First-Principles Molecular Dynamics Simulation of SiC Devices: "Generation of Amorphous SiO$_2$/SiC Interface"

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Silicon carbide (SiC) semiconductor device is expected to be used under a severe environment like the nuclear reactor and the space environment. However, an interfacial defect that originates in the SiC epitaxial layer defect or the structural change of the SiO$_2$/SiC interface exists. On the semiconductor device interface, the microscopic electric charge state of the defect decides a macroscopic electric characteristic. To emulate interfacial structure on the computer the SiO$_2$/SiC interface structure is generated and the electronic geometry is decided by the first-principle molecular dynamics (MD) simulation with the earth simulator. The amorphous SiO$_2$/SiC interface structure is made by medium-scale model of about 400 atoms. The heating temperature is 4000K, the heating time is 3.0ps, the speed of rapid cooling is -1000K/ps, and SiC movable layers in the interface are assumed to be 4 layers. In temperature 2200K the SiO$_2$ terminal was opened to make the SiO$_2$ layer more amorphous. The model has almost abrupt interface, however, some energy levels were still observed in the band gap. The defects energy levels are originated from interfacial oxygen and the as localized electronic distribution of the dangling bond causes defect energy levels.

Keywords: SiC device, first-principles calculation, molecular dynamics, interfacial defect, rapid cooling

1. Introduction

Silicon carbide (SiC) semiconductor device has a radiation-tolerant property that is difficult to obtain by usual Si or GaAs semiconductor devices. It is expected to be used under a severe environment like the nuclear reactor and the space environment. In addition, insulating layer of SiO$_2$ is easily obtained with thermal oxidization of SiC. There is an advantage that conventional Si processing technology can be used for the SiC processing unlike other exotic materials. However, an interfacial defect that originates in the SiC epitaxial layer defect or the structural change of the SiO$_2$/SiC interface exists. The relation among an atomic structure, an interfacial defect and an electric characteristic is not clear. A basic research that clarifies atomic structure on SiO$_2$/SiC interface by difference of oxidation method, investigates origin of interfacial defect and ties interfacial defect structure and electric characteristic are indispensable to solve this problem fundamentally. The purpose of this research is in the acquisition of the basic data to clarify relation between physical structure and electric characteristic of SiO$_2$/SiC interface by calculating the atomic structure on the interface with the earth simulator.

There is a precedent research in a theoretical calculation of the electric characteristic (electronic structure) generated with the atomic structure on the SiO$_2$/SiC interface[1]. Energy levels have been calculated by using the super computer on the condition that dangling bonds of Si and C that exist in the interface make defects. However, because the number of atoms included in these calculations was about 100 atoms at most, and the number of interfacial atoms was about 6-10, a complex SiO$_2$/SiC interface structure was not able to be simulated. By using the earth simulator, it is thought that the number of atoms included in an atomic model can be increased more than 1000 atoms that were not able to be calculated in the past, and the band structure simulation in an interfacial interlayer and a clustered carbon, etc. becomes possible.

A lot of researches exist that clarified only a physical structure of an interface, and that handled only an interfacial electric characteristic. It is difficult to decide the electric charge state of the defect though the structure of an interfacial defect can be identified from the measurement of a physical structure. On the other hand, it is difficult to know a physical structure though it can know the electric charge state of the defect from electric evaluation of characteristics. On the semiconductor device interface, the microscopic

electric charge state of the defect decides a macroscopic electric characteristic. The purpose of this research is a thing to know the relation between the atomic level defect structure and the electric charge state in the interface where the periodicity of the atom has collapsed, and to clarify the relations between a physical characteristic and electric characteristic.

