Large-scale Quantum Chemical Molecular Dynamics Study on the SiC/SiO₂ Interface for SiC-based Devices

John Paul Yacapin¹, Ai Suzuki², Hideyuki Tsuboi¹, Nozomu Hatakeyama¹, Akira Endou¹, Hiromitsu Takaba³, Momoji Kubo⁴, and Akira Miyamoto^{2,1,3}

¹Tohoku Univ., Dept. Appl. Chem., Grad. School Eng., 6-6-11-1302 Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan Phone: +81-22-795-7233 E-mail: yacapin@aki.che.tohoku.ac.jp

²Tohoku Univ., NICHe, 6-6-11-1302 Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan

³Tohoku Univ., Dept. Chem. Eng., Grad. School Eng., 6-6-11-1302 Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan ⁴Tohoku Univ., FRRI, Grad. School Eng., 6-6-11-701 Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan

1. Introduction

Wide-bandgap semiconductors are expected to replace Si in high-performance power electronic systems. SiC appears most promising in applications that require much higher efficiency, power density, and reliability. Commercialization of SiC-based devices, however, is hindered by defects found in the SiC/SiO₂ interface as characterized by the density of interface traps (D_{it}) in the interface bandgap [1]. Atomistic understanding on the nature of these defects and its treatment is very important.

Using our tight-binding quantum chemical molecular dynamics simulation method, we investigated the electronic structure of the SiC/SiO₂ interface. Known possible defect structures were later considered into the interface. After establishing the validity of these defect structures, treatment of these defects by H passivation was also studied.

2. Method

Tight-binding quantum chemical calculations

The quantum chemical molecular dynamics calculations were carried out using the "Colors" program [2] developed in our laboratory to calculate electronic structure properties of the SiC/SiO₂ interface, as well as its defect levels. This method is based on our original tightbinding approximation in which long-range Coulombic interaction is considered explicitly. The total energy of a system is calculated by the following equation:

$$E = \sum_{i=1}^{N} \frac{1}{2} m_i v_i^2 + \sum_{k=1}^{OCC} \varepsilon_k + \sum_{i=1}^{N} \sum_{j>i}^{N} \frac{Z_i Z_j e^2}{R_{ij}} + \sum_{i=1}^{N} \sum_{j>i}^{N} E_{repuls} \left(R_{ij} \right)$$
(1)

$$E_{repuls}\left(R_{ij}\right) = b_{ij} \exp\left(\frac{a_{ij} - R_{ij}}{b_{ij}}\right)$$
(2)

Here Z_i is the atomic charge, e is the elementary electric charge, and r_{ij} is the interatomic distance. The four terms in Eq. (1) refer to the kinetic energy, eigenvalues of all occupied orbitals, Coulombic interactions, and short-range exchange repulsion energy, respectively. The parameters a and b in Eq. (2) represent the size and stiffness of atoms, respectively.

Molecular dynamics simulations

Molecular dynamics simulations were carried out by the Ryudo program developed in our laboratory to obtain the interface structure. This program makes use of the consistent valence force field (CVFF) given by:

$$E = \sum_{b} D_{b} \left[1 - e^{-\alpha(b-b_{0})} \right]^{2} + \sum_{\theta} H_{\theta} \left(\theta - \theta_{0} \right)^{2}$$
(3)
+
$$\sum_{\phi} H_{\phi} \left[1 + \cos(n\phi - \phi) \right] + \sum_{i} \sum_{j>i} \left[\frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^{6}} + \frac{Z_{i}Z_{j}e^{2}}{r_{ij}} \right]$$
(3)

The four terms in Eq. (3) refer to the following potentials in respective order: Morse, angle bending, bond rotation, and noncovalent (Lennard-Jones and Coulomb). The Verlet algorithm was used for the calculation of atomic motions and the Ewald method for the electrostatic interactions.

The dynamic features of the molecular dynamics simulations were visualized and further analyzed using our computer graphics visualization program RYUGA [3].

3. Results and Discussions

*Structure and electronic properties of the SiC/SiO*₂ *interface*

The interfacial bonding pattern in the SiC/SiO_2 interface is modeled as an abrupt interface model with bond density reductions. Shown in Fig. 1 is the optimized interface model along with its electronic structure properties calculated using "Colors" at 300 K. Valence states near the Fermi level are predominated by C, while the conduction states by Si, due mainly to their relative electronegativities.



Fig. 1. (a) SiC/SiO₂ abrupt interface structure; (b) electronic structure showing total density of states with Si and C atomic decompositions.

