

Atomic Level Analysis of SiC Devices Using Numerical Simulation

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ABSTRACT

Research and development of power semiconductor devices with SiC (silicon carbide) has been very active because of the increasing need for low-loss power electronics equipment. The electrical properties of the SiC-metal-oxide-semiconductor field-effect transistors (SiC-MOSFETs) are affected by charge trapping that is thought to be caused by the atomic level disorder at the interface between the gate oxide and SiC (SiC/SiO₂ interface). In order to analyze the origin of the disorder at the interface, we have been implementing the atomic level analysis using both the X-ray photoelectron spectroscopy and the simulation based on the first principles calculations. As a result, we were able to estimate the chemical state of Si at SiC/SiO₂ interface, as well as its terminated structure via nitrogen when the interface is nitrided.

1. Introduction

Recently, there has been an increasing need for low-loss power electronics equipment for the purpose of realizing a low-carbon society. Fuji Electric has commercialized a great number of power electronics equipment products for uninterruptible power systems (UPSs), various types of electric power application equipment, transportation infrastructures and distribution infrastructures. In order to dramatically reduce the loss of these power electronics equipment products, it is essential to improve the efficiency of inverters by having technological innovation in power semiconductor devices, circuits and control. Currently, wide band gap semiconductors such as silicon carbide (SiC) and gallium nitride (GaN) are attracting attention as the next-generation semiconductor to replace silicon (Si), which is a mainstream material of power semiconductor devices. Vigorous research and development of power semiconductor devices that use these materials is under way.

Fuji Electric has already commercialized Schottky barrier diodes (SBDs) and is currently developing SiC-metal-oxide-semiconductor field-effect transistors (SiC-MOSFETs). To reduce the loss of these SiC-MOSFETs, it is important to improve electrical characteristics such as channel mobility. One possible predominant factor of the electrical characteristics is charge trapping resulting from an atomic level disorder at the interface between the gate oxide (SiO₂) and SiC (SiC/SiO₂ interface). Accordingly, the key to improving electrical characteristics is to identify the substance of this charge trapping.

As an analysis technology for estimating the substance of charge trapping, this paper describes an

atomic level analysis technology for SiC devices that employs first-principles calculation as a simulation method in addition to instrumental analysis.

2. SiC-MOSFET

Figure 1 shows the device structure of a SiC-MOSFET. In a MOSFET, voltage is applied to the gate electrode to form an inversion layer in the p well layer at the interface between the gate oxide and SiC substrate. Then, voltage between the source and drain is applied to let electrons to flow into the channel.

Important characteristics of a MOSFET include channel mobility, which has an effect on the on-resistance, and the threshold voltage V_{th} , at which the MOSFET is turned on. If the mobility can be increased, the on-resistance can be decreased, and this will make it possible to reduce the power consumption of equipment that uses the MOSFET.

Figure 2 shows an example of the mobility characteristics of SiC-MOSFETs. The horizontal axis represents the gate voltage V_g . It indicates that the degree of mobility and V_{th} may differ depending on the process. This difference is assumed to be due to the presence of

