Jpn. J. Appl. Phys. Vol. 41 (2002) pp. 800–804
Part 1, No. 2A, February 2002

Measurements of the Depth Profile of the Refractive Indices in Oxide Films on SiC by Spectroscopic Ellipsometry

Takeshi IIDA*, Yuichi TOMIOKA, Kazuo YOSHIMOTO, Masahiko MIDORIKAWA, Hiroyuki TUKADA, Misao ORIHARA, Yasuto HIJIKATA, Hiroyuki YAGUCHI, Masahito YOSHIKAWA[1], Hisayoshi ITOH[1], Yuuki ISHIDA[2] and Sadafumi YOSHIDA

Department of Electrical and Electronic Systems, Saitama University, 255 Shimo-Ohkubo, Saitama 338-8570, Japan
[1]*Japan Atomic Energy Research Institute, 1233 Watanuki, Takasaki, Gunma 370-1292, Japan*
[2]*National Institute of Advanced Industrial Science and Technology, 1-1-1 Umezono, Tsukuba, Ibaraki 305-8568, Japan*

(Received August 8, 2001; accepted for publication November 5, 2001)

The depth profiles of the refractive indices in thermally oxidized films on SiC have been measured by spectroscopic ellipsometry. Oxide films etched at an angle were used to obtain the depth profiles of the refractive indices in the oxide films. The apparent refractive indices n_{app} and thicknesses have been evaluated, assuming that the films have optically uniform single layer structures. The experimental results show that the values of n_{app} increase with oxide film thickness, and approach the values for oxide films on Si at around 60 nm in thickness. This feature is almost the same as the changes of refractive indices of oxide films with oxidation time reported previously. These results reveal that the oxide films are not optically uniform and that the optical properties change with depth from the surface. It has been found that the film structure model where the oxide film is composed of two layers, a thin interface layer around 1 nm in thickness with a higher refractive index than those of SiC and SiO_2 and a stoichiometric SiO_2 layer, the thickness of which changes with film thickness, can explain the thickness dependence of n_{app} observed. These results suggest that there exists an interface layer with high refractive indices at oxide film/SiC interfaces. [DOI: 10.1143/JJAP.41.800]

KEYWORDS: spectroscopic ellipsometry, 6H-SiC, refractive indices, oxide films, SiC/SiO_2 interface

1. Introduction

The physical properties of SiC, such as a wide band gap, high thermal conductivity, high saturated electron drift velocities, and high-breakdown electric fields, make SiC attractive for electronic device applications including high-power and high-frequency devices whose specifications cannot be obtained using Si and GaAs. In addition, SiC can be thermally oxidized to grow insulating SiO_2 layers, which are known to have superior dielectric properties for metal-oxide-semiconductor (MOS) applications, similar to Si.[1)] SiC-metal-oxide-semiconductor field-effect transistor (MOSFET) is expected to have on-resistance (R_{on}) two orders of magnitude smaller than that of Si-MOSFET at the same breakdown voltage.[2)] However, to date, such a small R_{on} has not been reported. For this reason, the electron mobility (μ_e) in the inversion layer is thought to be severely degraded, probably due to the residual carbon at the SiO_2/SiC interfaces.[3)] However, the mechanism of the small electron mobility has not yet been clarified. Therefore, it is important to characterize the structures of the SiC/SiO_2 interface in order to realize SiC-MOSFETs with the specifications expected.

Many studies have been carried out to investigate the SiC/oxide layer interfaces by, for example, C–V,[4–7)] X-ray photoelectron spectroscopy (XPS) and secondary ion mass spectroscopy (SIMS) measurements.[8–11)] In the previous report,[12)] we evaluated for the first time the optical constants of thermally oxidized films on SiC by spectroscopic ellipsometry. It was found that the apparent refractive indices n_{app} assuming an optically single layer structure are smaller than those of the oxide films on Si. The values of n_{app} increase with oxide film thickness, reaching the values of Si oxides of around 60 nm in thickness.

