Angle-resolved Photoelectron Spectroscopy studies of initial stage of thermal oxidation on 4H-SiC (0001)

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Abstract

We have investigated the initial stage of thermal oxidation on 4H-SiC (0001) using Angle-resolved Photoelectron Spectroscopy. Analyses of C 1s photoelectron spectra show that the amount of C-O in oxide in the case of 4H-SiC(0001) is smaller than that in the case of 4H-SiC(0001).

1. Introduction

The practical use of power devices that use SiC has already been reported. [1] However, the performance of a SiC MOSFET has not reached the level predicted based on the physical properties of SiC. One of the reasons is that interface state density (D_{it}) at SiO₂/SiC is more than an order of magnitude higher than that at SiO₂/Si. [2] Therefore, the reduction of the D_{it} is important for device performance improvement. Many studies have been performed to reveal the origin of D_{it} . [3] Also some types of interface defects have been identified, such as carbon clusters, Si/C dangling bonds, and silicon oxycarbides (SiO_xC_y) species. [4] However, the chemical structure of the interface transition region still remains unclear, resulting in the insufficient understanding of the origin of D_{it} and the atomic structure of SiO₂/SiC interface. Therefore, it is a key for improving the performance of SiC MOSFET to clarify SiO₂/SiC interface structure formed by thermal oxidation, and to control interface structure based on the knowledge. We have reported the results of the changes in chemical bonding state of $SiO_2/4H-SiC$ (0001) (C-face) structure with the progress of thermal oxidation using angle-resolved X-ray photoelectron spectroscopy (AR-XPS). [5] In this paper, we report the results for the case of 4H-SiC (0001) (Si-face) compared with the results for the case of 4H-SiC (0001).

2. Experimental Method

4H-SiC (0001) epitaxial films with 4° off-oriented were used in this study. The samples were prepared as follows. The sample was cleaned in the mixture of H₂SO₄ and H₂O₂ (H₂SO₄:H₂O₂=4:1) at 80-85 °C, and the native oxide was removed by dipping in 5% hydrofluoric acid (HF) followed by a rinse in deionized water. The sample was oxidized at 850 °C in dry oxygen with a pressure of 133 Pa. Then, the sample was oxidized in dry oxygen with a pressure of 133 Pa at 900 °C. Subsequently, the sample was oxidized in dry oxygen with a pressure of 133 Pa at 950 °C, 1000 °C and 1050 °C. The Si 2*p* and C 1*s* photoelectron spectra, excited by monochromatic AlK α radiation, were measured at a photoelectron take-off angle of 15° and 90° with an energy resolution of 0.37 eV and an acceptance angle of 3.3°, using an ESCA-300 manufactured by Scienta Instruments AB [6].

3. Result and Discussion

Figures 1 (a) and (b) show Si $2p_{3/2}$ photoelectron spectra arising from the sample of 4H-SiC(0001) and the decomposed Si $2p_{3/2}$ spectrum, respectively. Here, this spectra is normalized by Si $2p_{3/2}$ photoelectron intensity arising from Si in SiC substrate. Figs. 2 (a) and (b) show C 1s photoelectron spectra arising from the sample of 4H-SiC(0001) and 4H-SiC(0001), respectively. Figs. 2 (c) and (d) show the decomposed C 1s spectrum arising from the sample of 4H-SiC(0001) and 4H-SiC(0001) with the oxide thickness of 1.3nm, respectively. As seen in Fig. 1 (a), the oxide increases with the increase of oxidation time. As seen in Figs. 2 (a) and (b), the component with higher binding energy than that of SiC substrate observed in the unoxidized sample. This is reduced by the oxidation. As seen in Fig. 2 (c) and (d), these spectra arising consist of four peaks which are related with C in SiC, C-C bond, C-O bond and unknown α bond. In addition, the intensity of C-O bond of the 4H-SiC(0001) is smaller than that of the 4H-SiC(0001) with same oxide thickness. As seen in Fig. 2 (b), the intensity of component related to C-O bond increase with increase of oxidation time in the case of 4H-SiC(000 $\overline{1}$). However, it decrease in the case of 4H-SiC(0001) as seen in Fig. 2 (a). The measured spectra in Si 2p and C 1s regions were also decomposed into peaks convolution of Gaussian and Lorentzian as shown in Fig. 1 (b), Figs. 2 (c) and (d). [7] Fig. 3 shows the oxide thickness dependence of intensity ratio of the 4H-SiC(0001) and 4H-SiC(0001). As seen in Fig. 3, the intensity ratio I_{CC}/I_{CS} in the case of the 4H-SiC(0001) and 4H-SiC(0001) does not change so much with progress of oxidation. On the other hand, I_{CO}/I_{CS} related to C-O bond in the case of 4H-SiC(000 1) increases and that in the case of 4H-SiC(0001) decreases. Here, I_{CS}, I_{CC} and I_{CO} denote the intensity of component related to C in SiC, C-C bond, and C-O bond, respectively. Figure 4 shows the oxidation time dependence of oxide thickness of the 4H-SiC(0001) and 4H-SiC(0001) oxidized at 850°C. As seen in Fig. 4, the oxidation rate decreases at the oxide thickness of 0.6nm in both the 4H-SiC(0001) and 4H-SiC(0001). This implies that the oxidation rate decreases when the 1 ML SiO_2 was formed by the oxidation. The oxidation rate of the 4H-SiC(0001) has been already slower than that of the 4H-SiC($000\overline{1}$) in an early stage of oxidation.

4. Conclusions

From the changes of the Si $2p_{3/2}$ and C 1s photoelectron spectra, a changes in chemical bonding state of SiO₂/SiC structure with the progress of thermal oxidation were observed. We found that the intensity of C-O bond in the case of 4H-SiC(0001) was smaller than that in the case of 4H-SiC(0001) with same oxide thickness.

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Fig. 1 (a) Si $2p_{3/2}$ photoelectron spectra arising from the sample of 4H-SiC(0001). (b) Decomposed Si $2p_{3/2}$ photoelectron spectrum.



Fig. 2 C 1s photoelectron spectra arising from the sample of
(a) 4H-SiC(0001) and (b) 4H-SiC(0001). Decomposed
C 1s photoelectron spectrum arising from the sample of (c) 4H-SiC(0001) and (d) 4H-SiC(0001).



Fig. 3 The oxide thickness dependence of normalized intensity of 4H-SiC(0001) and 4H-SiC(0001).



Fig. 4 The oxidation time dependence of oxide thickness of the 4H-SiC(0001) and 4H-SiC(000 $\overline{1}$) oxidized at 850°C.