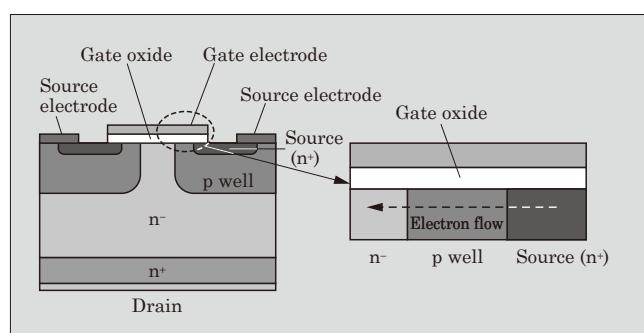


Fig.1 Outline of device structure of SiC-MOSFET

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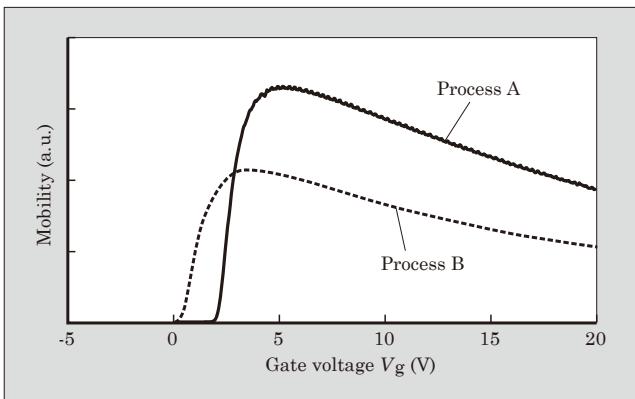


Fig.2 Example of mobility characteristics of SiC-MOSFETs

charge trapping resulting from the atomic level disorder at the SiC/SiO₂ interface. This charge trapping is considered to cause a decrease in mobility due to Coulomb scattering^{*1} and variation of V_{th} . Accordingly, to lower the on-resistance and to improve reliability by suppressing the variation of V_{th} , reducing the atomic level disorder is the key.

One indicator of atomic level disorder is interface state density. SiC substrates have different crystal surfaces such as the Si-face and the C-face, and they show different interface state densities. For example, Dhar et al. have reported that, when the oxide is formed by dry oxidation, the interface state density of the Si-face is lower than that of the C-face⁽¹⁾. It has also been reported that the interface state density is reduced by nitriding the interface^{(1) to (3)}. In this way, interface characteristics may depend on the crystallographic orientation of the surface and the process.

In order to reduce the interface state density, which is considered to result from the atomic level disorder, it is necessary to understand the substance (chemical states, bonding structures and geometry) of the interface state. To that end, Fuji Electric is working on atomic level analysis of the SiC/SiO₂ interface. For example, we observe the SiO₂ interface by transmission electron microscopy and X-ray photoelectron spectroscopy (XPS) using synchrotron radiation facility, to evaluate the chemical state and bonding structure of the Si atoms and others at the interface. Furthermore, for estimating the link between the bonding structure obtained by the analysis and the electrical characteristics, we conduct analysis that incorporates the first-principles calculation, which will be described later. Unlike Si, SiC is indeed difficult to grasp the substance of the interface states because of its compound nature, but analysis incorporating the first-principles calculation is considered to allow us to estimate the bonding structure and interface state.

*1: Coulomb scattering: Refer to Supplemental explanation 2 on page 62.

3. Analysis by XPS

3.1 Synchrotron radiation XPS

This section describes the analysis of the SiC/SiO₂ interface by XPS using synchrotron radiation facility.

XPS is a method of obtaining atomic information at a depth of a few nanometers from the surface of a sample and it allows quantitative analysis of the chemical state of atoms.

By using this analysis method, we analyzed the chemical state of the interface between SiC and the oxide formed in an oxygen ambient (dry oxidation) or in a nitrous ambient (N₂O oxidation). Both Si-face and C-face SiC surface were used for the measurement.

In order to obtain information about the minute amount of atoms at the interface, we etched the oxide of the samples to the thickness of about 1.5 nm and measured it at a synchrotron radiation facility (SPring-8^{*2} BL27SU).

Figure 3 shows a schematic diagram of the SiC/SiO₂ interface. SiO_x indicates a region where the oxidation state of Si at the interface has changed. In that region, it is considered that the chemical states of Si atoms continuously change with different numbers of the bonding oxygen. As the components of chemical states of Si, we assumed 3 types of suboxide components (Si¹⁺, Si²⁺ and Si³⁺^{*3}) in addition to SiC and SiO₂ components⁽⁴⁾⁽⁵⁾. We modeled the data envelope to separate each component with different chemical state for

