Materials Science Forum Vols. 615-617 (2009) pp 505-508
online at http://www.scientific.net
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Characterization of 4H-SiC–SiO_2 Interfaces by a Deep Ultraviolet Spectroscopic Ellipsometer

H. Seki[a], T. Wakabayashi[b], Y. Hijikata[c], H. Yaguchi[d], and S. Yoshida[e]

Division of Mathematics, Electronics and Informatics, Saitama University, 255 Shimo-Okubo, Sakura-ku, Saitama-shi, Saitama, 338-8570, Japan

[a]aseki@opt.ees.saitama-u.ac.jp, [b]wakabaya@opt.ees.saitama-u.ac.jp, [c]yasuto@opt.ees.saitama-u.ac.jp, [d]yaguchi@opt.ees.saitama-u.ac.jp, [e]yoshida@opt.ees.saitama-u.ac.jp

Keywords: 4H-SiC, spectroscopic ellipsometry, refractive index, SiC–SiO_2 interface, Si emission model

Abstract. We have characterized 4H-SiC–oxide interfaces fabricated by thermal oxidation of SiC using spectroscopic ellipsometry in the wide spectral range from visible to deep UV region. It was found that there exists an interface layer, around 1 nm in thickness, regardless of the oxide thickness from 15 nm to 40 nm. The optical constants of the interface layer have similar spectral dependence to those of SiC, though the absolute value of the refractive indices is 0.5–1 larger than that of SiC. We have discussed the structure of the interface layer based on the oxidation mechanism of SiC, like the Si-emission model.

Introduction

The physical properties of SiC, such as high-breakdown electric field and high thermal conductivity, are attractive for the realization of high-speed switching and/or low-power-loss electronic devices, compared with Si. In addition, SiC can be thermally oxidized and SiO_2 can be formed as a gate insulator for applications of metal-oxide-semiconductor (MOS) devices similarly to Si. However, SiC-MOSFETs have some problems to be solved before practical use, such as their higher on-resistance than that predicted from the physical properties of SiC. It has been considered that this poor electrical characteristic is attributed to high interface state density at the SiC–oxide interfaces. Therefore, it is important to investigate the interface structure to clarify the origin of the interface states. XPS and TEM studies found these exists the interface layer between SiC and oxide layer [1–4].

In our previous work, we have characterized the oxide layers on SiC by performing spectroscopic ellipsometry using slope-shaped oxide layers and found that there exists a high refractive index interface layer of about 1 nm in thickness between SiC and oxide layer [5]. We have studied the oxidation method and face polarity dependence of the refractive indices of the interface layer, and found that the value of refractive indices strongly is related to that of the interface state density. However, since the precise determination of the thickness of the interface layer was difficult in the analysis of optical data, we have assumed the thickness of the interface layers is 1 nm to derive the optical constants of the interface layers, based on the results from the XPS studies on SiC–oxide interfaces [1].

It has been reported in the studies on Si/oxide interfaces that the wavelength dependence of optical constants near the direct transition energy (E_0) gives the information on a structural defect near the interfaces, such as oxide-induced stacking fault [6] and interfacial strain [7] because these defects bring about the shift of E_0 peak. Although we had performed spectroscopic ellipsometry in the spectral range from 1.4 to 4.3 eV, optical measurements covering deep UV region is considered to be

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more desirable to characterize the SiC–oxide interface because the E_0 value for 4H-SiC is 5.65 eV [7].

In this study, to obtain the information on the interface structure in more detail, we have extended the wavelength range of the spectroscopic ellipsometry to deep ultraviolet (UV) region, i.e., to 200 nm, or 6.0 eV, which covers the E_0 peak of 4H-SiC. In the optical analysis, we have determined the thicknesses of the oxide and interface layers in the visible spectral range first, and then derived the optical constants of the interface layer in the wide spectral range by using the thicknesses determined in the visible range. We have characterized the SiO_2 layer thickness dependence of the optical constants and thickness of the interface layer by using a deep ultraviolet spectroscopic ellipsometer, and discussed the structure of the interface layer in terms of the oxidation mechanism of SiC.