In this study, we have measured the thickness dependence of refractive indices of oxide films on SiC for oxide films etched at an angle using spectroscopic ellipsometry, and evaluated the depth profile of the optical constants of oxide films.

2. Experiments

6H-SiC epilayers, 5 μm in thickness and 5×10^{15} cm^{-3} in carrier concentration (n-type) (Cree, Inc.), were used for the measurements. The (0001) Si surfaces of the SiC epilayers were oxidized in dry oxygen flow at 1100°C. The thicknesses of the oxide films obtained were around 60 nm for an oxidation of 16 h. After oxidation, the SiC substrates with the oxide layers were immersed gradually in diluted hydrofluoric acid of 8% at a constant speed to etch the oxide layer at an angle. Using the sloped oxide films, we can measure the optical properties of the oxide films with various thickness using one sample, which means only the film thickness changes along the slope and that the interface structures are the same for all positions, i.e., for all thicknesses.[12)] We can also obtain oxide films with various thicknesses by changing the oxidation time. However, in this case, there is a possibility that the film structures, particularly the interface structure, change with the oxidation time. The details of the fabrication method of oxide films etched at an angle have been reported elsewhere.[13)]

Following the etching, spectroscopic ellipsometric (SE) measurements have been carried out using a spectroscopic ellipsometer GESP-5 (Sopra) at wavelength intervals of every 2 nm in the wavelength range between 250 and 850 nm at an angle of incidence of 75°. The measurements have been performed at every 5 nm for the regions where the film thicknesses are more than 10 nm, and at every 0.5 nm for the regions where they are less than 10 nm. As the slope is very small, in the order of 10 nm per 1 cm, the effect of the thickness changes in the optical beam (~0.1 mm) can be

*Present address: NEC Electron Devices, NEC Corporation, 1753 Shimonumabe, Nakahara-ku, Kawasaki 221-8666, Japan.

neglected in the analysis.

3. Evaluation of the Apparent Refractive Indices

We have obtained the optical constants of the oxide films, as well as the film thicknesses, assuming an optically uniform single layer structure with uniform optical properties. The wavelength-dependence of the refractive indices of the oxide films were assumed to follow Sellmeier's dispersion law,

$$n_{\mathrm{app}} = \sqrt{1 + \frac{(A^2 - 1)\lambda^2}{\lambda^2 - B}}, \tag{1}$$

where parameter A indicates the refractive index of the wavelength at infinity, while the square root of parameter B indicates the wavelength corresponding to intrinsic oscillation. The extinction coefficient k was assumed to be equal to 0. The values of the film thickness and parameters A and B were evaluated by the curve fitting of the calculated ellipsometric parameters Ψ and Δ to those measured between 250–850 nm.

Figure 1 shows the oxide film thickness distribution along the slope evaluated from the SE measurements, assuming the oxide films are optically uniform. The figure shows that the oxide film thickness changes almost linearly with the measured position, except in the region less than 5 nm in thickness, which reveals that the oxide films were etched at an angle. Figure 2 shows the changes in the apparent refractive indices n_{app} of the oxide films on SiC along the slope at the wavelength of, for example, 630 nm. Figure 3 shows those as a function of oxide thickness. As the values of B are almost constant while the values of A decrease with film thickness, the refractive indices decrease with film thickness at all of the wavelengths measured. The evaluation of these parameters was carried out along the slope starting from the thickest end, and the parameter values for the former calculation, i.e., for thicker film, were used as initial values, in order to avoid converging on improper answers. We obtained the values of thickness, A and B in the errors of ± 0.002–0.02, which lead to the deviation of ± 0.002–0.006 in the values of refractive index. It is shown that n_{app} at the position corresponding to 60 nm in thickness is almost the same as that reported for stoichiometric SiO_2. Along the slope, i.e., with decreasing oxide film thickness, n_{app} decreases gradually. At less than 5 nm in thickness, n_{app} decreases markedly with decreasing oxide film thickness, and n_{app} approaches 1 at the position corresponding to the oxide film thickness equal to 0. This feature, i.e., that n_{app} decreases with decreasing oxide film thickness, is almost the same as those observed for oxide films with various oxidation times reported previously.[12]