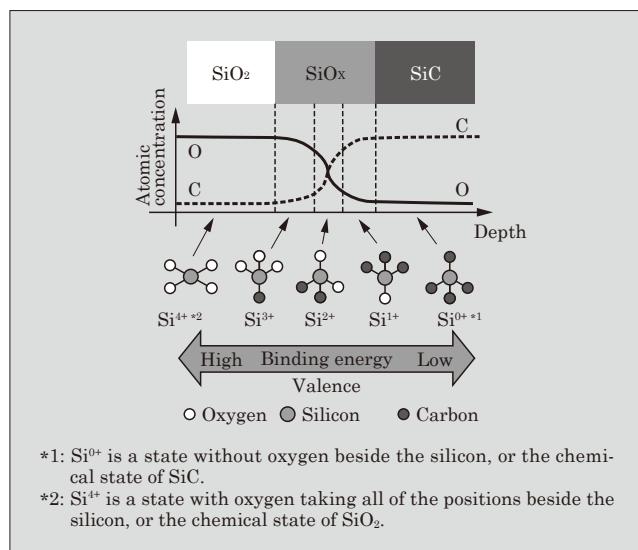


Fig.3 Schematic diagram of SiC/SiO₂ interface

*2: SPring-8: Large synchrotron radiation facility capable of emitting the world's highest-performance synchrotron radiation. It is comprehensively managed by the Institute of Physical and Chemical Research (RIKEN) as the facility operator. It is expected to be applied to wide-ranging fields including material science, earth science, life science, environmental science and medical science.

spectra obtained by XPS.

3.2 Analysis of Si spectra

Figure 4 shows Si spectra at the N₂O oxidized SiC/SiO₂ interface. As a result of comparing the amounts of the respective suboxide components, we found the Si¹⁺ component showed the largest amount for both the C-face and the Si-face. The amount of the Si³⁺ component for the C-face was about 4 times as large as that for the Si-face.

The tendency of suboxide components at the dry-oxidized interface showed a result similar to that of N₂O oxidation, which is not indicated in the figure.

3.3 Analysis of nitrogen spectra of N₂O oxidation

Figure 5 shows nitrogen spectra at the N₂O oxidized interface. The main components can be attributed to 3-coordinate Si₃N based on the peak position for both the C-face and Si-face⁽⁶⁾. In addition, a shoulder was observed on the high energy side of the nitrogen spectrum for both the C-face and the Si-face. This shoulder is attributed to distortion of Si₃N and chemi-

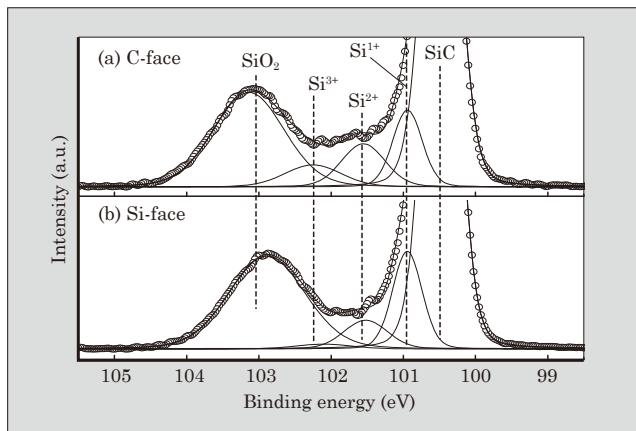


Fig.4 Spectra of Si at SiC/SiO₂ interface oxidized with N₂O

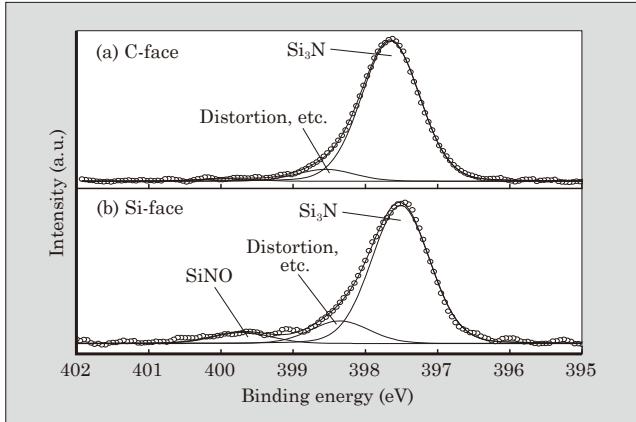


Fig.5 Spectra of nitrogen at SiC/SiO₂ interface oxidized with N₂O

*3: These indexes shows the number of oxygen atoms existing around the Si atom.

cal states other than Si₃N such as CN and NO_x⁽⁶⁾.

