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Characterization of Oxide Films on SiC by Spectroscopic Ellipsometry

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We have, for the first time, evaluated the optical constants of thermally oxidized films on SiC by spectroscopic ellipsometry, and discussed the characteristics of SiC/SiO_2 interfaces. It was found that the effective refractive indices are smaller than those of the oxide films on Si. They increase with oxidation time, or oxide thickness, reaching to the values of Si oxides. The refractive indices also depend on the oxidation methods, and the pyrogenic oxidation brings about larger refractive indices than dry oxidation. The origin of the small refractive indices of oxide films on SiC was discussed in terms of interface structures and composition in comparison with those of oxide films on Si.

KEYWORDS: spectroscopic ellipsometry, 6H-SiC, refractive index, oxidation, SiC/SiO_2 interface

1. Introduction

Silicon carbide (SiC) can be thermally oxidized to grow insulating SiO_2 layers which are known to have superior dielectric properties for metal-oxide-semiconductor (MOS) application, as in the case of Si. However, high-interface-trapped charge densities and oxide-trapped charge densities have been reported for SiC MOS structures[1)] which is a serious problem to be solved before the practical application of SiC MOS field effect transistors. To reduce the occurrence of these densities, many ideas have been proposed for the fabrication process of SiC MOS structures, such as re-oxidation,[2)] post-oxidation annealing in hydrogen atmosphere.[3)] Many studies have been also carried out to investigate the SiC/oxide layer interfaces by C–V measurements,[4,5)] X-ray photoelectron spectroscopy (XPS)[6–8)] and internal photoemission spectroscopy (IPS).[9)] Önneby and Pantano[8)] reported that there exists silicon oxycarbide SiC_xO_y from 0.3 to 1 nm in thickness at the interface. Afanas'ev and coworkers[9,10)] observed the interface states in the energy range up to 1.5 eV above the top of the SiC valence band, and suggested the existence of carbon clusters at the interfaces from atomic force microscope (AFM) observation of the SiC surface after removing the oxide layers. Jernigan and coworkers[11)] reported that no excess carbon was detected in the oxide or at the SiC/oxide interface. They reported, however, that the oxide is structurally different from the oxide grown on Si, though the oxide is stoichiometric SiO_2. In the case of oxide films on Si, on the contrary, the existence of transition layers between Si and SiO_2, i.e., suboxide, was reported.[12)] Hebert and coworkers[13,14)] measured the refractive index of ultrathin oxide films on Si by means of Fowler Nordheim tunneling current oscillations and ellipsometry and showed that the refractive indices of oxide films increase with decreasing film thickness in the thickness range below 10 nm.

In this study, we have, for the first time, evaluated the optical constants of thermally oxidized films on SiC by spectroscopic ellipsometry, and discussed the characteristics of SiC/SiO_2 interfaces in comparison with those of oxide films on Si.

2. Experiments

6H-SiC epilayers, 5 μm in thickness and 5×10^{15} cm^{-3} in carrier concentration (n-type) (Cree Research, Inc.), were used for oxidation experiments. The (0001) Si surfaces of the SiC epilayers were oxidized by two methods, pyrogenic oxidation and oxidation in dry oxygen flow. Pyrogenic oxidation was conducted at 1100°C in a flow of oxygen and hydrogen gases. Dry oxidation was conducted at 1100°C in a flow of oxygen gas. The thicknesses of the oxide films obtained were from 16 to 60 nm in the case of pyrogenic oxidation for 1–8 h and 20 to 60 nm in the case of dry oxidation for 4–16 h. Spectroscopic ellipsometric measurements have been carried out using a spectroscopic ellipsometer GESP-5 (Sopra) in the wavelength range between 250 and 850 nm at an angle of incidence of 75°. The optical constants of the oxide films, as well as the film thicknesses, assuming an optically single layer structure, were evaluated by the curve fitting of the calculated ellipsometric parameters Ψ and Δ to those measured as a function of wavelength, where the wavelength-dependence of the refractive indices of oxide films were assumed to follow Sellmeier's law. The optical constants of 6H-SiC used for the calculation were obtained from the ellipsometric measurements for SiC epilayers before oxidation. The surface roughness of the oxide films on SiC was examined by means of AFM measurements.

