

The Investigation of 4H-SiC/SiO₂ Interfaces by Optical and Electrical Measurements

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ABSTRACT. We have investigated SiO₂/4H-SiC interfaces by using capacitance-voltage (*CV*) measurements, spectroscopic ellipsometry (SE) and Fourier-transformed infrared (FTIR). From *CV* measurements, fairly large amounts of interface traps and negatively trapped charges in oxide layers were observed near the SiO₂/4H-SiC interface. By using spectroscopic ellipsometry (SE), we found interface layers between 4H-SiC substrates and SiO₂ layers, which have higher refractive indices than those of SiO₂ and 4H-SiC. The FTIR measurements showed that the Si-O-Si bonds near the SiO₂/4H-SiC interface had a lower stretching frequency compared to that of fused quartz. These results suggest that the interface layers are suboxides.

1. INTRODUCTION

Silicon carbide (SiC) is one of the most attractive materials for high power and high temperature devices because of its wide band gap and intrinsic properties. Particularly, the fact that SiC can be thermally oxidized to grow insulating SiO₂ layers makes it a promising material for metal-oxide-semiconductor field effect transistors (MOSFETs). However, the electrical characteristics of oxide/SiC structures are poorly understood compared with those of oxide/Si structures and the channel mobilities of SiC MOSFETs are much lower than the value expected from the bulk mobility. Many studies have been carried out to resolve these problems [1-5], nevertheless, the origin which lowers device characteristics has not yet been clarified. In this report, we have examined the optical and electrical characteristics of SiO₂/4H-SiC interfaces by capacitance-voltage (*CV*), spectroscopic ellipsometry (SE), Fourier-transformed infrared reflection absorption spectroscopy (FTIR-RAS) and Fourier-transformed infrared reflection attenuated total reflection (FTIR-ATR) measurements in order to make clear the interface structures.

2. EXPERIMENTS

Epitaxial wafers of 4H-SiC with 8° off-oriented (0001) Si face and n-type with the carrier density of approximately $5 \times 10^{15} \text{ cm}^{-3}$ were used for the measurements. Standard RCA cleaning process was carried out to these wafers. Following the cleaning, thermal oxides were grown in pure O₂ ambience at 1200 °C. Two samples were oxidized together in same furnace, one of which is for electrical measurements and the other is for optical measurements. The thickness of the oxide layers obtained was in the range 30-50 nm. The samples were immediately removed from the furnace to quench the oxides. For spectroscopic ellipsometry measurements and FTIR-RAS,

the samples were etched at an angle by dipping gradually into diluted hydrofluoric acid at a constant speed. The both optical measurements were performed along the slope of the oxides films to obtain the data as a function of oxide thickness. Because it is difficult to obtain enough sensitivity for thinner layer by FTIR-RAS measurement, we performed FTIR-ATR measurements for layer thickness below 3 nm. The samples for the FTIR-ATR measurements were made by etching thick oxide layers of 50 nm in thickness to a desired thickness using hydrofluoric acid. In order to connect optical properties obtained from the methods mentioned above with electrical properties, CV measurements were carried out using the samples which were oxidized side by side in the furnace with those for optical measurements. For CV measurements, oxide layers of 50 nm in thickness were used. Metal-oxide-semiconductor (MOS) structures were formed as follows. Gold was deposited on the oxide layers to form gate electrodes of 0.5 mm in diameter. To make ohmic electrodes, the oxide layers on the substrate backsides were removed and aluminum was deposited on the bared surfaces. High-frequency CV curves were obtained for the MOS structures to estimate the net number of interface traps per unit area (N_{it}) and the gate voltage corresponding to flat band condition (V_{fb}). SE measurements were carried out using a spectroscopic ellipsometer GESP-5 (Sopra) in the wavelength range between 250 and 850 nm at the angle of incidence of 75° . In the evaluation of the refractive indices, we assumed that the wavelength dependence of the refractive indices follows Sellmeier's dispersion law. The thickness of oxide layers and the values of parameters A and B in Sellmeier's equation were evaluated from the experimental data of (ψ, Δ) by a curve fitting method. FTIR was carried out using a Nicolet Magna-760. ATR spectra were taken with s- and p-polarized IR lights, and only p-polarized IR light was used for RAS measurements. The spectral resolution and accumulation were 2 cm^{-1} and 1024 times for ATR measurements, and 4 cm^{-1} and 512 times for RAS measurements. The ATR measurements were made with a Ge prism ($50 \times 20 \times 1\text{ mm}$) beveled at an angle of 60° as the ATR element. For the RAS measurements, the incident light was focused to $0.5\text{ mm}\phi$, and the angle of incidence was 80° .