Experiments

Epitaxial wafers of 4H-SiC with 8° off-oriented (0001) Si-face, *n*-types were used in this study. After RCA cleaning was executed, a sample was oxidized at 1100˚C in a dry oxygen atmosphere. By the oxidation for 2.4, 4.1, 5.4, 6.7, 9.2, and 14.5 h, we obtained the oxide layers from 15.7 to 42.2 nm in thickness. The photon energy dependence of ellipsometric parameters (Ψ, Δ) was measured by use of a spectroscopic ellipsometer (GESP-5, *Sopra inc.*) in the photon energy range between 2.0 and 6.0 eV at an angle of incidence of 75°. In the optical analysis of oxide layers on SiC, we assumed that an oxide is composed of two layers, *i.e.*, an oxide layer having stoichiometric SiO_2 composition and an interface layer. Firstly, we determined the oxide layer and interface layer thicknesses by curve fitting of the calculated (Ψ, Δ) spectra to the measured ones in the range from 2.0 and 4.0 eV. As the optical absorption is supposed to be sufficiently small in this spectral range, we used the modified Sellmeier's dispersion relation, including weak absorption [8]. Finally, the optical constants (n, k) of the interface layer were derived for each photon energy in the range between 2.0–6.0 eV from the measured ellipsometric parameters (Ψ, Δ) by using the SiO_2 and interface layer thicknesses determined in the visible spectral range.

Results and discussion

Figure 1 shows the oxide layer thickness (d_1) dependence of the interface layer thickness (d_2) for dry oxidation at 1100°C. This figure suggests that the values of d_2 are around 1 nm at all the oxide layer thicknesses measured in this study. It is also suggested that d_2 decreases a little with oxidation thicknesses larger than around 20 nm. Yamamoto *et al.* have performed real time observations of SiC oxidation using an in-situ spectroscopic ellipsometry and reported that the growth-rates in thin oxide regime are much larger than the values predicted from D-G model [9,10]. In the case of SiC Si-face, the growth rate enhancement occurs below the oxide thickness of around 10 nm at 1100°C. Therefore, the change in d_2 does not correspond directly to the change in the

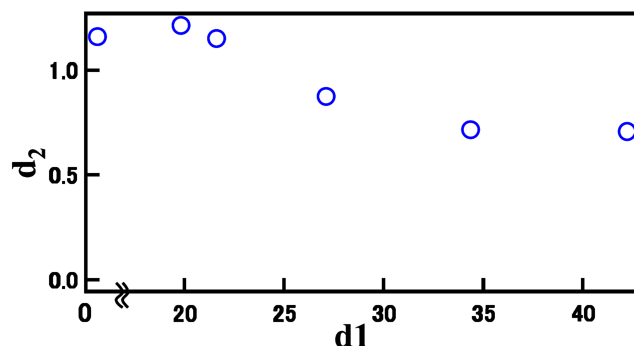

Fig.1 Oxide thickness dependence of the thickness of the interface layer for dry oxidation at 1100°C,

grown oxide thickness. Although we have no idea to explain the origin of the decrease in interface layer thickness at around 20 nm at present, more precise determination of the interface layers is needed to discuss the origin.

Figure 2 shows the photon energy dependence of refractive index, *n*, and extinction coefficient, *k*, of the interface layer at various oxide thicknesses. The optical constants of 4H-SiC are also shown in the figure. The values of *n* and *k* between 2–6 eV derived from the measured values of (Ψ, Δ) at each photon energy agree well with those calculated from the Sellmeier's dispersion relation determined by curve fitting in the range between 2–4 eV. This suggests the validity of the optical model used in the analysis. As shown in this figure, the photon energy dependence of the refractive index *n* of the interface layer is similar to that of SiC, though the absolute values are 0.5–1 larger than that of SiC, and the refractive index of the interface layer slightly decreases with oxide thickness. The differences in *n* between the interface layer and SiC tend to increase with photon energy. While, the photon energy dependence of *k* looks similar to that of SiC in the whole energy range, *i.e.*, almost zero below 4 eV and a rise around 5 eV. Only for the thickest oxide sample, 42.2 nm in thickness, the value of *k* starts rising up at the lower energy compared with the other samples.

The experimental results can be summarized as follows; there exists an interface layer of about 1 nm in thickness, the optical constants of the interface layer have a similar energy dispersion to those of SiC in the spectral range from visible to deep ultraviolet region, the values of refractive index are 0.5–1 larger than that of SiC, and the values of extinction coefficient are almost the same as those of SiC.

It was also found that the thickness and optical constants of the interface layer show a little dependence on the oxide thickness. These experimental results suggest the presence of an interface layer having a similar structure as SiC. Namely, the interface layer is considered to be not the transition layer between SiC and SiO_2, like SiO_x or SiC_xO_y, but a layer having the modified structure and/or composition from SiC, locating at the SiC-side of SiC–oxide interface.