3. Results and Discussion

The refractive indices of the oxide films on SiC oxidized with two different methods are shown as a function of wavelength in Fig. 1. The thicknesses of the pyrogenic oxide film and the dry oxide film are both about 20 nm. The values for oxide films on Si are also shown in the figure for comparison. It was found that the refractive indices for both the films are smaller than those of oxide films on Si in the entire wavelength range measured. The figure also shows that the dry oxidation brings about smaller refractive indices than the pyrogenic oxidation.

Figures 2(a) and 2(b) show the refractive indices of the oxide films with the dry oxidation for various oxidation times from 4 to 16 h, and those in the case of pyrogenic oxidation from 1 to 8 h, respectively. Both the figures reveal that, though the refractive indices of all the films are smaller than those of oxide films on Si, they increase with oxidation time or oxide film thickness and reaching to the values for oxide films on Si. The thickness dependences of the refractive indices at the wavelength of 630 nm are shown in Figs. 3(a) and 3(b). In

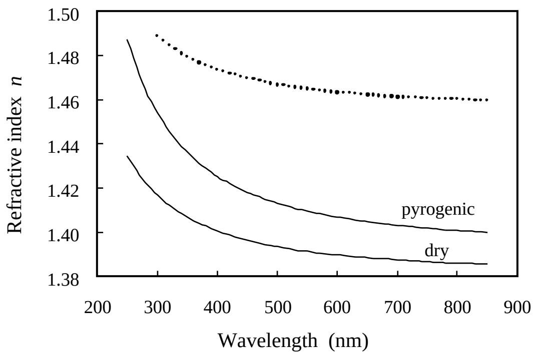

Fig. 1. Refractive indices of oxide films on SiC oxidized with two different methods, dry oxidation and pyrogenic oxidation. The thicknesses of the oxide films are both about 20 nm. The dotted line indicates the values for oxide films on Si.

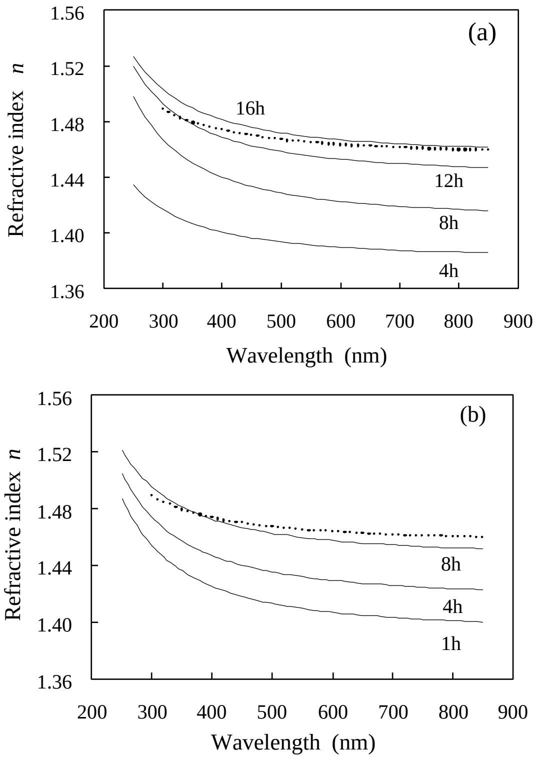

Fig. 2. Variations of refractive indices of oxide films on SiC with oxidation time; (a) dry oxidation, (b) pyrogenic oxidation. The dotted line indicates the values for oxide films on Si.

the cases of both dry oxidation and pyrogenic oxidation, the refractive indices decrease with decreasing oxide film thickness. These features are significantly different from those reported in the case of oxide films on Si,[13,14] i.e., the refractive indices of oxide films on Si have been reported to increase with decreasing film thickness, as denoted by the broken line in Figs. 3(a) and 3(b). This has been explained by the existence of the transition layers, i.e., suboxide layers, at Si/SiO_2 interfaces, whose refractive indices are larger than those of SiO_2. The decrease of refractive indices of SiC oxide films cannot be explained by the existence of a SiC-SiO_2 transition layer. As the refractive indices of SiC are larger than those of SiO_2, the refractive indices of the SiC-SiO_2 mixed layer or SiC_xO_y should be larger than those of SiO_2.