2. Simulation result

2.1. Generation of amorphous SiO_2/SiC interface

The defect structure of the oxide and the semiconductor interface are important factors to decide the characteristic of the SiC device. To emulate this interfacial structure on the computer, and to decide how the interfacial defect structure determines the device characteristic, the SiO_2/SiC interface structure is generated and the electronic geometry is decided by the first-principle molecular dynamics (MD) simulation with the earth simulator. The calculations have been performed using the ab-initio total-energy and molecular-dynamics program VASP (Vienna ab-initio simulation program) developed at the Institut für Materialphysik of the Universität Wien[3-5]. In last year's research project, an amorphous SiO_2 layer was formed by using a small-scale model of about 100 atoms crystal SiO_2 (beta-quartz)/crystal SiC by melting and rapid cooling and it searched for the temperature condition etc. of the melting and rapid cooling[2]. As a result, it has been understood the SiO_2 layer was made amorphous and free energy of the entire system was minimized when the heating temperature was 3000K, the heating time was 3.0ps, and the speed of rapid cooling was -1000K/ps. When the temperatures were lower than 3000K, the SiO_2 layer was not made amorphous enough. However, when the temperatures were higher than 3000K, it was seen that the SiO_2 layer part separates (Fig. 1). Then, at current year, we fixed the terminal in the SiO_2 area and made a sandwich model that was a structure to place a movable layer between fixed layers. It is tried to improve a disorderly interface by melting and rapid cooling this model, therefore it has been under-

stood to be able to generate an amorphous structure without causing the model's destruction even in 4000K (Fig. 2). As a result, a more disordered amorphous area was able to be obtained than before.

Based on the result of a preliminary calculation in these small-scale models of about 100 atoms, we generated the amorphous SiO_2/SiC interface structure by using a medium-scale model of about 400 atoms. The heating temperature is 4000K, the heating time is 3.0ps, the speed of rapid cooling is -1000K/ps, and SiC movable layers in the interface are assumed to be 4 or 6 layers. In addition, in temperature (2200K) to which model doesn't separate because degree of freedom of system decreased, the fixed SiO_2 terminal was opened to make the SiO_2 layer more amorphous.

As a result, in the four layers movable SiC system after cooled to the room temperature, total energy of the system that opens the SiO_2 fixed terminal is lower than total energy
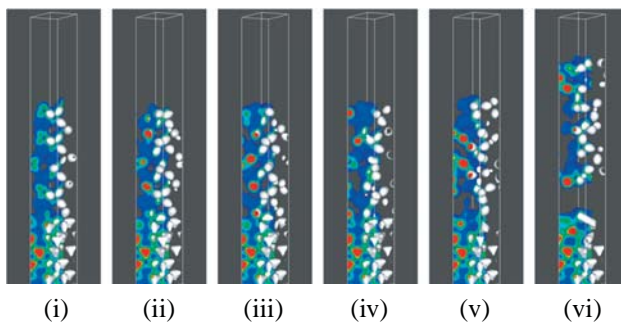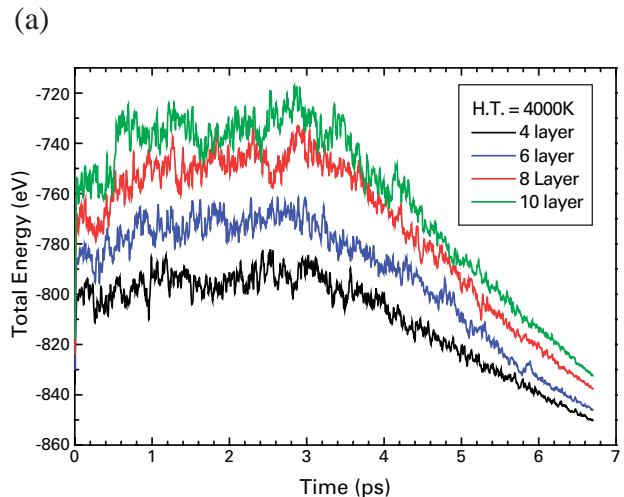
(a)

(b)