4. Analysis by First-Principles Calculation

To analyze the difference between the C-face and the Si-face obtained by the XPS analysis and to estimate the bonding structure of the SiC/SiO₂ interface, we used the first-principles calculation. We assumed ideal bonding structures of the SiC/SiO₂ interface and compared them with the results of the XPS analysis, thereby analyzing the interface bonding structure.

The first-principles calculation, which means a calculation based on the most fundamental principles, is a technique of solving the state of electrons in a substance by numerical calculation at the atomic or nanoscale dimension based on quantum mechanics. The first-principles calculation makes it possible to investigate the properties of unknown substances and physical and chemical phenomena at the atomic level that cannot be measured experimentally.

DMol³^{*4}⁽⁷⁾⁽⁸⁾ was used to perform the first-principles calculations presented in this paper.

4.1 Analysis of interface bonding structure

(1) Dry oxidation

We created a model of an ideal interface structure with an abrupt SiC/SiO₂ interface as the starting point of interface analysis for dry oxidation. We constructed a C-face and a Si-face surface model, which is shown in Fig. 6, from the crystal structure of SiC, followed by making of SiO₂ crystal surface, and bonded the surfaces together so that no C-O bond would be generated between the surfaces. To combine SiC and SiO₂, we take into consideration the suboxides obtained by the XPS analysis. Then, from the state of combination, the ideal interface structure was determined by performing a geometry optimization calculation to find the most stable atomic positions. The results are shown in Fig. 7. Figure 7 only shows some of the atoms at the interface. In the ideal interface structure obtained on the C-face shown in Fig. 7(a), Si that exists at the interface is in a chemical state Si³⁺. With this ideal interface structure

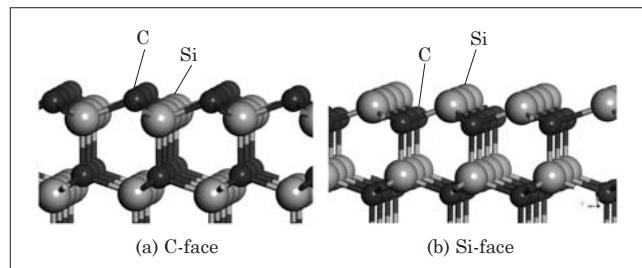


Fig.6 Models of surface structure created from SiC crystal structure

*4: DMol³: Part of the Materials Studio software environment. Materials Studio is a trademark or registered trademark of Dassault Systèmes S.A.

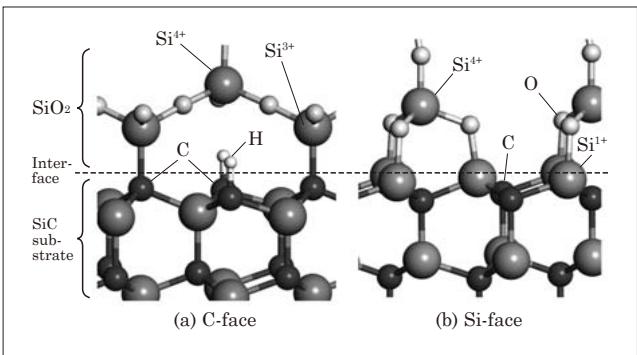


Fig.7 Estimated structural models of dry oxide interface assuming ideal interface based on structure optimization calculation

considered, Si^{3+} observed in the XPS analysis of the C-face is estimated to result from an interface structure as shown in Fig. 7(a). Si^{1+} and Si^{2+} is estimated to result from interface disorder.

