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X-Ray Photoelectron Spectroscopy Studies of Post-Oxidation Process Effects on Oxide/SiC Interfaces

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Abstract. In this report, we carried out x-ray photoelectron spectroscopy measurements on slope shaped oxide films to explore the changes of interfacial structures by post oxidation processes. By the observation of Si2p, C1s and O1s spectra, the bonding states which influence the electrical properties of MOS structures were suggested to be bonds related to carbon. We also discuss the reasons for the improvement of MOS properties by these post oxidation processes.

Introduction

Silicon carbide metal-oxide-semiconductor field-effect-transistors (SiC MOSFETs) have some problems to be solved before practical use, such as their low channel mobilities and higher on-resistances than those predicted, nevertheless the bulk SiC has superior characteristics. It has been reported that[1] high interface trap density and high oxide-trapped charges of SiC MOS structures, which are estimated by capacitance-voltage (*C-V*) measurements, are concerned with the inferior properties of SiC MOSFETs. Also, it has been reported that some post oxidation processes, such as re-oxidation[2] and hydrogen post oxidation annealing[3], improve their *C-V* characteristics. While, we have reported that[4,5], in the results of x-ray photoelectron spectroscopy (XPS) measurements for slope shaped oxide films without post oxidation processes, several photoemission peaks corresponding to other bonding states than Si-C and Si-O bonds, such as Si-Si, Si-O-C, C and single atom O, were observed at the oxide/SiC interfaces. In this report, we try to explore the changes of interfacial structures by post oxidation processes in terms of bonding states.

The oxide layers of specimens were chemical etched to form slants. We obtained various oxide thickness with the same thermal treatment by measuring along the slope. Moreover, we observed the depth profile of an oxide which has experienced electrical measurements. In the final, we discuss the bonds which influence *C-V* characteristics by comparing the change of interfacial bonding states with that of *C-V* characteristics due to these processes.

Experimental details

The surfaces of 6H-SiC homo-epilayers, 5 μm in thickness and 5×10^{15} cm^{-3} in carrier

concentration (n-type) (Cree,Inc.), were cleaned by a standard RCA cleaning process and a native oxide on the surface was removed by buffered HF. The (0001) Si faces of SiC epilayers were oxidized in a pure O_2 flow at 1100 ^{0}C for 3 hours. After the oxidation ceased, one of the samples was cooled down immediately ((a) quench), the second one was post-oxidation-annealed in Ar atmosphere at 1150 ^{0}C for 3 hours ((b) Ar POA), and the third one was wet re-oxidized at 950 ^{0}C for 3 hours ((c) Re-oxi.) In the wet re-oxidation process, the temperature of distilled water was 75 ^{0}C, that is, the concentration ratio of H_2O vapor to O_2 gas was approximately 1 : 3. From the results obtained by spectroscopic ellipsometry, the oxide thicknesses of (a), (b) and (c) were 25, 23 and 22 nm, respectively. Aluminum were deposited on the top of the oxide films and on the back of the samples to make gate electrodes and ohmic contacts, respectively, for *C-V* measurements. After the *C-V* measurements, the three specimens were immersed gradually into buffered hydrofluoric acid (HF (50 volume %) : NH_4F (40 weight %) = 1 : 9, at room temperature) at a constant speed to etch the oxide layers at an angle[6]. The maximum oxide thickness of (a), (b) and (c) after slant etching was 4.0, 8.9 and 5.7 nm, respectively, and the length of the slopes of the specimens were 10 mm. XPS measurements were performed using Mg X-rays ($h\nu$ = 1253.6 eV). An acceptance aperture was used to permit only photoelectrons emitted from 1 × 1 mm^2. The measuring point of XPS was scanned along the slope of the samples from the points of maximum oxide thickness with 0.5 mm step.