There is a possibility that rough surfaces of the SiC oxide films lead to the evaluation of smaller refractive indices. We measured the surface roughness of the oxide films on SiC as well as that of the SiC epilayers before oxidation. The AFM measurements suggest that the surface roughnesses of the oxide films and epilayers are well below 1 nm. Figures 4(a) and 4(b) show, respectively, the AFM image and the line profile of the oxide film with dry oxidation for 4 h (20 nm in thickness). The root mean squares of the surface roughness of the oxide film are around 0.2 nm. Then, we attempted to take into account the effects of rough surface layers with the thickness of 1 nm in the evaluation of the refractive indices of oxide films. In the calculation, we assumed three layer structures, a rough surface layer with the mean refractive indices of air and oxide layer, an oxide layer and the SiC substrate. The changes in the evaluated values of the refractive indices were on the order of 10^{-3}. Therefore, the surface roughness is not the origin of the result of smaller refractive indices for oxide films on SiC.

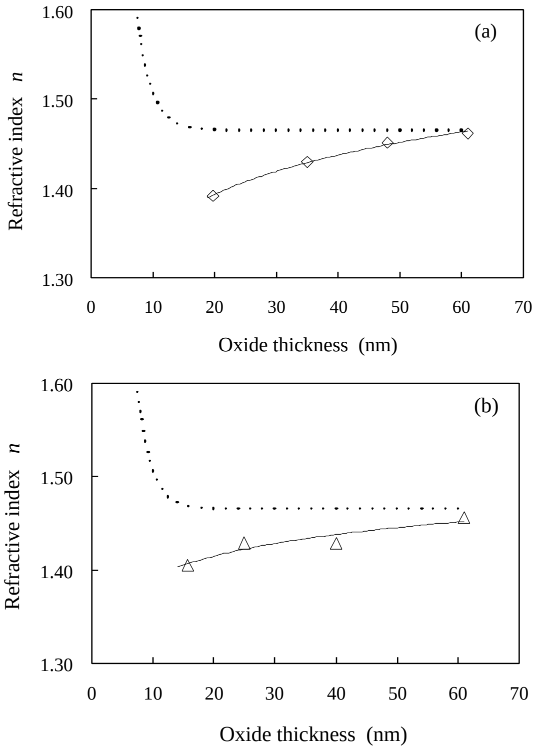

Fig. 3. Thickness dependence of the refractive indices of oxide films on SiC at the wavelength of 630 nm; (a) dry oxidation, (b) pyrogenic oxidation. The broken line indicates the values for oxide films on Si.

From these results, we can conclude that the effective refractive indices of the oxide films on SiC are smaller than those of oxide films on Si, assuming an optically single layer structure. The increase of the refractive indices with film thickness can be explained as follows: there exist thin layers with small refractive indices near the SiO_2/SiC interface, and the thickness of the SiO_2 layer on these interface layers increases with oxidation time. Therefore, we attempted to obtain the refractive indices of the interface layers, assuming that the oxide film consists of two layers, the SiO_2 layer and the interface layer. However, it was difficult to obtain these by curve fitting due to the lack of measured parameters compared with the number of unknown parameters to be evaluated. More studies will be required to obtain more detailed information about the SiC/oxide interface layers having

