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Generation of Amorphous SiO_2/SiC Interface Structure by the First-Principles Molecular Dynamics Simulation

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Abstract. The performance of SiC MOSFET devices to date is below theoretically expected performance levels. This is widely considered to be attributed to defect at the SiO_2/SiC interface that degrade the electrical performance of the device. To analyze the relationship between defect structures near the interface and electrical performances, advanced computer simulations were performed. A slab model using 444 atoms for an amorphous oxide layer on a 4H-SiC (0001) substrate was made by using first-principles molecular dynamic simulation code optimized for the Earth-Simulator. Simulated heating and rapid quenching was performed for the slab model in order to obtain a more realistic structure and electronic geometry of a-SiO_2/4H-SiC interface. The heating temperature, the heating time and the speed of rapid quenching were 4000 K, 3.0 ps and -1000 K/ps, respectively. The interatomic distance and the bond angles of SiO_2 layers after the calculation are agree well with the most probable values of bulk a-SiO_2 layers, and no coordination defects were observed in the neighborhood of SiC substrate.

Introduction

Silicon carbide (SiC) semiconductor devices are expected to be used in severe environments such as outer space and nuclear power plants. However, SiC devices do not reach theoretically expected performance levels. This is widely considered to be attributed to interface defects between the SiC and the oxide (SiO_2) layer that degrade the electrical characteristics of devices. At this stage, the relation among atomic structures, interfacial defects and electrical characteristics is not clear. In this study, we tried to solve these problems by the computer simulation of electronic structure of the SiO_2/SiC interface. The oxide layer of the real device has an amorphous structure, and there is an interlayer in the SiO_2/SiC interface. To generate the real device interface structure with the computer simulation, it is important to construct the amorphous SiO_2 (a-SiO_2) structure on SiC. In case of a conventional calculation, a-SiO_2/SiC interface structure has been simulated with the crystal-SiO2/crystal-SiC structure that can be easily constructed by small-scale computer calculation [1,2]. To simulate the interface characteristic more accurately, we aimed to generate a-SiO_2/SiC structure by computer calculation using a large-scale interface model in which the amorphous structure was constructed. In the use of the large-scale interface structure, it is possible to introduce not only small size defects like dangling bonds but also big size defects like the carbon cluster.

Simulation result

Generation of a-SiO_2/SiC interface. The heating and rapid quenching method using first-principles molecular dynamics (MD) simulation code was carried out to make an a-SiO_2/SiC interface structure.

In previously published research, the Si/SiO_2 interface structure was generated by heating and rapid quenching calculation [3]. A slab model using 444 atoms for a-SiO_2 on a 4H-SiC (0001) crystal layer was constructed in order to obtain a more realistic interface structure and electronic geometry of a-SiO_2/4H-SiC interface. The calculations have been performed using the ab-initio total-energy and molecular-dynamics program Vienna ab-initio simulation program (VASP) [4] on the Earth-Simulator (ES) under support of JAMSTEC. The simulation code has been strongly optimized for the ES. Prior to the calculation, supercells of the crystalline form of SiO_2 (beta-quartz) on a 4H-SiC (0001) crystal layer were employed as an initial simulation structure. Because quite a lot of CPU time is needed for a large-scale calculation, it is necessary to shorten the heating time as much as possible. The crystal becomes amorphous at shorter heating time if a higher temperature is used. We decided the heating temperature, the heating time and the speed of rapid quenching to 4000 K, 3.0 ps and -1000 K/ps, respectively. In order to preserve the crystalline structure of the 4H-SiC layers, atoms of SiC substrates other than in a few interfacial layers have been fixed during the calculation. Even if the SiC substrate is fixed, the atomic structure of SiO_2 breaks easily [5] when it is heated at a high temperature above the boiling point of quartz (2950˚C).

