

Characterization of Oxide Films on SiC Epitaxial (000-1) Faces by Angle-Resolved Photoemission Spectroscopy Measurements using Synchrotron Radiation

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Abstract. Thermal oxide films on SiC epitaxial (000-1) C-faces have been characterized by angle-resolved photoemission spectroscopy (AR-PES). The structure of wet oxide/SiC C-face interface was compared with that of dry oxide/SiC C-face, as well as that of dry oxide/SiC Si-face, in order to clarify why a MOS device of SiC C-face achieved good electrical properties. The improvement in electrical properties was confirmed by AR-PES measurements, evidencing differences in binding energy between SiC and the Si⁴⁺ components in Si2*p* and valence band region, and in binding energy between SiC and the CH_x components in C1*s*. The reason for the improvement in electrical property of MOS devices by use of SiC C-face are discussed in terms of depth profiles of oxide films calculated from the AR-PES results.

Introduction

SiC MOSFETs have some problems to be solved before practical use, such as their higher on-resistances than those predicted from bulk properties. It has been considered that this poor electrical property is due to the low channel mobility μ_{ch} in inversion layer of SiC MOSFET, and the small μ_{ch} results from the high interface state density. Therefore, controlling the structure of the oxide/SiC interface is a key to the developments of SiC MOSFET. On the other hand, oxidation rate of (000-1) C-face is the largest among all hexagonal SiC faces, which is approximately ten times larger than that of SiC (0001) Si-face.[1] Therefore, the production time of SiC MOSFETs can be dramatically reduced by the utilization of SiC C-face. It has been long time while no report showing that MOSFETs fabricated on SiC C-face have better electrical properties than those on SiC Si-face. However, recent works succeeded in growing high-quality epitaxial films on SiC C-face, and achieved μ_{ch} of over 100 cm²/Vs by a pyrogenic oxidation followed by a hydrogen annealing.[2,3] The electrical properties of MOS devices obtained by a dry oxidation of SiC C-face have been reported to be poor compared with that of wet oxidation of SiC C-face, on the contrary in the case of SiC Si-face.

In this work, to clarify the reason for improvement in the electrical property of SiC MOSFET, we examine the MOS structure on C epi-face by the observation of composition and bonding structure at oxide/SiC interfaces of wet and dry oxide films, as well as that on Si-face, using high-resolution angle-resolved photoemission spectroscopy (AR-PES.)

Experiments

We performed AR-PES measurements on three kinds of sample. 4H-SiC epi-films with 8° off-oriented, *n*-type, $N_d - N_a \sim 10^{16} \text{ cm}^{-3}$ were used in this study. After standard RCA cleaning, C-face and Si-face specimens were oxidized in pure dry O_2 flow at 1100°C , followed by quenching at room temperature (denoted as samples (C-Dry) and (Si-Dry)). Another C-face specimen was oxidized in wet O_2 flow ($\text{O}_2 : \text{H}_2\text{O} = 3:1$) at 900°C , also followed by quenching (denoted as sample (C-Wet)). The oxide thicknesses measured by a spectroscopic ellipsometer were all around 1.3 nm. AR-PES measurements were performed with synchrotron radiation (undulator beam line BL27US of Spring-8) and hemispherical analyzer (*Scienta ESCA300*) as a light source and an electron analyzer, respectively. The photon energies of 1050 and 400 eV were selected for the core level and valence band spectra, respectively. The normalized energy resolution $\Delta E/E$ was about 2×10^{-4} .

Results and Discussion

The photoemission spectra in $\text{Si}2p$ region for samples (C-Dry), (C-Wet) and (Si-Dry) at 55° in in-take angle of photoelectron, θ_e , are shown in Figs. 1(a). The measured spectra were decomposed into peaks with Gaussian. By the analysis, it was found that the Lorentzian contribution is small enough to be ignored, and the spin orbit splitting and the branching ratio are 0.5 eV and 0.5, respectively, for the best curve fitting. The component peaks and the sum of all component peaks are shown by thin and thick solid lines, respectively, together with the measured spectra. The photoemission spectra in

