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Characterization of the Interfaces between SiC and Oxide Films by Spectroscopic Ellipsometry

Y. Tomioka[1], T. Iida[1], M. Midorikawa[1], H. Tukada[1], K. Yoshimoto[1], Y. Hijikata[1], H. Yaguchi[1], M. Yoshikawa[2], Y. Ishida[3], R. Kosugi[3] and S. Yoshida[1,3]

[1] Saitama University, 255, Shimo-Ohkubo, Saitama, Saitama 338-8570, Japan

[2] Japan Atomic Energy Research Institute, 1233 Watanuki, Takasaki, Gunma 370-1292, Japan

[3] National Institute of Advanced Industrial Science and Technology, Umezono, Tsukuba, Ibaraki 305-8568, Japan

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Abstract
Spectroscopic ellipsometry has been used to investigate, for the first time, the optical properties of oxide films on SiC to discuss the difference of the structures of SiC/SiO_2 interfaces with oxidation processes, thermal oxidation in dry oxygen, pyrogenic oxidation and low temperature deposition of oxides by chemical vapor deposition. It was found that there exist interface layers with high refractive indices between SiC and SiO_2, the values of which are larger than those of SiC and SiO_2 and depend on the oxidation process. The validity of the evaluation of refractive indices of the interfaces has also been discussed.

Introduction
SiC-MOSFET is expected to have two orders of magnitude smaller on-resistance (R_{on}) than those of Si-MOSFET at the same breakdown voltage[1]. However, so far, such a small R_{on} has not been reported. For this reason, the electron mobility in the inversion layer is thought to be severely degraded, probably due to residual carbon[2], suboxides[3], and/or dangling bonds[4,5] at SiO_2/SiC interfaces. Diverse oxidation and annealing methods have been studied to improve the characteristic of SiO_2/SiC interfaces. Many studies have been carried out to investigate the SiO_2/SiC interfaces by use of, for example, C-V, X-ray photoelectron spectroscopy (XPS) and secondary ion mass spectroscopy (SIMS) measurements. In a previous report, we have evaluated, for the first time, the optical constants of oxide films on SiC by spectroscopic ellipsometry[6]. In this study, we have measured the optical constants of oxide films on SiC by various oxidation ways by using spectroscopic ellipsometry, and have tried to elucidate the difference of the structures of SiO_2/SiC interfaces by comparing their refractive index-profiles.

Experimental
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. Oxide layers were formed on the (0001) Si surfaces of SiC epilayers by three processes, thermal oxidation of SiC surfaces in oxygen (dry oxidation), pyrogenic oxidation and low temperature deposition of oxide (LTO) films. Dry oxidation was done in pure O_2 flow at 1100 ^{0}C for 16 h. Pyrogenic oxidation was done in a hydrogen-oxygen flame at 1100 ^{0}C for 8 h. LTO films were deposited by low-pressure chemical vapor deposition (LPCVD) at 400 ^{0}C. The SiC substrates with the oxide layers were immersed gradually into diluted hydrofluoric acid at a constant speed to etch the oxide

layers at an angle. We have measured the ellipsometric parameters (Ψ,Δ) along the slopes in the wavelength range between 250 and 850 nm at an angle of incidence of 75 ^{0}.

Results and Discussion

The optical constants of the oxide films, as well as the film thicknesses, assuming an optically single layer structure with uniform optical properties, were evaluated by the curve fitting of the calculated wavelength variation of ellipsometric parameters to the measured ones. The wavelength-dependence of the apparent refractive indices of the oxide films was assumed to follow the Sellmeier's dispersion law,

$$n_{app}=\{1+[(A^2-1)\,\lambda^2]/(\lambda^2-B)\}^{1/2} \qquad (1)$$

and the extinction coefficient k was assumed to be equal to 0. The parameter A indicates the refractive index at infinite wavelength, while square root of the parameter B indicates the wavelength corresponding to an intrinsic oscillation.

Figure 1 shows the thickness distribution of a dry oxide film along the slope, which reveals the oxide film was etched at an angle. Figure 2 shows the thickness dependence of n_{app} for a dry oxidation film at the wavelength, as an example, λ = 630 nm, where the values of n_{app} were calculated using the values of parameters A and B obtained. In the thick region, n_{app} increases with film thickness and approaches to the refractive index of bulk SiO_2 (n = 1.46). In the very thin region, on the contrary, n_{app} decreases steeply with decreasing film thickness, approaching to 1. In the both cases of pyrogenic oxidation and LTO films, n_{app} changes with film thickness as in the case of dry oxidation.