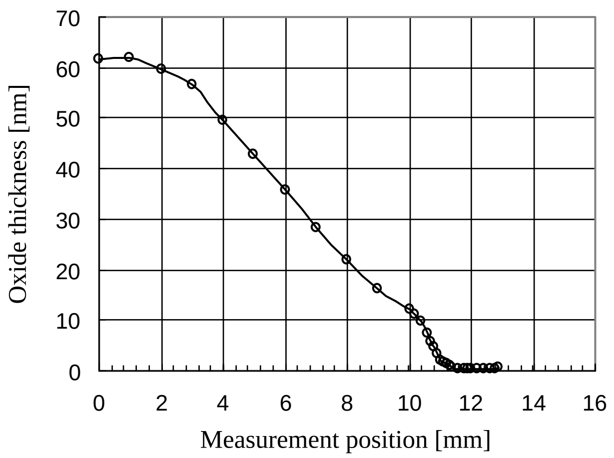

Fig. 1. Film thickness distribution of a sloped oxide film on SiC, along the slope.

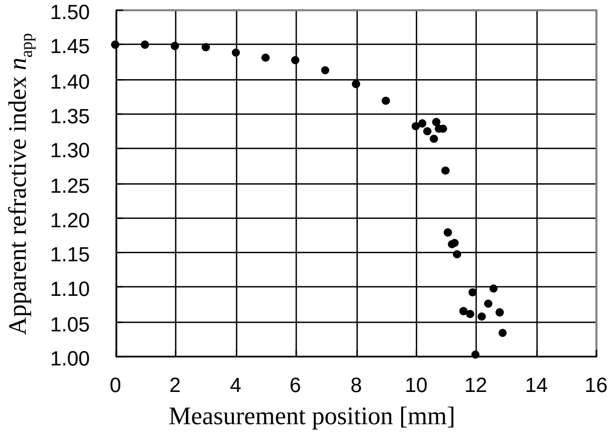

Fig. 2. Changes of the apparent refractive indices n_{app} of an oxide film on SiC along the slope at the wavelength of 630 nm.

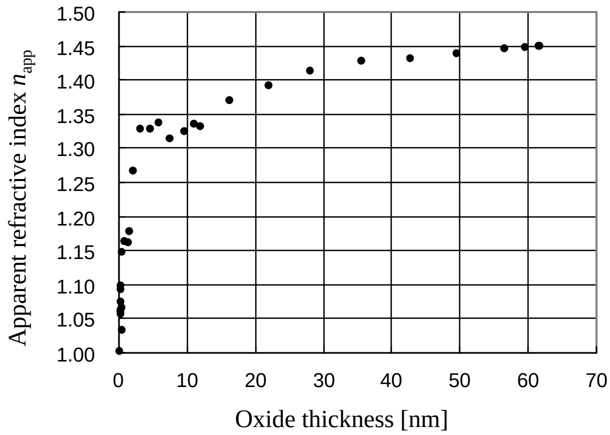

Fig. 3. Thickness dependence of n_{app} of an oxide film on SiC at the wavelength of 630 nm.