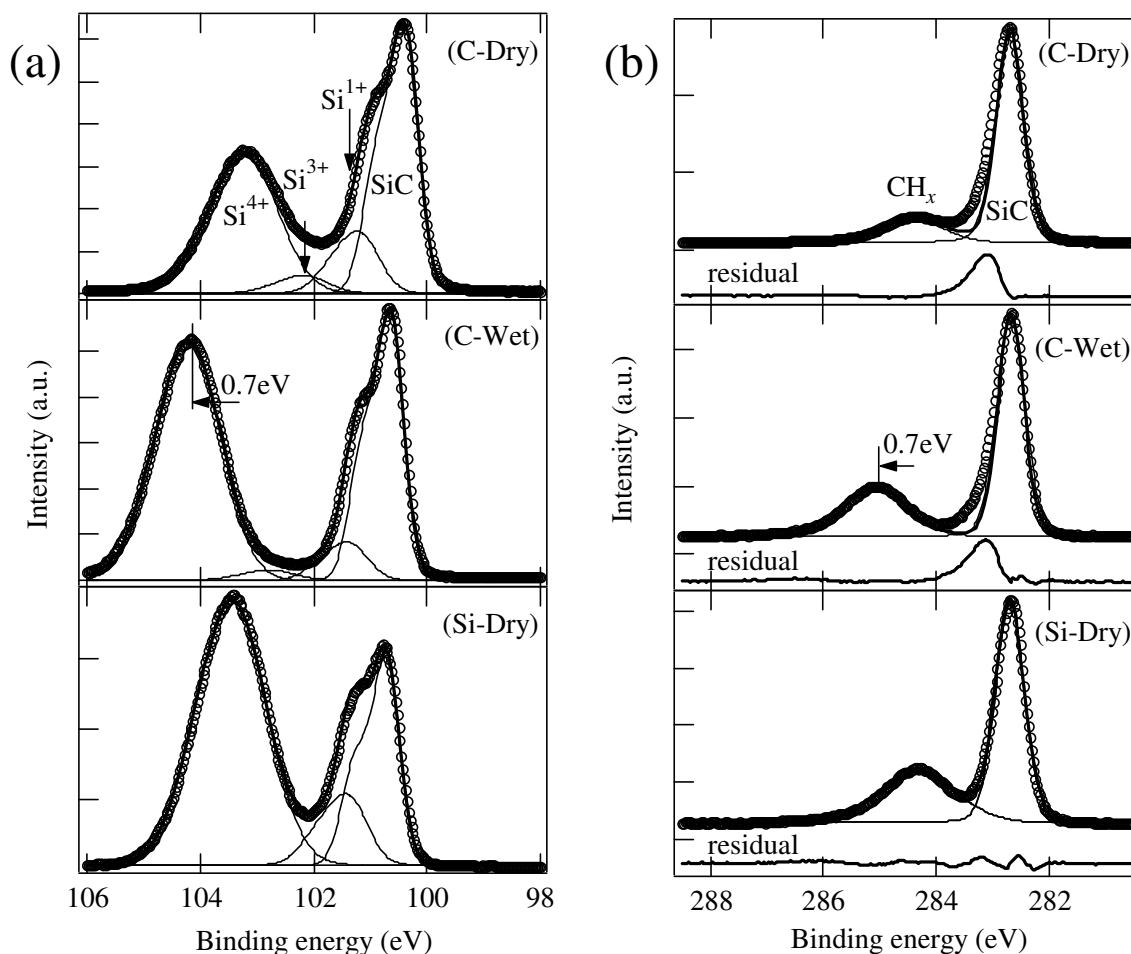


Fig. 1. Core level spectra for the samples (C-Dry), (C-Wet) and (Si-Dry) at $\theta_e = 55^\circ$; (a) $\text{Si}2p$ region, (b) $\text{C}1s$ region.