Fig. 1 Interfacial electronic density after rapid cooling. Heating temperature is (i) Initial state, (ii) 2000K, (iii) 2500K, (iv) 3000K, (v) 3500K, (vi) 4000K, respectively.
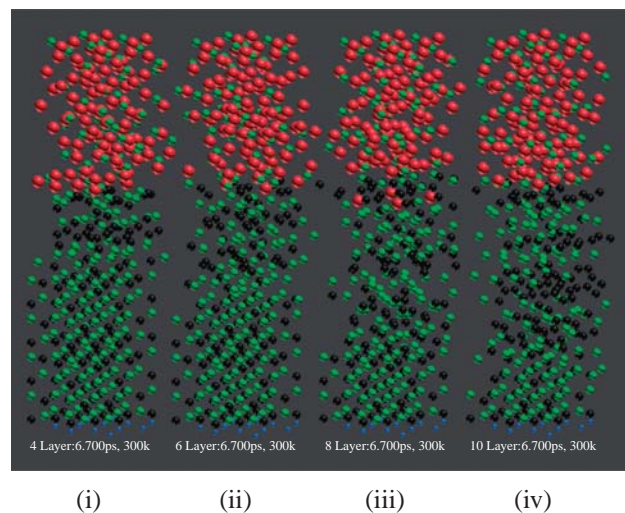
Fig. 2 Free energy and atomic structure of the fixed terminal models. (a) Free energy, (b) Atomic structure after cooling, Free SiC area is (i) 4 layers, (ii) 6 layers, (iii) 8 layers, (iv) 10 layers, respectively.

(a)

(b)

04 Layer:6.700ps, 300K

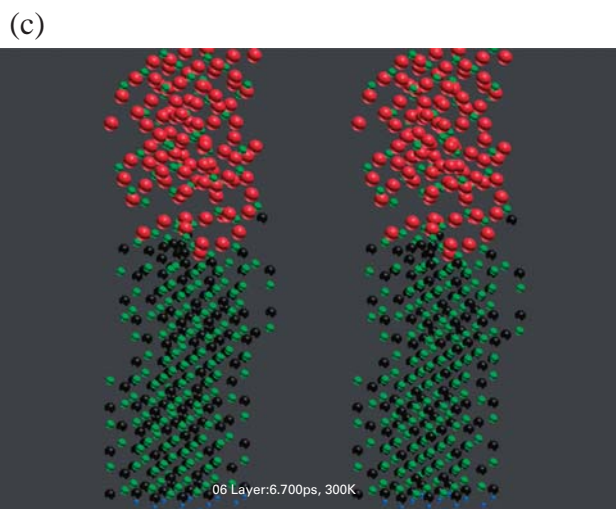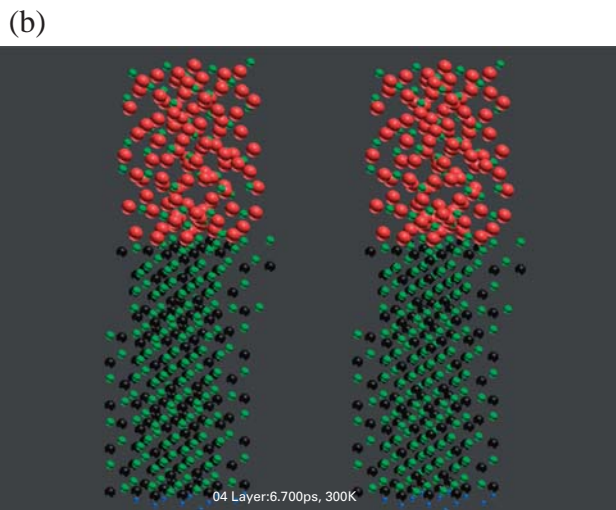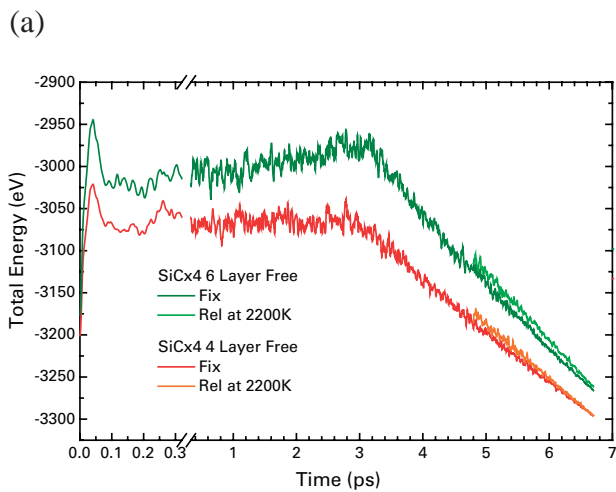(c)

06 Layer:6.700ps, 300K

Fig. 3 Free energy and atomic structure of the relaxed terminal models. (a) Free energy of 4 or 6 free layer models, Atomic structure after cooling of (b) 4 free layers and (c) 6 free layers models (stereograph).