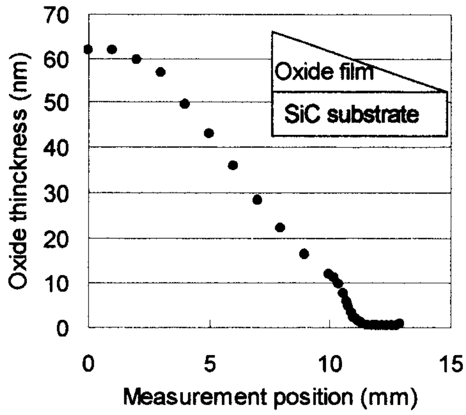

Fig.1. Variation of thickness of a dry oxide film along the slope

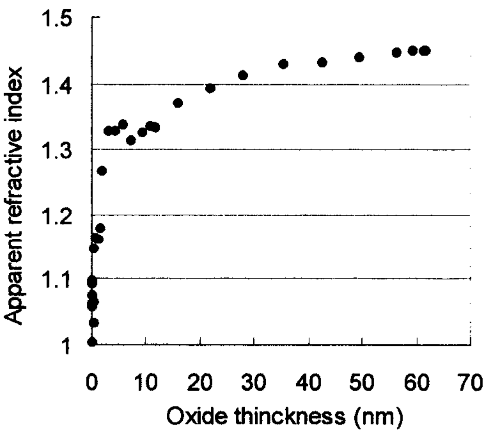

Fig.2. Thickness dependence of refractive index n_{app} at λ = 630nm for a dry oxide film.

The thickness dependence of the refractive index n_{app} obtained is inconsistent with the assumption of an optically single layer structure with uniform optical properties. These results suggest that the refractive indices of the oxide films are not uniform but change with the depth from the surfaces. Therefore, it is needed to suppose another structure model which can explain the results of the ellipsometric measurements. Some reports have suggested the presence of an interface layer between Si and SiO_2 [7,8]. Therefore, we have considered that the films consist of two layers, a thin interface layer and a SiO_2 layer, the thickness of which changes along the slope. Here, the thickness of an interface layer was assumed to be 1 nm and its refractance index was assumed to obey Sellmeier's dispersion law and its extinction coefficient equals to be 0. We have evaluated the values of A and B in the Sellmeier's equation for the refractive indices of interface layers, as well as the thickness of the SiO_2 layers by use of curve fitting method.

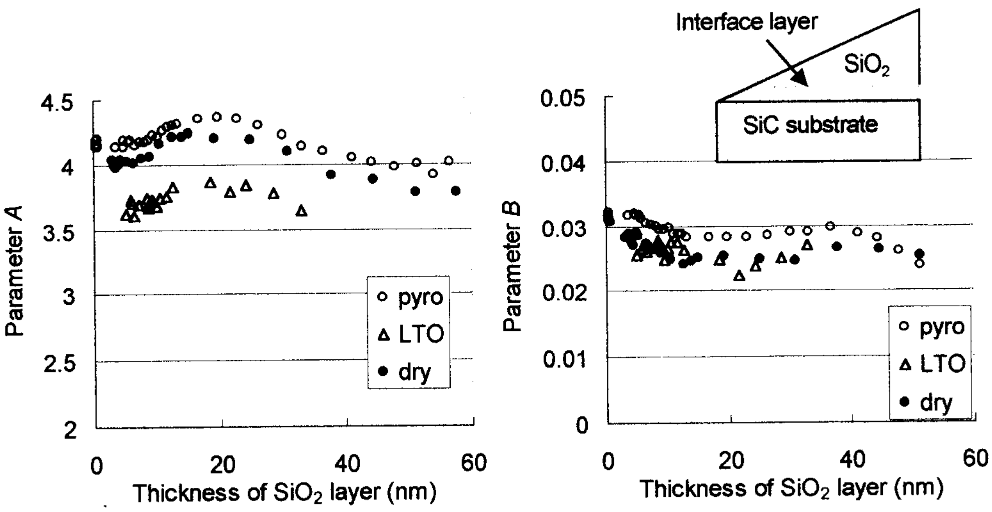

Fig.3. The values of the parameter A and B in the Sellmeier's dispersion equation for a LTO film, and pyrogenic and dry oxidation films.