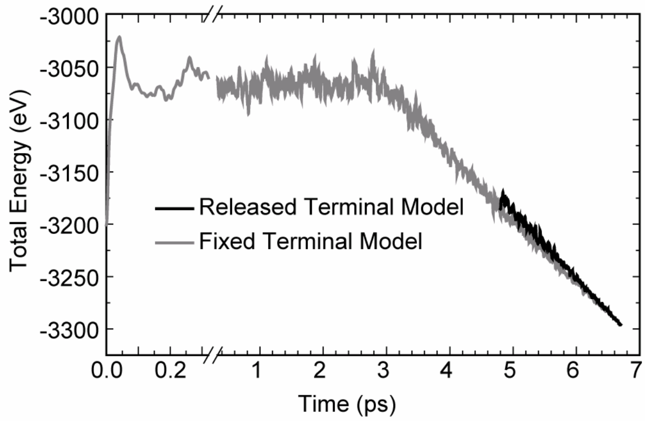


Fig. 1. Total energy of the released terminal model (black) and fixed terminal model (gray) during heating and rapid quenching process.

To prevent destruction of atomic structure, we fixed not only SiC substrate but also the terminal of the SiO_2 layer. Therefore, in this model, movable layer is sandwiched between two fixed layers. In using this sandwich model the movable SiO_2 layer can be made amorphous in a short time without causing the destruction of the atomic structure even if the heating temperature is 4000 K. If the SiO_2 terminal is fixed during all the heating and rapid quenching calculations (fixed terminal model), the interface does not become a preferable structure because the fixed terminal neighborhood layers are not made amorphous. To make the SiO_2 layer a better amorphous structure, the fixed SiO_2 terminal was released while rapid quenching (released terminal model) at the temperature below 2200 K in which the destruction of the atomic structure did not happen. However, although the total energy of the released terminal model became larger than that of fixed terminal model during heating, it became almost the same value after quenching to the room temperature. This shows that the released terminal model has been become a stable structure in room temperature.

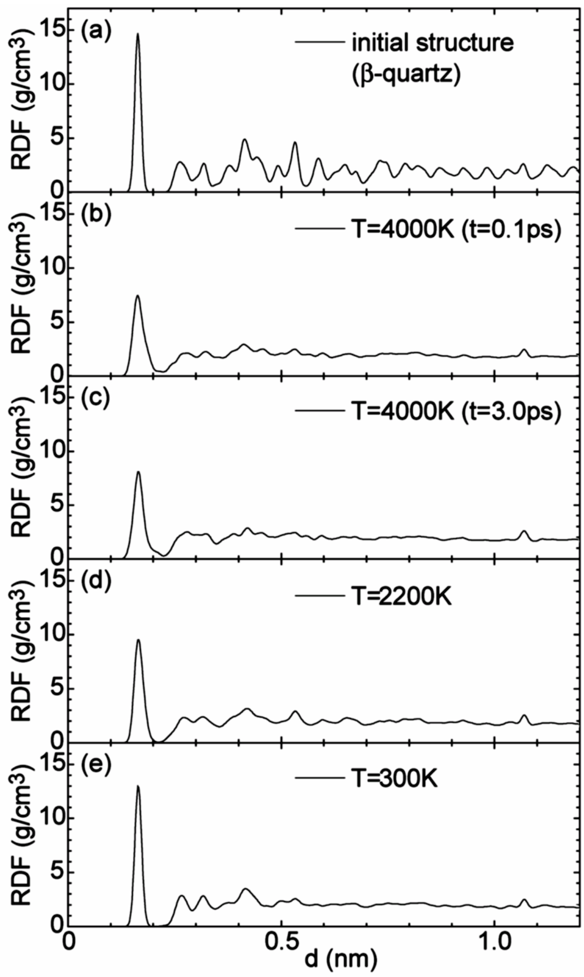


Fig. 2. The RDF of the SiO_2 layers during heating and rapid quenching process.