4. Evaluation of the Depth Profiles of the Refractive Indices

X-ray photoemission studies on the SiC/SiO_2 interface have suggested the existence of an interface layer, around 1 nm in thickness, whose composition and/or bonding states are different from those of SiC and SiO_2.[13] The ellipsometric measurements using oxide films etched at an angle show that the values of n_{app} decrease with decreasing oxide film thickness. This result contradicts the assumption that the films are optically single layer structures with uniform optical properties, which suggests that the oxide films are not optically uniform but their refractive indices change in the depth direction. In particular, the result that n_{app} decreases markedly in the very low thickness region suggests a large change of refractive indices near the interfaces. Therefore, we have attempted to obtain film structure models that can explain the thickness dependence of the apparent refractive index of oxide films on SiC. It is well known that in the case of oxide films on Si, there exist transition layers, the composition of which varies from Si to SiO_2.[14,15] There is a possibility that at the oxide films/SiC interface, there exists a transition layer whose optical constant varies gradually from that of SiC to that of SiO_2, as in the case of oxide films on Si. We have attempted to explain the thickness dependence of the refractive indices of SiC oxide films, taking into account the existence of the transition interface layer whose optical constant changes exponentially from that of SiC to that of SiO_2. However, the thickness dependence of n_{app} observed could not be explained by the transition layer model.

This result means that the refractive indices of the interfaces are larger than that of SiC ($n = 2.6$ at $\lambda = 630$ nm) or smaller than that of SiO_2 ($n = 1.45$). Thus, we attempt to explain the thickness dependence of the refractive indices of oxide film by using a model in which there exist interface layers with lower refractive indices than that of SiO_2. That is, the oxide films are composed of two layers, a thin interface layer with low refractive indices, and a SiO_2 layer with the same refractive indices as stoichiometric SiO_2. We attempted to explain the changes of n_{app} along the slope, i.e., the thickness dependence of n_{app} by the change in SiO_2 layer thickness. We have evaluated the refractive indices and thicknesses of interface layers and the thicknesses of SiO_2 layers by curve fitting for all of the positions along the slope. However, negative values were obtained for the thickness of the interface layer in the regions where the SiO_2 layer thicknesses are between 40 nm and 60 nm. This means that the two-layer model with a low refractive index interface layer cannot explain the thickness dependence of n_{app} observed throughout the thickness range.

Next, we attempt to explain the changes of the refractive indices n_{app} using the model in which there exist interface layers with higher refractive indices than that of SiC. That is, the films are composed of two layers, a thin interface layer with high refractive indices, and a SiO_2 layer. The wavelength dependence of the refractive indices of the interface layer was assumed to follow Sellmeier's dispersion law. We have evaluated the fitting parameters A and B appearing in Sellmeier's equation eq. (1) and the thicknesses of the highly refractive interface layer and the SiO_2 layer. Figures 4 and 5 show the obtained values of the thicknesses of the SiO_2 layers and the highly refractive interface layer, and the values of A and B, respectively, as a function of the measurement position. The figures show that the thickness and the Sellmeier parameters A and B of the highly refractive interface layer are almost constant for all of the positions measured, and the thickness of the SiO_2 layer changes almost linearly along the slope. This means that the thickness dependence of n_{app} in oxide films on SiC can be explained only by the change in the thickness of the SiO_2 layer that lies on the interface layer with $A \sim 4$ and $B \sim 0.15$. As parameter A in Sellmeier's equation indicates the refractive index at long wavelengths, this suggests that there exist interface layers with high refractive indices. These values are higher than those of SiC and SiO_2, which reveals that the interface layers are not mixed layers between SiC and SiO_2.

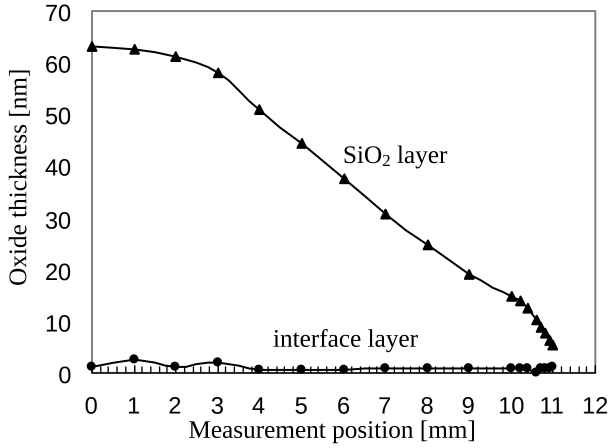

Fig. 4. Thicknesses of the SiO_2 layer and the highly refractive interface layer as a function of the measurement position.

