.

In this study, we give a guideline for the issue of SiC/SiO₂ interface problem by considering the atomistic behavior of NO molecules absorbed on a 4H-SiC(0001) surface on the basis of first-principles calculations within the framework of density functional theory (DFT).

2. Method

In this study, we prepared a 72 atoms repeated slab model with eight atomic layers 4H-SiC and a 10Å vacuum region. We also considered two types SiC (0001) surfaces. One is a $\sqrt{3}\times\sqrt{3}$ Si-terminated (0001) reconstructed surface (Fig.1(a)). The other is H-terminated (0001) surface (Fig.1(b)). We studied NO molecules absorption on the two types (0001) surface and investigated the most stable structure by optimizing the structure including NO molecules. We used ultrasoft pseudopotentials for Si, C, O, H and N. Wavefunctions were expanded by a planewave basis set with a cutoff energy of 36 Ry, and $2\times 2\times 2$ k -points are used for the Brillouin zone integration. Structural optimizations were performed until all the atomic forces were less than

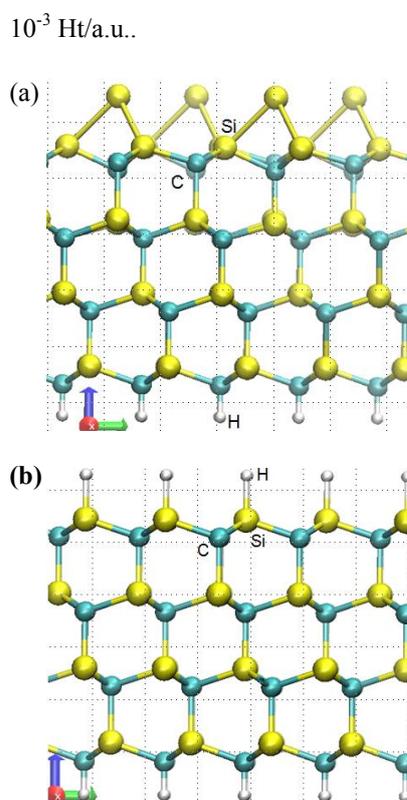


Fig.1: A 72 atoms repeated slab model with eight atomic layers 4H-SiC. (a) $\sqrt{3}\times\sqrt{3}$ Si-terminated (0001) reconstructed surface. (b) H-terminated (0001) surface.

3. Result and Discussion

3.1 NO adsorption on $\sqrt{3}\times\sqrt{3}$ reconstructed SiC surfaces

We first discuss $\sqrt{3}\times\sqrt{3}$ Si-terminated reconstructed surface. We found that an absorbed NO molecule separates into a N atom and an O atom. As a result, the absorbed N atom formed three-fold coordinated covalent bonds with surface Si atoms (Fig.2(a)) and several surface Si-Si bonds were extended compared to experimental Si-Si bonds 2.34Å. We also found that N behaves similarly when an additional NO molecule was absorbed on the SiC surface. Actually, the additional NO molecule is absorbed on the

one-NO-absorbed surface given in Fig.2(b), the second NO molecule also separates into a N atom and an O atom, leading to the formation of three N-Si bonds.

These results indicate that N atoms are likely to form three-fold coordinated covalent bonds on high-atomic-density SiC surface. It is noted that N atoms can terminate odd number of dangling bonds because the suitable coordination number of N is three. On the other hand, O atoms can terminate two dangling bonds. Therefore, a small number of N incorporation is effective to improve interface properties as illustrated in Fig.3. Consequently, we can conclude that N incorporation during SiC oxidation is effective to improve SiC interface properties.

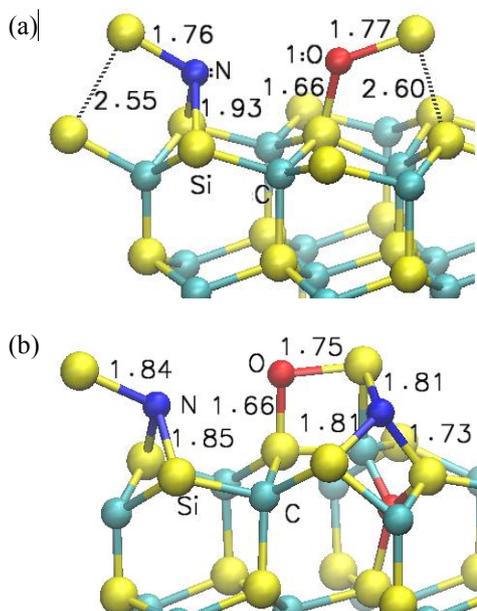


Fig.2: Optimized $\sqrt{3}\times\sqrt{3}$ Si-terminated SiC(0001) surface structures after one and two NO molecule adsorption. (a) An optimized structure after one NO adsorption (b) An optimized structure after two NO molecules adsorption.