Radial distribution function of a-SiO_2 layer. The radial pair distribution function (RDF) of the SiO_2 layers was calculated. The RDF can be understood as a bond-length distribution between all pairs of atoms within the crystal. Figure 2 shows the RDF of the SiO_2 layers during heating and rapid quenching process when the device function (peak broadening width) is assumed to be 0.02 nm. Initial SiO_2 layer has the beta-quartz structure. The fine structure of RDF that existed in distance of more than 0.2 nm was lost at once when heating started at temperature up to 4000 K. This shows the long range order of the atomic structure was lost. The position of the peak that existed in 0.165 nm of RDF was kept during heating. However the peak width broadened compared with that of the initial structure. This shows the nearest neighbor interatomic distance did not change so much though that of dispersion became large. Figure 3 shows the RDF of the SiO2 layers after quenching to the room temperature. The RDF of layers between individual elements was shown in Figure 3 while only total atoms RDF had been shown in Figure 2. The nearest neighbor interatomic distance between Si and O became 0.165 nm. It almost became equal with Si-O bond length of 0.161 nm in the alpha crystal. The nearest neighbor interatomic distance between Si and Si became 0.315 nm. When this distance is converted into Si-O-Si bond angle, it becomes 145º. This angle agrees well with 145º ± 10º that is Si-O-Si bond angle in the silica glass. The nearest neighbor interatomic distance between O and O became 0.266 nm, and is converted into O-Si-O bond angle of 107º. This angle is almost equal to bond angle of 109.5º in Si-atom-centered tetrahedra. While the short range order of the atomic structure recovered that of the crystal, the long range order had been lost even if returning to room temperature. Therefore, it was confirmed to be able to generate the a-SiO_2 layer with the simulation of the heating and rapid quenching method.

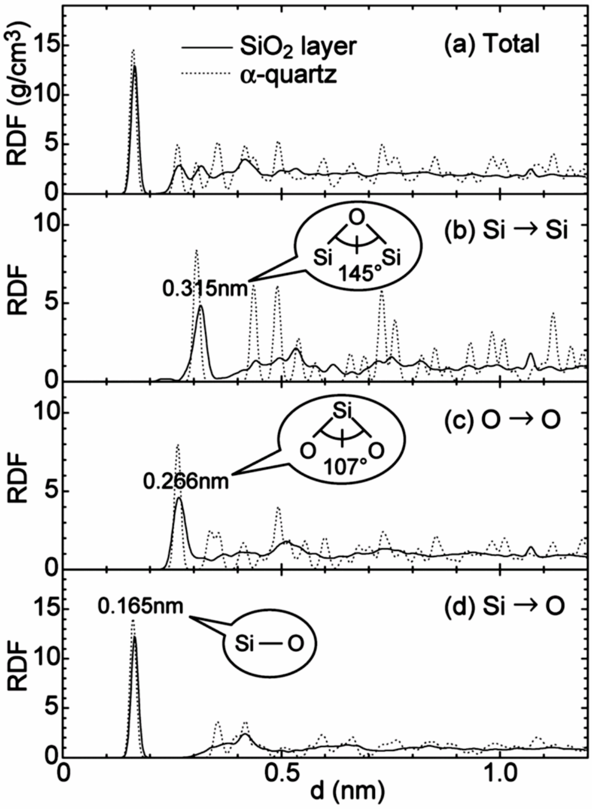


Fig. 3. The RDF of the SiO_2 layers after quenching to the room temperature of (a) total atoms, (b) Si to Si atoms, (c) O to O atoms and (d) Si to O atoms (solid). The alpha-quartz RDF is shown respectively for the reference (dashed).

Electronic structure of a-SiO_2/SiC interface. After quenching to the room temperature, the atomic structure became clean and abrupt a-SiO_2/SiC interface. The coordination defects that existed in every three Si of the neighborhood of substrate in the initial structure disappeared completely. However, a few defects energy levels at 0.25 eV and 0.35 eV above the edge of a valence band were still observed in the band gap at density of state (DOS) of the interface structure (Fig. 4). We examined to which wave functions