Results and discussion

Figures 1-3 show the photoelectron spectra of Si2p, C1s and O1s core levels as a function of position, *i.e.* oxide thickness, respectively. In these figures, deconvolution peaks were attached to some spectra. In Fig. 1, Si^{4+} peak indicates the photoemission peak originated from stoichiometric SiO_2. The oxide thickness of each position was derived from the area ratio of Si^{4+} peak to Si-C peak. By the results of deconvolution of the spectra, Si-O-C bonds were found in all of the specimens, and the maximum peak intensities of Si-O-C peaks normalized by Si-C peak in (a), (b) and (c) were 0.280, 0.355 and 0.385, respectively. The number of Si-O-C bonds decreased apparently by quench. Si^{x+} peaks ($1 \le x \le 4$, in case of $x < 4$, which means that the layer consists of suboxide) did not disappear even if we measured the position where oxide had been completely removed by chemical etching. It can be explained that native oxides were formed quickly onto the

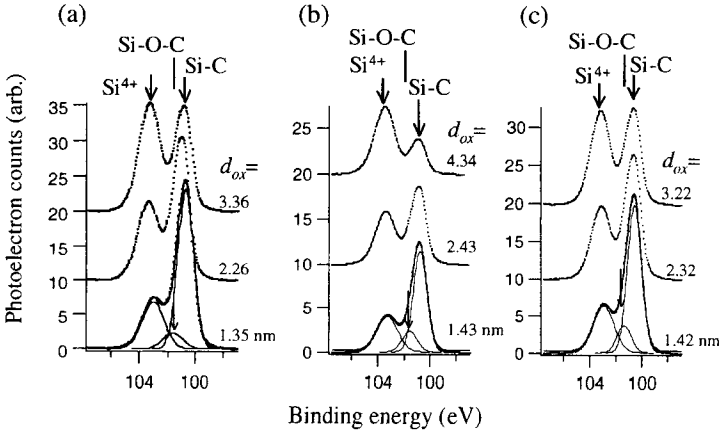

Fig.1 Photoelectron spectra of Si2p as a function of oxide thickness. (a)-(c) denote quench, Ar POA, wet re-oxidation, respectively.

chemical etched SiC surface since the first atomic layer of the SiC surface including dangling bond or back bond must be very activated to the air.

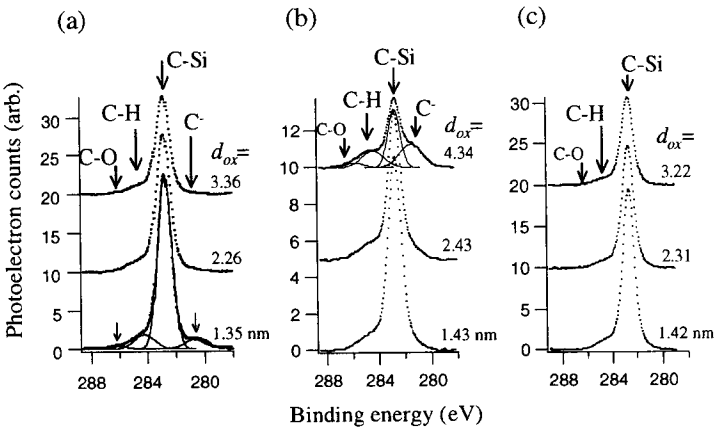

Fig.2 Photoelectron spectra of C1s as a function of oxide thichness. (a)-(c) denote quench, Ar POA, wet re-oxidation, respectively.

In Fig. 2, C-O, C$^-$ bonding peaks are seen as well as C-Si, C-H bonding peaks. C$^-$ bonding peak is probably originated from a dissociation of C-Si bond because a negative charge of C(-Si) may be stronger than that of C-Si when C-Si bond dissociates, and bringing about the photoemission peak at lower binding energy than C-Si peak. In the results of deconvolution mentioned above, the maximum peak intensities of C-O peaks normalized by C-Si peak in (a), (b) and (c) were 0.017, 0.078 and 0.010, respectively. Therefore, the number of C-O bonds increases by Ar POA. Next, the maximum peak intensities of C$^-$ bonds normalized by C-Si peak in (a), (b) and (c) were 0.055, 0.390 and 0.030, respectively. The numbers of C$^-$ and C-H bonds decrease by wet re-oxidation compared with (a) and (b). It can be considered that C$^-$ bonds are terminated by hydrogen in the wet atmosphere, and then, C-H bonds are burried away during the oxidation.