4 Free SiC Layer Model
Heating: 4000K, 3ps
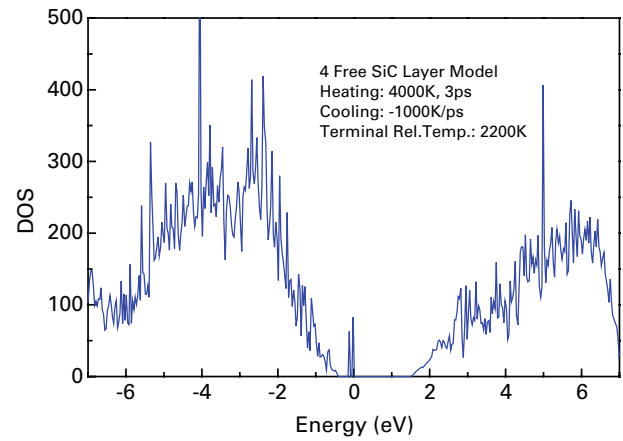Cooling: -1000K/ps
Terminal Rel.Temp.: 2200K

Fig. 4 Total electronic density of state of the relaxed terminal model

gy of the fixed system, and the atomic structure is observed to be separating in SiO_2, it has been understood not to be able to keep a stable amorphous structure. Therefore, four layers movable SiC system is suitable to generate the interfacial defect structure.

2.2. Electronic structure of amorphous SiO_2/SiC interface

In the interface generated with four layer movable SiC layer 2200K relaxation model, the bond not to take part in an interfacial connection (dangling bond) has disappeared that exists by one per three atom of interface in conventional crystal SiO_2/crystal SiC connection model, and almost abrupt interface is reproduced. However, when the entire electronic density of state (DOS) was calculated, some energy levels were still observed in the band gap (Fig. 4). Two defect energy levels exist from the top of a valence band at the level of about 0.4eV. We examined to which wave function the energy level belonged, and calculated the ratio of the atom that made the wave function. We examined the energy level belonged to which wave function, and calculated the ratio of the atom that made the wave function. As a result, it was decided that both energy levels were made by almost single atoms. Figure 5 shows the charge density distribution by all electrons and defects energy levels, respectively. The defects energy levels are originated from interfacial oxygen. This O has bonding with interfacial Si, however the other side is not bonded to any atoms, and it becomes a dangling bond. The localized electronic distribution that cannot contribute to bonding causes defect energy levels.

3. Conclusion

On the semiconductor device interface, the microscopic electric charge state of the defect decides a macroscopic electric characteristic. To emulate interfacial structure, the SiO_2/SiC interface structure is generated and the electronic geometry is decided by the first-principle molecular dynamics simulation. The amorphous SiO_2/SiC interface structure