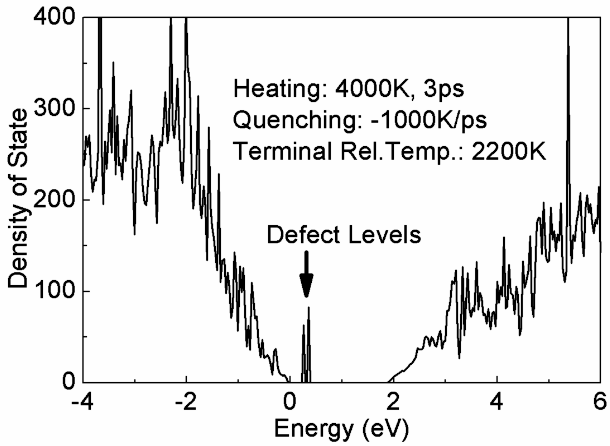
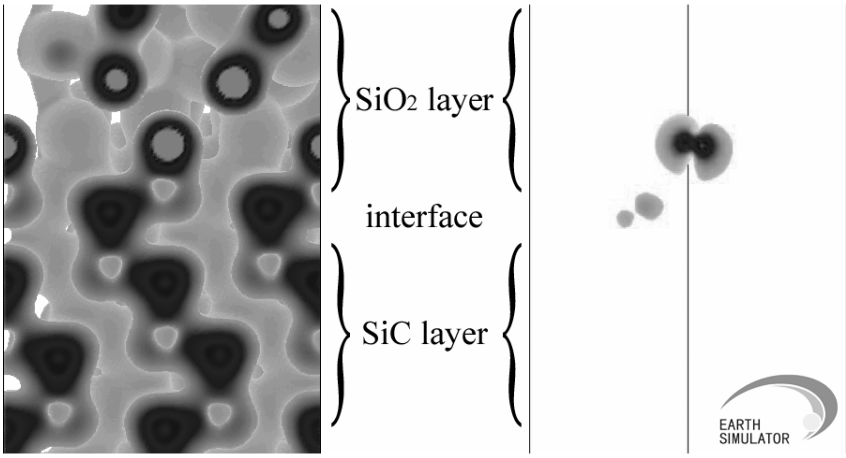


Fig. 4. The DOS of the released terminal model interface structure. The defects energy levels exist at 0.25 eV and 0.35 eV above the edge of a VB. (The absolute band gap value is not accurate because it becomes smaller than actual value in the first-principle calculation used here.)



(a) Total charge density (b) Charge density of the defect

Fig. 5. The cross section image of the charge density of atomic structure near the interface.

the defect energy levels belonged, and calculated the ratio of the atoms that made the wave functions. As a result, it was understood that both defect energy levels had been made from almost single atom. Figure 5 shows the charge density distribution by all electrons (Fig. 5(a)) and one of the defect energy level (Fig. 5(b)), respectively. The defects energy levels are originated from interfacial oxygen. This oxygen has bonding with interfacial Si, however another bonding is a dangling bond, and it connects to no atom. The oxygen dangling bond caused the defect energy levels.

Summary

The heating and rapid quenching method using first-principles molecular dynamics (MD) simulation code was carried out to make an a-SiO_2/SiC interface structure. A slab model using 444 atoms for a-SiO_2 on a 4H-SiC (0001) crystal layers was constructed in order to obtain a more realistic interface structure and electronic geometry of a-SiO_2/4H-SiC interface. The heating temperature, the heating time and the speed of rapid quenching were 4000 K, 3.0 ps and -1000 K/ps, respectively. To make the SiO_2 layer a better amorphous structure, the fixed SiO_2 terminal was released while rapid quenching at the temperature below 2200 K. The released terminal model became more stable atomic structure than the fixed terminal model. The radial distribution function of the SiO_2 layers was calculated. The interatomic distance and the bond angles of SiO_2 layers agreed well with the most probable values in bulk a-SiO_2. After quenching to the room temperature, the atomic structure became clean and abrupt a-SiO_2/SiC interface. The coordination defects that existed in every three Si of the neighborhood of substrate in the initial structure disappeared completely. However, two energy levels observed at 0.25 eV and 0.35 eV above the edge of a valence band were still exist in the band gap at DOS of the interface structure after calculation, which indicates two different types of localized electronic distributions that originate from a oxygen at the SiO_2/4H-SiC interface.

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