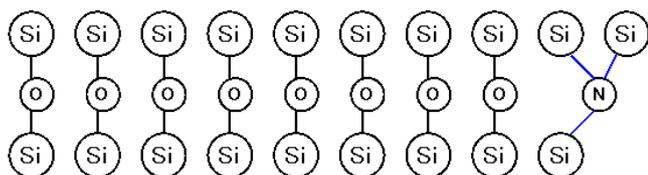


Fig.3: Schematic illustration of the role of N in the termination of SiC/SiO₂ interfaces. A small number of N incorporation is effective to improve interface properties.

3.2 NO adsorption on H-terminated SiC surfaces

Next, we discuss the NO adsorption on a H-terminated surface. Our calculation showed that a NO molecule was absorbed on SiC surface, maintaining NO molecule form as shown in Fig. 4(a). It is noted that a NO molecule was adsorbed on SiC surface from N atom. However, the O atom of NO molecule was not absorbed on a SiC surface. Thus, the N atom can form three-fold coordinated covalent bonds with surface Si, H, and O atoms. On the other hand, the O

atom has only one covalent bond. Moreover, we also found that NO molecules behave similarly when an additional NO molecule was absorbed on H-terminated SiC surface. Actually, when the second NO molecule was absorbed on the one-NO-absorbed surface, the N atom was inserted into Si-C bond (Fig. 4(a)). Whereas, an O atom stayed on the surface. These results indicate that the N atom in NO molecule has higher reactivity on SiC surfaces than the O atom.

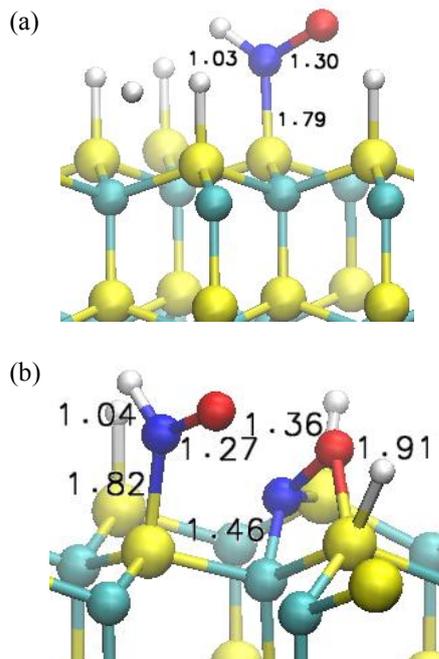


Fig.4: Optimized H-terminated SiC(0001) surface structures after one and two NO molecule adsorption. (a) An optimized structure after one NO adsorption (b) An optimized structure after two NO molecules adsorption.

4. Summary

We investigated the effect of N atom incorporation during SiC oxidation. We found that N atoms form three-fold coordinated covalent bonds on both of $\sqrt{3}\times\sqrt{3}$ Si-terminated SiC surface and H-terminated SiC surface. On $\sqrt{3}\times\sqrt{3}$ Si-terminated SiC surface, NO molecule separates into a N atom and an O atom and the absorbed N atom formed three-fold coordinated covalent bonds with surface Si atoms. On the other hand, a NO molecule tends to adsorb from a N atom on H-terminated SiC surface.

It is noted that N atoms terminate odd number of dangling bonds at a SiC/SiO₂ interface. O atoms can terminate two dangling bonds. In oxidized SiC surface, a small number of N incorporation is effective to terminate odd number of dangling bonds which cannot be terminated only by O atoms.

References

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- [2] D. Okamoto, H. Yano, T. Hatayama and T. Fuyuki, Appl. Phys. Lett. 96, 203508 (2010)