of the system that fixed the terminal, it is able to be confirmed that the system of open terminal is taking a steady atomic structure (Fig. 3). However, in the six layers movable SiC system after cooled to the room temperature, total energy of the open terminal system doesn't decrease to the ener-
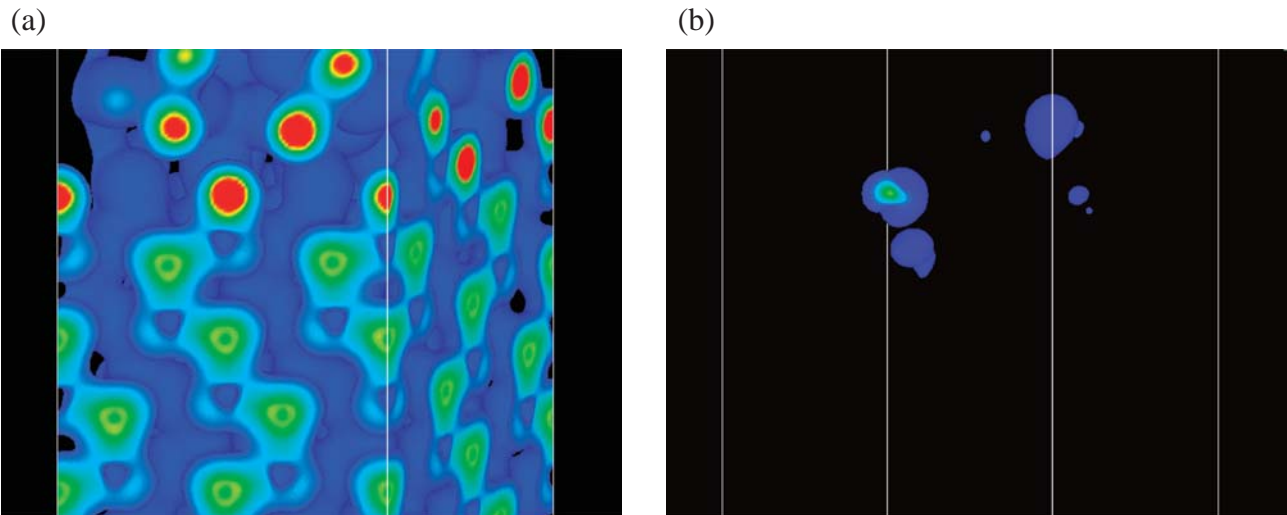
(a)

(b)

Fig. 5 Charge density distribution of the relaxed terminal model near the interface by (a) all electrons and (b) defect energy level, respectively.

is made by medium-scale model of about 400 atoms. The heating temperature is 4000K, the heating time is 3.0ps, the speed of rapid cooling is -1000K/ps, and SiC movable layers in the interface are assumed to be 4 layers. In temperature 2200K the SiO_2 terminal was opened to make the SiO_2 layer more amorphous. Therefore, four layers movable SiC system is suitable to generate the interfacial defect structure. In the interface generated with four layer movable SiC layer 2200K relaxation model, the dangling bond has disappeared, and almost abrupt interface is reproduced. However, some energy levels were still observed in the band gap. Two defect energy levels exist from the top of a valence band at the level of about 0.4eV. It was decided that both energy levels were made by almost single atoms. The defects energy levels are originated from interfacial oxygen. The localized electronic distribution that cannot contribute to bonding causes defect energy levels. The interfacial model size will be expanded to 1000 atom size in the coming year, and various defect structures that exist in an actual semiconductor device are scheduled to be simulated.

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SiCデバイスの第一原理分子動力学シミュレーション：
「アモルファスSiO_2/SiC界面の生成」

プロジェクト責任者

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　Siに比べ優れた物理特性を持つSiCを用いた半導体デバイスは、従来のSiやGaAs半導体デバイスでは動作が困難な、原子炉や宇宙環境等、極限環境下で用いられる素子として期待されている。しかしながら、SiCの酸化膜とSiCの界面には、SiCエピタキシャル膜内の欠陥やSiO_2/SiC界面の構造変化に起因する界面欠陥が存在している。半導体素子界面では、ミクロな原子レベルの欠陥の荷電状態がマクロな電気特性を支配しており、この界面構造を計算機上で模擬し、界面欠陥構造がどのようにデバイス特性に影響するのかを導出するため、地球シミュレータを用いた第一原理分子動力学計算でSiO_2/SiC界面構造を構築し電子構造を決定する。400原子程度の中規模モデルを用いてアモルファスSiO_2/SiC界面構造生成を行った。加熱温度は4000K、加熱時間は3ps、急冷速度は-1000K/ps、界面でのSiC可動層は4層とし、2200KでSiO_2側終端固定層を開放し自由端とすることによって、SiO_2層でのアモルファス化を促進させた。生成された界面はダングリングボンドが消滅しており、清浄界面に近い状態が再現されている。しかしながら、まだバンドギャップ中に準位が存在するのが観察され、欠陥準位は界面に存在するOから生じており、結合に寄与できない局在した電子分布が準位の原因となっている事が分かった。

キーワード：SiCデバイス，第一原理計算，分子動力学，界面欠陥，急冷計算