For the Si-face, as shown in Fig. 7(b), Si that exists at the interface is in a chemical state Si^{1+} . The Si^{1+} observed in the XPS analysis of the Si surface is estimated to result from an interface structure as shown in Fig. 7(b).

(2) N_2O oxidation

Regarding a bonding structure with nitrogen atoms introduced into the SiC/SiO_2 interface, on the Si-face, nitrogen atoms at the interface are known to enter the positions of carbon atoms of SiC to bond with Si atoms⁽⁹⁾. Accordingly, for interface analysis for N_2O oxidation, nitrogen atoms were assumed to enter the positions of the carbon atoms on the C-face in the same way. We used an ideal interface structure that simulates dry oxidation and considered the suboxides and the bonding structure Si_3N_4 obtained by the XPS analysis when we arrange the atoms so that the carbon atom positions would be replaced by nitrogen atoms. Then, to find the most stable atomic positions, we carried out first-principles calculation to perform geometry optimization calculations, thereby assuming the ideal interface structures.

The results obtained are shown in Fig. 8. For the C-face shown in Fig. 8(a), with the structure of Si_3N_4 taken into account, the structure with all of the 3 bonds of nitrogen atoms bonded with Si in SiC seems appropriate. In addition, the structure with one of the bonds of nitrogen atoms oriented toward the SiO_2 , which is not shown, is also regarded to be appropriate.

For the Si-face shown in Fig. 8(b), a structure with 2 of the bonds of nitrogen atoms oriented toward the SiO_2 film is thought to be appropriate. Incorporation of nitrogen atoms like these is similar to the bonding structure with nitrogen atoms, which is reported by Xu et al.⁽⁶⁾ and Shirasawa et al.⁽¹⁰⁾

As described above, creating an interface bonding structure by the first-principles calculation has made it possible to analyze the results obtained by XPS analysis in detail.

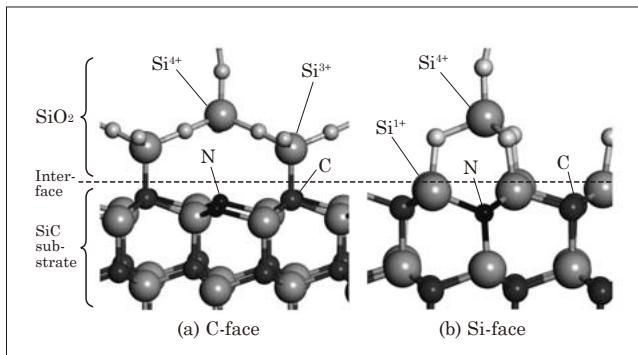


Fig.8 Models of nitrogen structure estimated at interface

4.2 Analysis of interface states

Examples of the SiC/SiO_2 interface model structures with dangling bonds (DBs) are shown in Fig. 9. In Fig. 9, DBs are indicated by white bars. For the C-face, we made the model interface that has 3 DBs of Si by removing one of the carbons at the interface shown in Fig. 7(a). The part of it is shown in Fig. 9(a). For the Si-face, we made the model interface with DBs by referring the paper by Okuno et al.⁽¹¹⁾, and the result is shown in Fig. 9(b). The Si atoms at the interface, as with the Si-face in Fig. 7(b), is the Si^{1+} bonding state observed in the XPS analysis.

The results of investigation of the interface state by these DBs using the first-principles calculation are shown in Fig. 10. It indicates that the interface state of a DB is formed within the band gap of SiC for both the C-face and Si-face. For the C-face, a state is also formed at the lower end of the conduction band side, which is estimated to result from the influence of the 3 DBs of Si existing adjacent to each other. The Si-face was found to be similar to the result of the paper by Okuno et al.⁽¹¹⁾

One possible factor of reduction of the interface state density by introducing nitrogen atoms into the interface^{(1) to (3)} is suggested to be that the nitrogen atoms bind the DBs of the Si atoms and form a terminated structure as shown in Fig. 8 to reduce the interface state.