Figure 3 shows the thickness dependence of the parameters A and B for various oxide films. As shown in this figure, the values of parameters A and B for three oxide films are almost constant against film thickness. Therefore, the results of the ellipsometric measurements along the slope for three oxide films can be explained by two layers model we proposed. All the values of the refractive indices calculated using the values of A and B obtained for three oxide films are higher than the refractive indices of bulk SiO_2 (n = 1.46 at 630 nm) and bulk SiC (n = 2.63 at 630 nm). This means that there exist thin interface layers with high refractive indices. The figure also reveals that the values of A depend on the oxidation process, and the values for LTO films are smaller than those for pyrogenic and dry oxidation. It has been reported that the LTO films have lower interface state densities and effective oxide charge densities than those of thermally oxidized films[9]. Therefore, these results suggest that the values of A of the interface may be related to the electrical properties of SiC MOS structures in some extent. The large refractive indices evaluated suggest the existence of bonds with large polarization, like Si-Si bonds at the interface. However, as the absolute values of A depend on, for example, thickness of the interface layers assumed, it is hard to discuss the difference of the interface structures with oxidation process quantitatively, like the quantities of the bonds having large polarization.

In the evaluation of the optical constants of the interface layers, we have assumed that the wavelength dependence of the refractive indices follows the Sellmeier's dispersion law and the extinction coefficient is equal to be 0. If there exist chemicals other than SiC and SiO_2 at the interfaces, their extinction coefficients are expected not to be zero. Thus we have tried to evaluate the optical constants (n,k) of the interface layers at each wavelength from the measured (Ψ,Δ) values under the assumption that the thickness of the interface layer is 1nm and that of the SiO_2 layer is same as that in Fig 3. Figure 4 shows the optical constants (n,k) of the interface layer for pyrogenic oxidation as a function of wavelengh for various thicknesses of SiO_2 layers. The figure shows the values of extinction coefficient are in the order of 0.1 though the values vary widely. The most important point of the results is that the values of refractive index of the interface are still higher than the refractive indices of bulk SiO_2 and SiC, even in the case of the evaluation without the assumption of k = 0. The solid line in Fig.4 indicates the refractive indices calculated from the values of A and B obtained under the assumption of k = 0 and the Sellmeier's dispersion law for n. The values of the refractive indices obtained at each wavelength almost agree with the values calculated from the Sellmeier's dispersion law. These results suggest that the assumption of the Sellmeier's dispersion law for n is also reasonable.

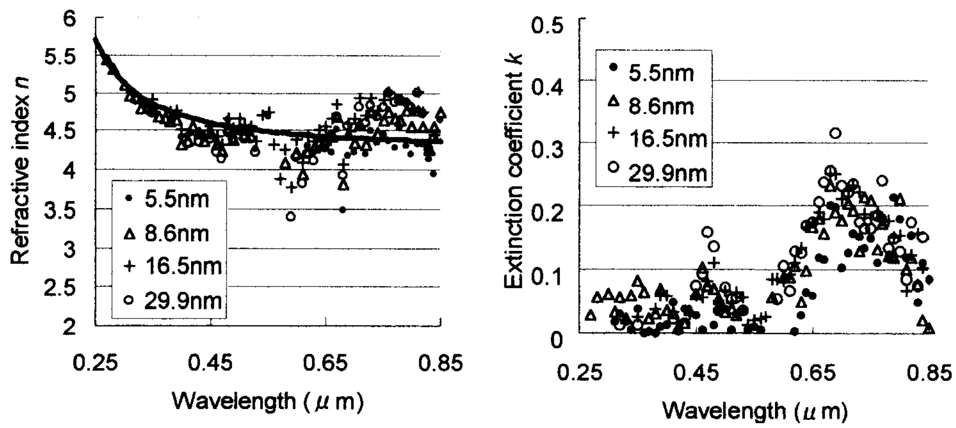

Fig.4. The values of optical constants (n,k) of the interface layer in pyrogenic oxidation as a function of wavelengh. The thicknesses of SiO_2 layers are shown in the inset.

Summary

We have evaluated the optical constants of oxide films on 6H-SiC by spectroscopic ellipsometry, for the first time, using oxide films etched at an angle. The difference in the optical constants of SiC/SiO_2 interfaces with oxidation processes, thermal oxidation in dry oxygen, pyrogenic oxidation and low temperature deposition of oxides by chemical vapor deposition has been studied. It was found that, for three cases, there exist interface layers with high refractive indices between SiC and SiO_2, the values of which are larger than those of SiC and SiO_2. It was also found that the refractive indices of the interfaces depend on the oxidation processes, *i.e.*, those for pyrogenic and dry oxidation films are larger than those for LTO films. This result well corresponds to the electrical properties of SiC/SiO_2 interfaces, like interface state densities, which suggests the ellipsometric measurements give some information on the interfaces related to their electrical properties.

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