3. RESULTS and DISCUSSION

Figure 1 shows the high-frequency CV characteristics for MOS structures with oxide layers grown in pure oxygen (dry oxides) for 3 hours. C_{fb} and C_{Lg} indicate the capacitance corresponding to flat band condition and the ledge of high-frequency CV curve swept from negative to positive gate voltage side, respectively. There is a split near the depletion region. This indicates that the interface traps exist near the interface. The value of N_{it} in dry oxides was over $7 \times 10^{12}\text{ cm}^{-2}$ and V_{fb} was determined to be $+18\text{ V}$. From the value of V_{fb} , the existence of large amounts of negatively trapped charges was suggested. In case of the CV curve swept from negative to positive gate voltage, the capacitance was not measured beyond $+19\text{ V}$ because of the electrical breakdown of the oxides. We also tried to measure the quasi-static CV curve. However, we failed to obtain the curve due to the large leakage current flowing in the oxides.

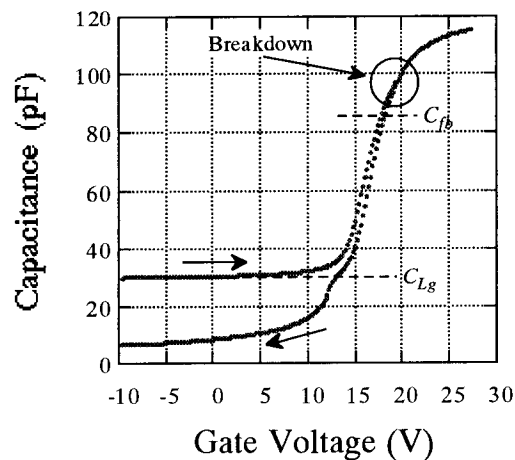


Fig. 1 High-frequency CV characteristics for MOS structures with dry oxide layers.

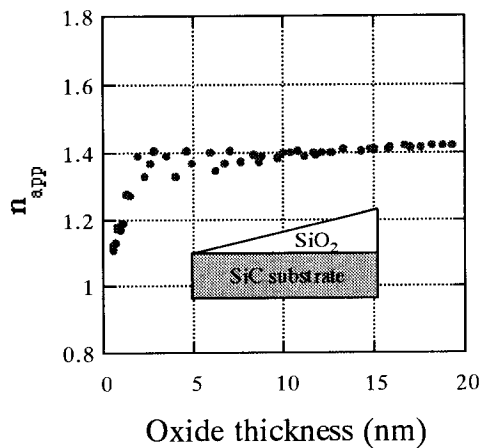


Fig. 2 Thickness dependence of refractive indices n_{app} for dry oxide layers. ($\lambda=630$ nm)

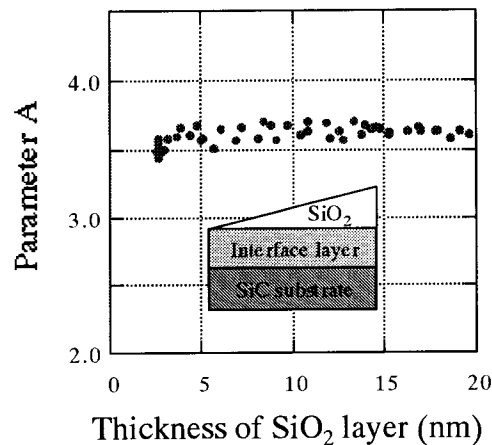


Fig. 3 The value of parameter A in the Sellmeier's dispersion equation for an interface layer.

All of the dry oxides over 30 nm in thickness showed this characteristics in this experiment.

Figure 2 shows the oxide thickness dependence of apparent refractive indices (n_{app}) at the wavelength of, for example, 630 nm obtained from the spectroscopic ellipsometric measurements under the assumption that the oxide films have uniform refractive indices. These values are not constant but decrease with film thickness, especially in the region below 5 nm in thickness. The change with thickness indicates the existence of interface layers. Therefore, we reanalyzed the results by using a two layer model, where the interface layers with the thickness of 1 nm exist under the SiO_2 layers having the same refractive indices as those of fused quartz. Figure 3 shows the values of Sellmeier's parameter A of interface layers as a function of the thickness of upper SiO_2 layers. The values are almost constant over all the thickness region and are higher than the refractive indices (n) of SiO_2 ($n=1.46$ at 630 nm) and SiC ($n=2.63$ at 630 nm). It is noted that the value of parameter A is almost equal to n at 630 nm in this experiment.