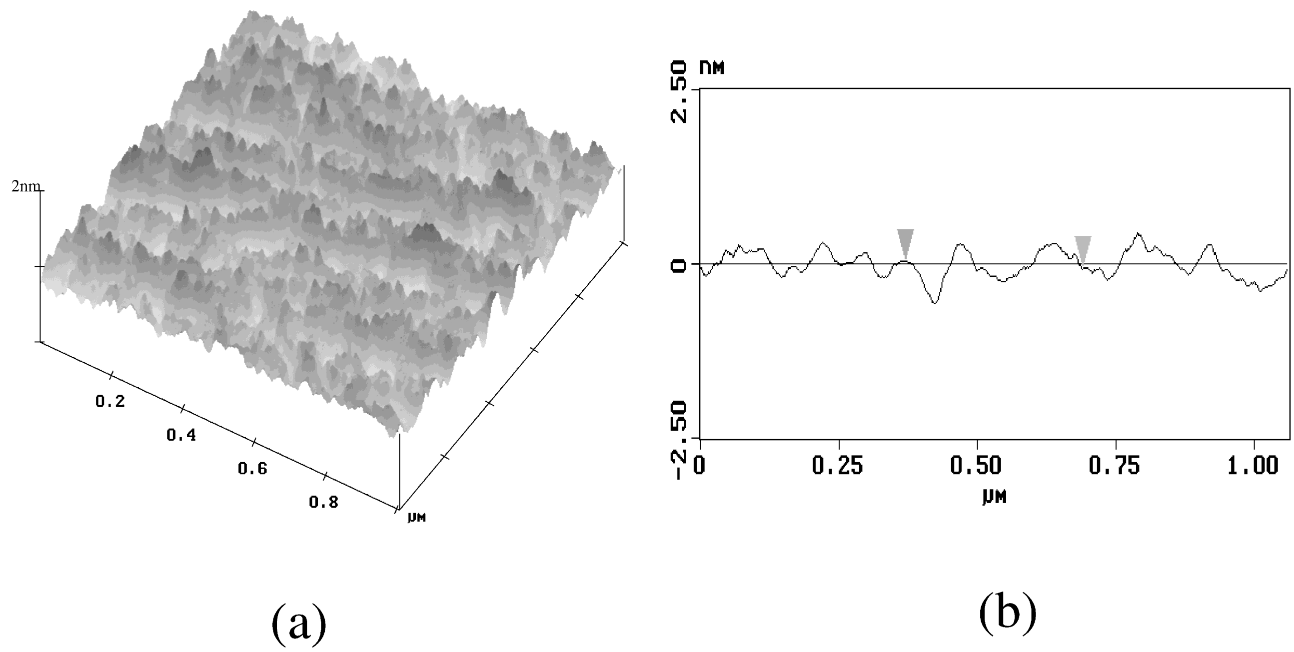

Fig. 4. AFM image and line profile of the oxide film on SiC with dry oxdation for 4 h.

smaller refractive indices.

As mentioned previously, the small refractive indices of the SiC/oxide interface layers cannot be explained by the existence of transition layers between SiC and SiO_2, i.e., SiC_xO_y layers. The inclusion of carbon clusters at the interfaces has been reported.[2] If there exist unpolarized C-C bonds in the interface layers, these may reduce the dielectric constant, resulting in smaller refractive indices. It has been reported that there exists stress or strain due to the difference between the thermal expansion coefficients of SiC and SiO_2,[15] and because of the evolution of gaseous CO or CO_2 through the oxide.[11] The stress or strain may change the refractive indices near the interfaces. To clarify the characteristics of the interface layers, more precise studies on very thin oxide films on SiC will be necessary.

4. Summary

We have measured the optical constants of oxide films on 6H-SiC by means of spectroscopic ellipsometry, for the first time, and found that the effective refractive indices are smaller than those of oxide films on Si. They increase with oxidation time, or oxide thickness, reaching to the values of SiO_2. The refractive indices also depend on the oxidation method; pyrogenic oxidation brings about larger refractive indices than dry oxidation. We have demonstrated that the surface roughness is not the origin of the result of small refractive indices for oxide films on SiC by means of ellipsometry.

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