Even in bonding states other than a DB, if inter-

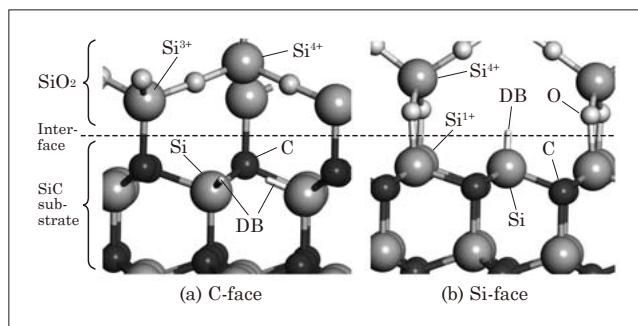


Fig.9 Ideal interface structures provided with dangling bonds (DBs)

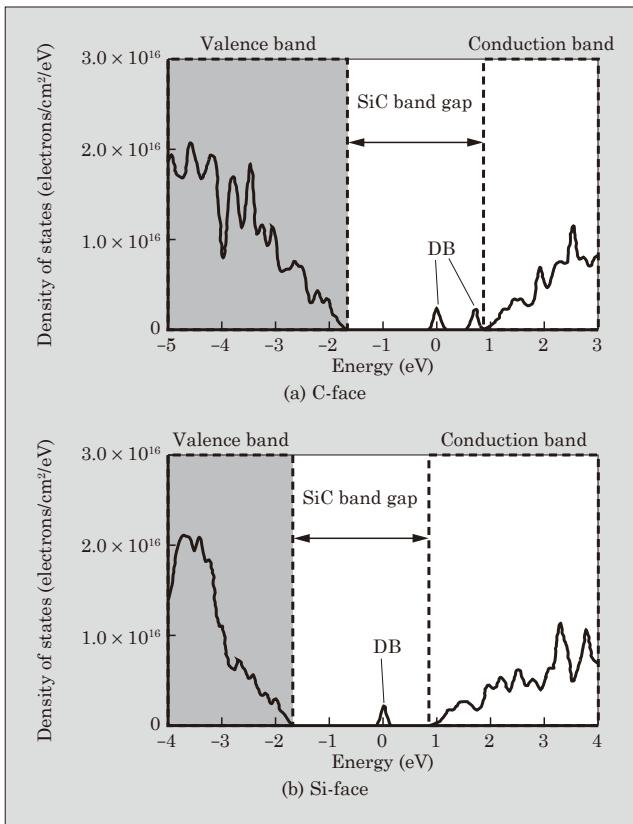


Fig.10 Density of states of interface structure with dangling bonds (DBs) of Si

face states exist within the SiC band gap, charge trapping occurs in the interface states, which may cause the mobility reduction due to Coulomb scattering and/or the variation of V_{th} .

4.3 Future issues

The first-principles calculation makes it possible not only to create a bonding structure but also to analyze the electronic state of a bonding structure for estimating whether it can be an interface state that has an effect on electrical characteristics. In addition, it makes it possible to analyze the ease of chemical reaction.

We have analyzed the change of the bonding state caused by introduction of nitrogen atoms into the interface and studied the mechanism of interface state reduction. In the future, we intend to investigate between the nitrogen introduction process and device characteristics, analysis, structural analysis by the first-principles calculation. Through these investigation, we will indicate the direction of characteristic improvement, thereby contributing to improved characteristics and processes of MOSFETs.

5. Postscript

This paper has described atomic level analysis of

SiC devices using simulation.

In order to understand the characteristics of SiC-MOSFETs, it is important to analyze the bonding structure existing in the minute region of about 1 nm in the vicinity of the SiO_2 interface, which determines the characteristics, and clarify how the bonding structure affects the characteristics. In the future, we intend to continue to make use of analysis and simulation to contribute to early commercialization of high-performance SiC-MOSFETs and to the realization of a low-carbon society by achieving energy savings of power electronics equipment.

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