Figure 4 shows the results of FTIR-RAS measurements for the same as SE measurements. The peak frequency of the TO mode of Si-O-Si stretching vibration shifts to a lower frequency in the region below 5 nm in thickness of the oxide. The FTIR-RAS measurements were performed with relatively low resolution (4 cm^{-1}) and the measurements at the region below 3 nm were impossible because of its low sensitivity. Therefore, in order to investigate thinner region and to obtain more accurate values of the peak frequency, we carried out FTIR-ATR measurements for the oxide layers, which were uniformly thinned by etching. Figure 5 shows the results obtained by FTIR-ATR measurements for s-polarized IR lights. The peak frequency of the TO modes of Si-O-Si stretching vibration shifts from 1075 cm^{-1} to 1071 cm^{-1} with decrease of thickness, while the peak frequency of 1075 cm^{-1} corresponds to that of fused quartz. Because the peak frequency at 6.9 nm was 1075 cm^{-1} from FTIR-ATR measurements, the region more than 5 nm in Fig. 4 is consider to correspond to the peak frequency of fused quartz. These results from FTIR measurements indicate that interface layers exist at SiO_2 /4H-SiC interface. The Si-O-Si bonds in upper SiO_2 layers had the same stretching frequency of fused quartz, though the Si-O-Si bonds near the interface had a lower stretching frequency compared to that of fused quartz.

Based on the results from electrical and optical measurements, we will discuss the origin of the interface layers. From the results of FTIR measurements, the peak frequency of Si-O-Si stretching vibration shifts toward a lower frequency near the interface. This suggests a decrease in

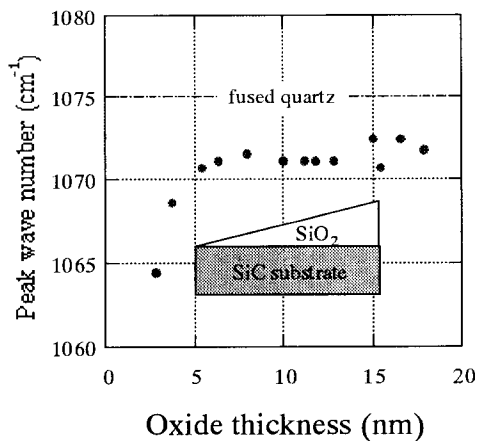


Fig. 4 TO mode frequency of dry oxide layers by FTIR-RAS.

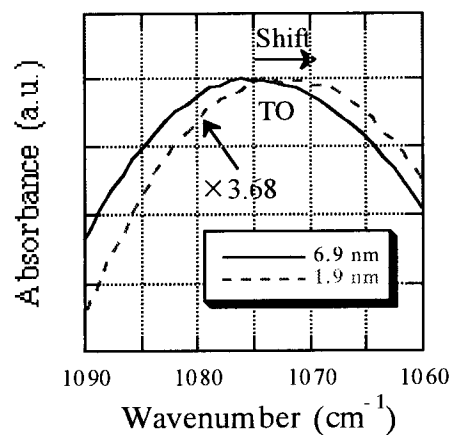


Fig. 5 S-polarized ATR spectra of dry oxide layers.

the Si-O-Si bond angle and/or the Si-O force constant, which can be expected if Si-Si bonds or Si-C bonds exist in SiO₂ [6,7]. From SE measurements, the interface layers having higher refractive indices than those of fused quartz were found. This suggests the interface layers contain large dipole moments than those in SiO₂ and SiC, like Si-Si bonds. Consequently, the results from optical measurements show the existence of the suboxide with Si-Si bonds. The origin of N_{it} is thought to be attribute to this suboxide. To make clear our consideration, further investigations, for example, the comparison between samples oxidized by different oxidation methods and the change of interface layer by post annealing treatment, are needed.

4. CONCLUSION

We studied SiO₂/4H-SiC interfaces by using FTIR, SE and *CV* measurements. In the case of oxide layers formed by dry O₂, we found high densities of interface traps, large shift of *CV* curve along the gate voltage axis and large leakage current from *CV* measurements. From the optical measurements, the existence of interface layers at SiO₂/SiC interface were suggested. The interface layers have higher refractive indices than those of SiO₂ and SiC, and a lower vibration frequency of the Si-O-Si stretching mode compared to that of fused quartz.

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