C1s region are shown in Figs. 1(b). The measured spectra in C1s region were also decomposed into peaks with superposition of Gaussian and Lorentzian. Intensity ratio of Lorentzian to Gaussian was found to be 0.1 for the best curve fitting. The spectra in C1s region from angle-resolved measurements (not shown here) indicate that the extra peak around 284.5 eV originates from CH_x. We can see from Figs. 1(a) and (b) that the binding energies, E_b , of the Si⁴⁺ component in Si2p region and CH_x peak in C1s region for (C-Wet) are around 0.7 eV higher than the others.

The valence band spectra are shown in Fig.

2. They indicate that the difference in valence band edge between SiC and oxide layer for (C-Wet) is around 0.7 eV larger than that of (C-Dry). This energy difference between (C-Dry) and (C-Wet) agrees with that observed in Si2p and C1s regions. Therefore, this energy difference can be explained by the difference of charges arise at the interface states. The energy difference of 0.7 eV corresponds to that of the number of interface state per unit area N_{it} of a few 10^{13} cm⁻², which agrees well with that obtained from C-V measurements.[3] It was found that there is a good correspondence between the shift of E_b in AR-PES measurements and the amount of interface trapping charge estimated by electrical measurements. In our previous report,[4] we have pointed out, in the case of Si-face, that the energy difference of valence band edge corresponds to N_{it} . Therefore, it is considered that this correspondence is made up for both cases of Si and C-faces.

In Figs. 1(a), the Si³⁺ component as well as the Si¹⁺ one were seen in the case of C-face. Virojanadara *et al.* have reported that only the Si²⁺ states are observed in the case of C-face.[5] In Figs. 1(b), the residual peak is seen at the higher energy side of SiC peak only in the cases of C-face. This extra peak can be assigned as C¹⁺, probably originating from C-OSi₃ at the topmost layer of SiC. Virojanadara *et al.* have reported that no component peak is observed at this binding energy.[5] By the way, as mentioned above, it was found that the amount of interface trapping charge for (C-Wet) is much smaller than the others, and that for (C-Dry) does not much differ from that for (Si-Dry). However, there is no correspondence between the relation in peak intensities of Si¹⁺, Si³⁺ and C¹⁺ states and that in amounts of interface trapping charge of them.

Figure 3(a) shows the relative energy from SiC E_b of Si¹⁺, Si³⁺ and Si⁴⁺ as a function of effective escape depth, *i.e.* $\lambda \sin \theta_e$ (λ : escape depth ~ 2.3 nm[6]), for the samples (C-Dry) and (C-Wet). It is found from the figure that the relative energies of Si¹⁺ and Si⁴⁺ in both the cases and that of Si³⁺ for (C-Wet) change scarcely with effective escape depth. However, the relative energy of Si³⁺ for (C-Dry) changes abruptly at the depth corresponding to SiC topmost layer. This indicates that the charge bringing about E_b shift distribute at the region from the SiC topmost layer to a few angstroms upper.

Figure 3(b) shows the peak intensity ratios, (Si¹⁺ + Si³⁺)/SiC and Si⁴⁺/SiC, as a function of effective escape depth for the samples (C-Dry) and (C-Wet). The structure of oxide film on SiC can be estimated roughly from angle-resolved data by use of the two layers attenuation model.[7] Here, an oxide film is assumed to be composed of two layers, an intermediate oxidation layer, containing Si¹⁺ and Si³⁺ states, and a Si⁴⁺ state layer. The broken and the solid curves in the figure indicate fitted ones for (C-Dry) and (C-Wet), respectively. From the calculation, the thickness of intermediate oxidation layer and that of Si⁴⁺ state layer for sample (C-Dry) was obtained as 0.28 and 0.92 nm, respectively. As mentioned above, there exist a lot of charges at the region from the SiC topmost layer to a few angstroms upper. The location agrees well with the thickness of topmost intermediate oxidation layer