An important feature of this interface is the carefully configured bonding in the interface, which allows for bond reduction as shown in Fig. 2. The SiC substrate shown in Fig. 2(a) exposes 12 Si dangling bonds on its surface. To reproduce the realistic density of the SiO₂ layer, bond reduction in the SiC/SiO₂ interface required. The bonding configurations shown in Fig. 2(b) allows for this required bond reduction while preserving the tetrahedral bonds of Si. Fig. 2(c) shows the 8 O atoms after bond reduction.



Fig. 2. Bond configurations within the interface: (a) SiC surface exposing 12 Si dangling bonds; (b) interfacial bonding configurations in the abrupt interface of SiC and SiO₂; (c) bond reduction from 12 down to 8 bonds.

Defect configurations in the SiC/SiO₂ interface

Incomplete removal of C in conventional oxidation of SiC leads to several C-related defects as previously proposed [1, 4, 5]. We considered a single C interstitial in SiC and a C-C pair defect in the interface. Known defects intrinsic to bulk SiO_2 were also studied. With our novel large-scale quantum chemical molecular dynamics simulator, modeling of defects in the form of C aggregates requiring larger simulation cells was also realized.

From the experimental findings of Afanas'ev *et al.* [1] and the proposed defect configurations by Knaup *et al.* [4], we analyzed the contribution of C-related defects in the density of interface states. As shown in Fig. 3, the atomic structures of these defects are embedded into the SiC/SiO₂ interface. The corresponding defect levels revealed the contribution of these defects in interface traps.

In Fig. 3(a), a C interstitial defect is shown to bond with 2 Si atoms and a C atom in the substrate surface. A similarly bonded interstitial species of a C-C pair is depicted in Fig. 3(b). Figs. 3(c) & (d) are defects related to vacancies. A C vacancy occupied by 2 O interstitial atoms and a C dumbbell occupying a Si vacancy are illustrated in Figs. 3(c) & (d), respectively. Defects are shown enclosed in elliptical marks.



Fig. 3. Defect configurations in the SiC/SiO_2 interface and corresponding defect levels in eV: (a) a C interstitial, (b) a C-C pair interstitial, (c) a C vacancy occupied by 2 O interstitials, and (d) a C dumbbell occupying a Si vacancy.

Discussion of defect levels

Opposite the illustration of defect configurations in Fig. 3 are the defect levels in comparison with the valence band maximum (VBM) and the conduction band minimum (CBM) of SiC. The VBM was set to 0 eV, and a CBM of 2.3 eV was obtained. For a C interstitial, defect levels of 0.7 eV beyond the VBM and 2.1 eV below the CBM of SiC were calculated. This suggests a contribution of this defect to the D_{it} found within the interface. A C-C pair interstitial, on the other hand, has a defect level of 0.4 eV beyond the SiC VBM and its CBM is beyond that of SiC's. With regards to the explanation of the D_{it} , a C-C pair interstitial does not contribute to the defect states near the conduction band and has very small contribution to the defect states near the valence band.

A C vacancy occupied by 2 C interstitials in Fig. 3(c) may not contribute to the D_{it} near the conduction band but shows a relatively high contribution in the valence band at 1.0 eV. A similar case can be observed for a C dumbbell occupying a Si vacancy as shown in Fig. 3(d). This defect contributes to the D_{it} near the valence band with a defect level of up to 1.1 eV.

From the calculation of these defect levels, it can be observed that those defects occupying a certain atomic vacancy in the SiC substrate have relatively high defect levels in the valence band, thus, the defects shown in Figs. 3(c) & (d) may be responsible for the D_{it} near the valence band.

4. Conclusions

An abrupt interface model was successfully generated in this study. Our large-scale quantum chemical molecular dynamics program "Colors" allows for the analyses of defect configurations previously not considered due to limitations of simulation cell size [4]. From the results, two of the defects as depicted in Figs. 3(c) & (d) may have the largest contribution in the traps near the valence band due to their high defect levels.

References

- V.V. Afanas'ev, M. Bassler, G. Pensl, & M. Schulz, *Phys. Stat. Sol. (a)* 162 (1997) 321.
- [2] T. Masuda, K. Sasata, M. Elanany, M. Koyama, M. Kubo, & A. Miyamoto, *Appl. Surf. Sci.* 244 (2005) 30.
- [3] R. Miura, H. Yamano, R. Yamauchi, M. Katagiri, M. Kubo, R. Vetrivel, & A. Miyamoto, *Catal. Today* 23 (1995) 409.
- [4] J.M. Knaup, P. Deák, Th. Frauenheim, *Phys. Rev. B* 72 (2005) 115323.
- [5] J.M. Knaup, P. Deák, Th. Frauenheim, *Phys. Rev. B* 71 (2005) 235321.