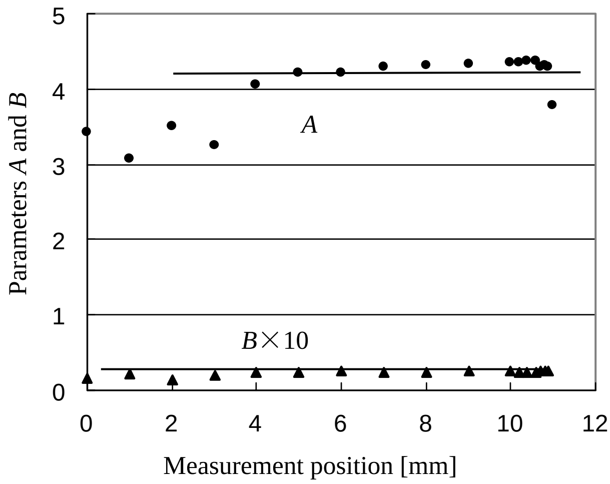

Fig. 5. Sellmeier parameters A and B of the highly refractive interface layers as a function of the measurement position.

X-ray photoemission studies also suggest that there exist Si–Si bonds at the interfaces, which result in $k \neq 0$ for interface layers. We evaluated the refractive indices of the interface layers, assuming that the wavelength dependence of the refractive indices follows Sellmeier's dispersion law and $k = 0$. This is not self-evident. Then, we attempted to evaluate the optical constants of the interface layers at every wavelength measured without assuming Sellmeier's dispersion law. We obtained the thicknesses of the interface layer and SiO_2 layer and the optical constants n and k of the interface layer, assuming the thickness of the interface layer is 1 nm. The optical constants obtained are shown in Fig. 6. Although the obtained values are scattered, the values of the refractive indices are around 3.5 and the absorption coefficients are around 0.2. The refractive indices obtained are slightly smaller than the value obtained assuming Sellmeier's dispersion law, but are still larger than those of SiC and SiO_2. These results also suggest that the interface layers have high refractive indices. Though the obtained values for n and k depend on the thicknesses of the interfaces assumed, the values of n obtained are higher than those of

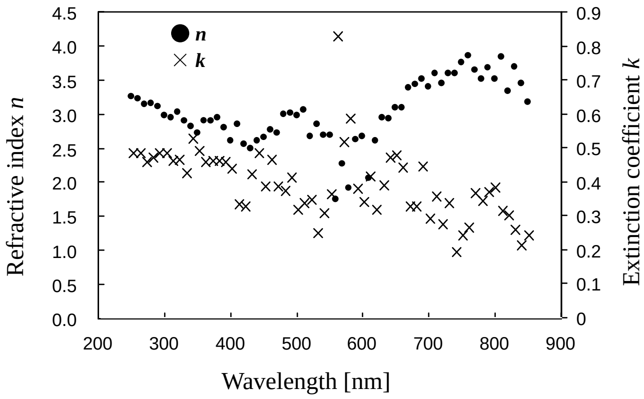

Fig. 6. Optical constants of the interface layer obtained without assuming Sellmeier's dispersion law.

SiC and SiO_2, which is in agreement with the results derived under the assumption of $k \neq 0$ for the interface layers.

It is well known that the refractive indices of SiO_x ($x < 2$) increase with decreasing oxygen composition x,[16] and the refractive indices of Si are reported to be around 3.5 at $\lambda = 630$ nm. The theoretical consideration of the oxidation mechanisms of SiC has predicted the presence of Si–Si bonds at the SiC/SiO_2 interfaces.[11] Therefore, the high refractive index of the interface layer is plausibly due to the presence of Si or Si–Si bonds at the interfaces.