In Fig. 3, the extra peaks (O) are seen at 3 eV lower than the binding energy of O-Si_2 peak. It is considered at present that O peak is originated from an absorption of single oxygen atom or an oxygen bridge (Si*-O-Si*; Si* denotes the first Si layer from the surface of oxide.) The maximum peak intensities of O peaks normalized by O-Si_2 peak in (a), (b) and (c) were 0.020, 0.013 and 0.005, respectively. O-Si_2 peaks did not disappear, similarly to the case of Si^{x+} mentioned above.

Several reports on the effect of post oxidation processes in terms of electrical characteristics have been brought to us. Then, we have carried out *C-V* measurements for the three specimens used in the XPS

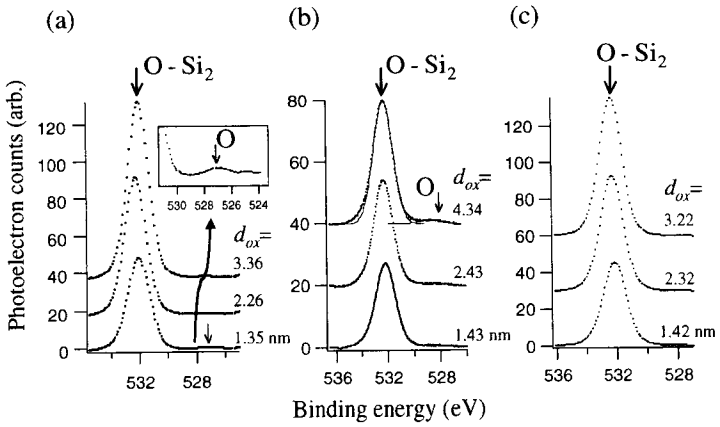

Fig.3 Photoelectron spectra of O1s as a function of oxide thichness. (a)-(c) denote quench, Ar POA, wet re-oxidation, respectively.

Table 1

The changes of electrical properties and interfacial bonding structures due to post oxidation processes.

	C-V characteristics		XPS (relative intensity %)				
	V_{fb} [a] [V]	D_{it} [b] / 10^{12} [$cm^{-2}eV^{-1}$]	Si-O-C	C-O	C-	C-H	O
quench 1	2.0	4 ~ 50	28.0	~ 0	5.5	10.0	2.0
Ar POA 1	~ - 0.2 [c]	unknown	35.5	7.8	39.0	26.6	1.3
Wet re-ox. 1	2.0	1.5 ~ 4	38.5	~ 0	3.0	8.5	~ 0
quench 2	1.0	5 ~ 10	25.6	~ 0	4.0	13.6	~ 0
Ar POA 2	0.5	0.3 ~ 20	25.8	~ 0	2.9	17.3	~ 0
Wet re-ox. 2	1.5	0.2 ~ 2	30.9	~ 0	4.8	10.5	~ 0

[a] Denotes a flat-band voltage; [b] Denotes an interfacial trap density

[c] Denotes a shift of negative direction

measurements. However, the detail of experimental results of *C-V* measurements are omitted here. The dependence of *C-V* characteristics on the post oxidation processes, as well as XPS results, were summarized in Table 1. The differences between upper layer (#1) and lower layer (#2) are of the oxidation furnace and the fabrication technique. If we compare #1 with #2 , C-O or C- bonds may be related to the shift of flat-band voltage (V_{fb}). Also, if we pay attention to the specimen which indicates the lowest interface trap density (D_{it}), C-H bonds may be related to D_{it}. Although we could not distinguish the bonds which influence the *C-V* characteristics clearly from the results, the differences of bonding structure and electrical property due to the post oxidation processes were found out.

Summary

We carried out XPS measurements for slope shaped oxide films with several post oxidation processes. The differences at oxide/SiC interfaces by these processes were the number of characteristic bonds, such as Si-Si, Si-O-C, C-O, C- and O bonds. Also, the bonds which influence the MOS property were discussed by comparing the results of XPS measurements with that of *C-V* measurements. Although we could not know the reasons for degrading the electrical properties of SiC MOS structures, the differences due to post oxidation processes in terms of bonding structure and electrical property have been pointed out.

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