Hijikata *et al.* [11] have reported that the Si emission model, which has been originally proposed for Si oxidation, accounts for the oxide thickness dependence of oxide growth rate of SiC C-face in the wide oxide thickness range. The concept of this model is that Si atoms are emitted from the SiC/oxide interface during oxidation due to the strain between SiO_2 and SiC, accumulate near the interface, and suppress the interfacial reaction rate. In this model, Si atoms are emitted not only into the SiO_2 layer but also into the substrate, *i.e.*, into SiC. The value of *n* is supposed to be larger than that of SiC, while that of *k* scarcely changes from that of SiC when

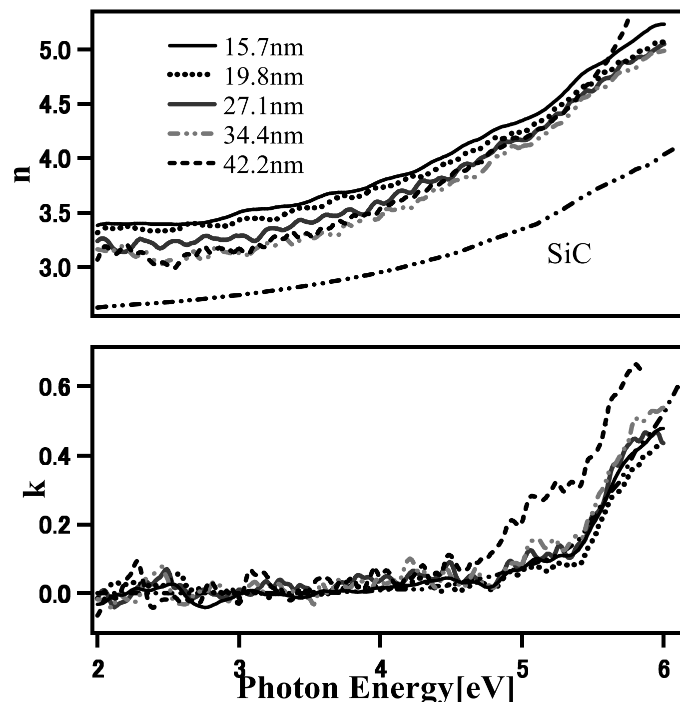

Fig.2 Photon energy dependence of the optical constants of the interface layers for various oxide thicknesses

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interfacial Si atoms are contained in SiC contains, which are in good agreement with the characteristics of the interface layers mentioned above. It is plausible that the presence of such an interface layer may bring about a formation of interface states and/or low channel mobility. The fact that *n*, *k* and thickness of interface layer depend little on oxide thickness suggests that the formation of interface layers correlates strongly with the interfacial oxidation reaction.

In the case of the thickest oxide sample, the rise up energy of *k* is smaller than that of 4H-SiC. There is a possibility that the increase of roughness at the surface of the oxide or interface layer with oxide thickness causes the increase of *k* in a short wavelength range. We have estimated the influence of the surface and interface roughness on the analysis of optical constants of the interfaces in our experiments, and found that such a roughness induces an increase of *k* at not only high energy but also lower energy region. Therefore, the shift of the rise up energy cannot be explained by the surface or interface roughness. In the case of Si oxidation, Nguyen *et al.* have reported that the interfacial strain between Si and SiO_2 causes a red-shift of E_0 energy of Si [6]. As in the case of SiC oxidation, the increase of *k* in the deep ultraviolet region can be explained by the red-shift of E_0 peak of SiC (5.65 eV for 4H-SiC [7]) due to the increase of interfacial strain with oxide thickness.

Summary

We have performed spectroscopic ellipsometry measurements in the wide spectral range from visible to deep UV region to clarify the structure at SiC–oxide interfaces for various oxide thicknesses. It was found that there exists an interface layer, around 1nm in thickness, between oxide layer and SiC, whose refractive index is lager than that of SiC and SiO_2, and the energy dependence of the extinction coefficient of the interface layer is similar to that of SiC. These results can be explained by the presence of modified SiC layers, like SiC layers containing Si interstitials emitted from the SiC–oxide interface with the progress of oxidation. It is also found that the optical constants and thickness of the interface layer are little dependent on the oxide thickness. This result indicates that the formation mechanism of the interface layer is correlated with not the oxidation process which is dependent on oxide thickness, such as oxidant diffusion in SiO_2, but the oxidation process near the SiC–SiO_2 interface.

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Silicon Carbide and Related Materials 2008
doi:10.4028/3-908454-16-6
Characterization of 4H-SiC–SiO₂ Interfaces by a Deep Ultraviolet Spectroscopic Ellipsometer
doi:10.4028/3-908454-16-6.505

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