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Theoretical Investigations on the Oxidation Mechanism of the 4H-SiC(0001) Surface and its Interface with SiO_2

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Introduction

The silicon carbide (SiC) material is known to have wide band gaps, high thermal conductivities, and high electrical breakdown field strengths much preferred for high power devices. Commercialization of SiC-based devices, however, has been hampered by large density of interface states (D_{it}) [1] found in the SiC/SiO_2 interface, the heart of metal-oxide semiconductor (MOS) devices. High values of D_{it} contribute to charge-trapping and Coulomb scattering, which, in turn, results to high on-state resistances manifested as low-inversion channel mobilities in the device [2].

Using our large-scale quantum chemical molecular dynamics simulation method, we performed a series of theoretical investigations on the 4H-SiC(0001) surface as well as its interface with SiO_2 to understand the oxidation mechanisms of this surface, which will give hint to the formation of defects within the interface.

Method

The quantum chemical molecular dynamics calculations were carried out using the “Colors” program [3] developed in our laboratory. This method is based on our original tight-binding approximation in which long-range Coulombic interaction is considered explicitly.

For the molecular dynamics simulations, the Ryudo program, also developed in our laboratory, was used. This program makes use of the consistent valence force field (CVFF). Atomic motions and electronic interactions were calculated using the Verlet algorithm and the Ewald method, respectively.

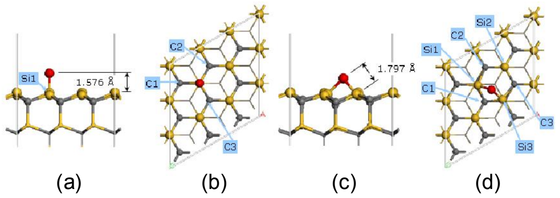

Fig. 1. (a) and (c) depict the side views of the on-top (OT) and bridge (BR) bonding sites for the O adatom on the 4H-SiC(0001) surface. (b) and (d) are the corresponding top views.

Results and Discussion

Four possible bonding sites for the O adatom with varying coordination numbers were configured on the 4H-SiC(0001) surface. These are the on-top (OT), bridge (BR), three-fold coordinated bonding to 3 Si surface atoms (T3), and four-fold coordinated bonding to 3 Si surface atoms and a C atom (T4) sites. These four bonding configurations were allowed to relax with the four bottom layers of alternating Si and C atoms kept fixed, including the saturating H atoms.

Only the OT and BR adatom configurations, as shown in Fig. 1, were equilibrium adsorption sites. The BR bonding site with a calculated adsorption energy of 4.009 eV, which is greater than that of the OT site, might be a more favorable bonding site. From the bond parameters, however, it was observed that the O adatom on the BR site contributed much strain on the two Si atoms it was bonded to. Without this O adatom, these two Si atoms maintained a distance of 3.078Å, while with the adatom present, this distance was reduced down to 2.583Å. To resolve this ambiguity, O atom pairs were also considered.

Further results will be presented in the conference. The generation of the SiC/SiO_2 interface as well as its electronic properties will also be discussed.

Table 1. Adsorption energies, Si-O distances, and O atom Mulliken charges of the four bonding sites.

Bonding site	E_{ads} (eV)	$d_{O\text{-}Si}$ (Å)	O atom Mulliken charge (|e|)
OT	3.737	1.576	-0.741
BR	4.009	1.797	-0.807
T3	-	-	-
T4	-	-	-

References

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3. T. Masuda *et al. Appl. Surf. Sci.,* **244** (2005) 30.