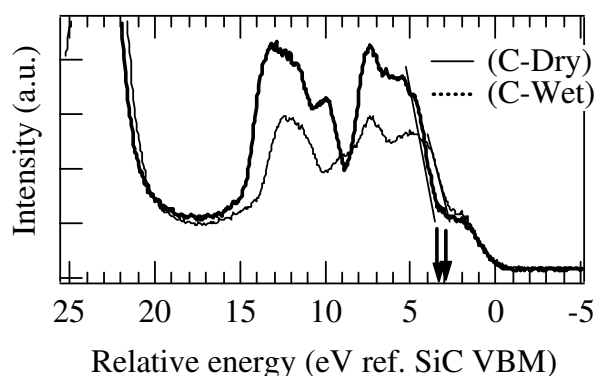


Fig. 2. Valence band spectra for the samples (C-Dry) and (C-Wet); $\theta_e = 30^\circ$. Solid line around 3 eV corresponds to superimposed valence band edge of oxide layer.

obtained from the calculation. Similarly, the thicknesses for samples (C-Wet) and (Si-Dry) were calculated as 0.18 and 1.27 nm, and as 0.30 and 1.21 nm, respectively. The results indicate that the thickness of the intermediate layer for (C-Wet) is 1/3 smaller than the others. There is a good correspondence between the thickness of intermediate layer and the amount of interface trapping charges. Therefore, these results suggest that the improvement of electrical characteristics for MOS devices fabricated by wet oxidation of SiC C-face is due to the improvement of interface structure, *i.e.* the reduction in the thickness of intermediate layer.

Summary

We have studied the thermal oxide films on 4H-SiC (000-1) epi-film by a high-resolution AR-PES. The difference in the amount of interface trapped charges between dry and wet oxidations was clearly observed as that in the E_b between the Si^{4+} and SiC components, as well as that in E_b between CH_x and SiC ones. Si^{1+} oxidation state was seen at the oxide/SiC interface in both of C-face and Si-face, however, Si^{3+} and C^{1+} states are seen only in the cases of C-faces. AR-PES results indicate that the interface trapping charges locate within a few angstroms upper from the SiC topmost layer. There is correspondence between the location of the charge and that of intermediate oxidation states. AR-PES results indicated that the decrease in thickness of intermediate layer corresponds to the decrease in the amount of interface trapping charge.

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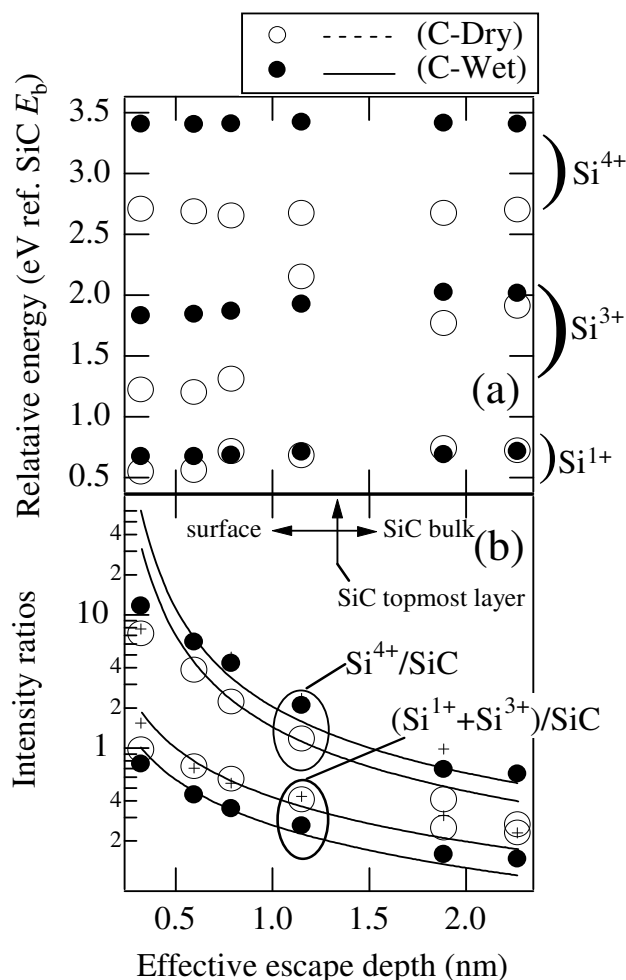


Fig. 3. Relative energy from SiC binding energy, (a); Intensity ratios normalized by intensity of SiC peak, (b); as a function of escape depth for the samples (C-Dry) and (C-Wet); Si2p region.