5. Changes of the Optical Properties after Etching

Figures 1 and 2 show that when the oxide thicknesses were less than 5 nm, the values of n_{app} decrease markedly with decreasing oxide film thickness, and approach unity. All of the data reported above were obtained by the spectroscopic measurements carried out immediately after etching at an angle. We also carried out ellipsometric measurements for the oxide films on SiC one month after the etching. Figure 7 shows the thickness dependence of the apparent refractive indices of oxide films on SiC at the wavelength of 630 nm, evaluated from the data measured one month after etching. The values obtained immediately after the etching are also plotted for comparison. When the thicknesses of the oxide films are from 10 nm to 60 nm, no appreciable change is observed in either thickness or the refractive indices. However, when the thicknesses of the oxide films are below 5 nm, the thickness dependence of the apparent refractive indices changes markedly, i.e., for one month after the etching the refractive indices increase with decreasing film thickness and approach approximately 2.6, while immediately after etching the refractive indices decrease with decreasing film thickness and approach unity.

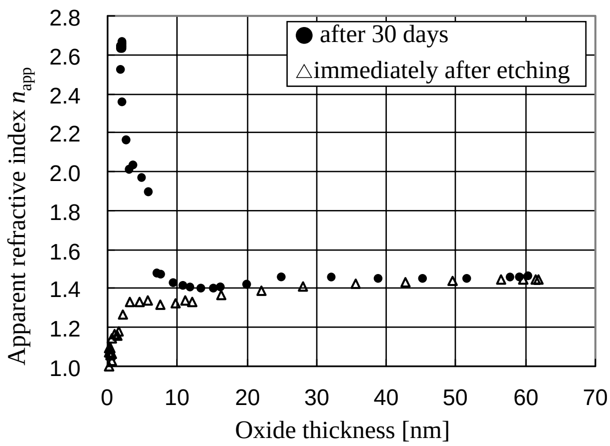

Fig. 7. Thickness dependence of n_{app} of an oxide film on SiC at the wavelength of 630 nm evaluated from data measured 1 month after etching.

This result suggests that the nature of the oxide films less than 5 nm from the interfaces is different from the nature of those more than 5 nm from the interfaces. Therefore, for discussion of the region corresponding to a thickness less than 5 nm, we have to take into account the changes in the refractive indices after etching, though the reasons for this change are not yet clear. We can evaluate the refractive index profile of the oxide layers, i.e., the interface information, from the data for the region corresponding to the oxide thickness more than 5 nm, where no appreciable change is observed in the atmosphere. This is one of the advantages of spectroscopic ellipsometry.

6. Summary

We have evaluated the thickness dependence of the apparent refractive indices n_{app} of oxide films on 6H-SiC, assuming an optically uniform single layer structure, from the spectroscopic ellipsometry measurements of the oxide films etched at an angle. It was found that n_{app} decreases with decreasing oxide film thickness and reaches 1 at oxide thickness = 0. These results indicate that the oxide films are not optically uniform, but the refractive indices change with depth from the surface. We have shown that the thickness dependence of n_{app} can be explained by the model in which the oxide films are composed of two layers, a thin interface layer of around 1 nm in thickness with a high refractive index compared with those of SiC and stoichiometric SiO_2 and a stoichiometric SiO_2 layer, the thickness of which changes with film thickness. These results suggest that there exist interface layers with high refractive indices at oxide/SiC interfaces.

Acknowledgements

This work was partially supported by the management of FED as a part of the METI Project (R&D of Ultra-Low-Loss Power Device Technologies) supported by NEDO and the Ministry of Education, Culture, Sports, Science and Technology through a 2001-2002 Grant-in-Aid for Scientific Research (B) (No. 13450120).

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