

Observation of SiC Oxidation in Ultra-thin Oxide Regime by In-situ Spectroscopic Ellipsometry

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Abstract. Thermal oxidation process of silicon carbide in ultra-thin oxide regime has been studied by performing *in-situ* and real time spectroscopic ellipsometry. We found the thermal oxidation at 700°C forms no or extremely thin interface layers between SiC and oxide layers. In contrast, the oxidation at 850°C forms an interface layer of around 1 nm in thickness, having similar thickness and optical constants of the interface layers formed by the oxidation at higher temperature than 1000°C. To make clear the conditions no interface layer is formed, *i.e.*, whether low temperature growth or thin oxide thickness is crucial, we have performed the oxidation at 850°C in the reduced oxygen pressure. Based on the results of these experiments, we discussed the origin of the formation of interface layers as well as the oxidation mechanism of SiC.

Introduction

SiC MOSFETs are expected to show a superior performance, such as high-power, high-frequency, and high-temperature operation and low power consumption compared with Si MOSFET because of the physical properties of SiC. At the present time, however, the electrical characteristics of SiC MOSFETs, such as on-resistance, are poorer than those predicted from the physical properties of SiC. It has been considered that such unsatisfactory electrical characteristics are attributed to high interface state density, which is related to the structure of SiC–oxide interfaces, in other words, the existence of an interface layer [1–3]. In order to improve the electrical characteristics of SiC MOSFETs, therefore, it is crucially important to investigate the SiC–oxide interface structures.

Hino *et al.* recently reported that high channel mobility is obtained for Al₂O₃/SiO_x/SiC-MOSFET when the SiO_x layer thinner than about 1 nm, whereas the channel mobility drastically decreased when the SiO_x is thicker than 1 nm [4]. In our previous work, we have performed real-time measurements of the oxidation rate of SiC using an *in-situ* spectroscopic ellipsometer and have successfully observed the oxide formation even at several nm thickness regime [5–7]. Accordingly, we thought that the real time observation of SiC oxidation in the ultra-thin oxide regime is a promising approach to know the cause for improvement in electrical characteristics of SiC MOS devices. In this work, we have studied SiC oxidation at low temperatures and under reduced oxygen pressure by performing *in-situ* and real time spectroscopic ellipsometry, and discussed the formation process of the interface layers in terms of SiC oxidation mechanism in ultra-thin thickness regime.

Experiments

Epitaxial layers of 4H-SiC (0001) Si-face with 8° off-angles (*n*-type, $N_d - N_a = 7 \times 10^{15} \text{ cm}^{-3}$) were used in this study. After RCA cleaning was executed, an epi-wafer was placed into the oxidation furnace with a spectroscopic ellipsometer [7] and was heated at 700 and 850°C. First, to determine the optical constants of SiC at the oxidation temperature, the wavelength dependence of ellipsometric

parameters (Ψ , Δ) was measured in Ar atmosphere. Then the furnace was evacuated and was filled with O_2 gas at 1 atm. The flow rate of O_2 during the oxidation was 1.0 slm. Ellipsometric measurements were carried out at wavelengths between 290 and 450 nm, and at an angle of incidence of 75.8° . Assuming the existence of an interfacial layer between SiC and SiO_2 , we derived the thicknesses of SiO_2 and interfacial layers from the (Ψ , Δ) spectra measured. The parameters Ψ and Δ are defined by $r_p / r_s = \tan\Psi \exp(i\Delta)$, where r_p and r_s are the reflected amplitudes for p- and s-polarized light, respectively. We also assumed that the optical constants (n , k) of the interface layer were described by the modified Sellmeier's equation included weak absorption. The thicknesses of SiO_2 and interfacial layers and the parameters included in the modified Sellmeier's equation were derived by the curve fitting of the calculated (Ψ , Δ) spectra to the measured ones.

Results and Discussion

Figure 1 shows the oxidation time dependence of the thicknesses of SiO_2 and interfacial layer for the oxidation at 850 and 700°C. At 850°C, both the SiO_2 and interface layer thicknesses increase with time, but the thickness of the interface layer is saturated to 1 nm at 2 hours in the oxidation time while the SiO_2 layer thickness continues to increase after 2 hours. For the oxidation at 700°C, on the contrary, the SiO_2 thickness increases rapidly up to around 1 nm and then the oxidation rate becomes very small, and the thickness is around 1.2 nm even after 8-hour oxidation. As shown in this figure, the interface layer thickness is almost zero up to 8 hours, indicating that no interface layer is formed between SiO_2 and SiC at 700°C.

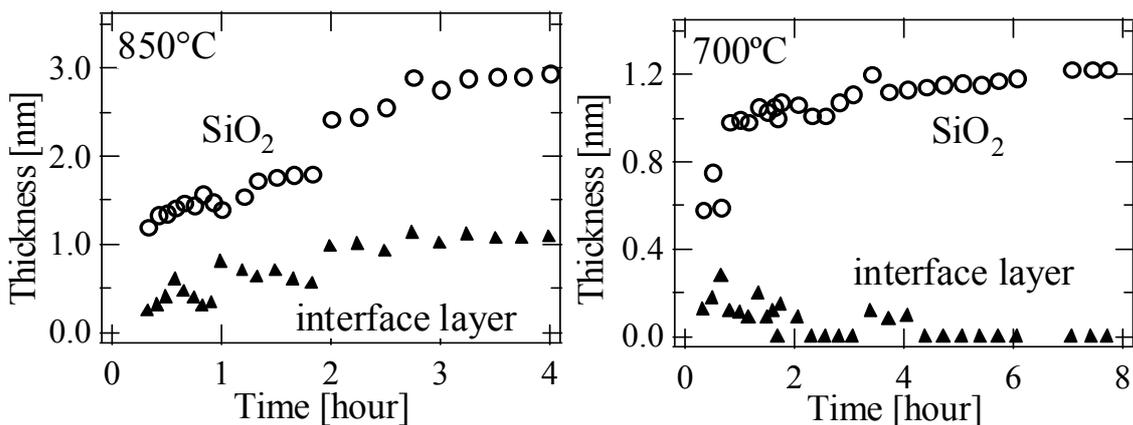


Fig. 1 Oxidation time dependences of thicknesses of the SiO_2 layer and the interface layer for the oxidation at 850 and 700°C.

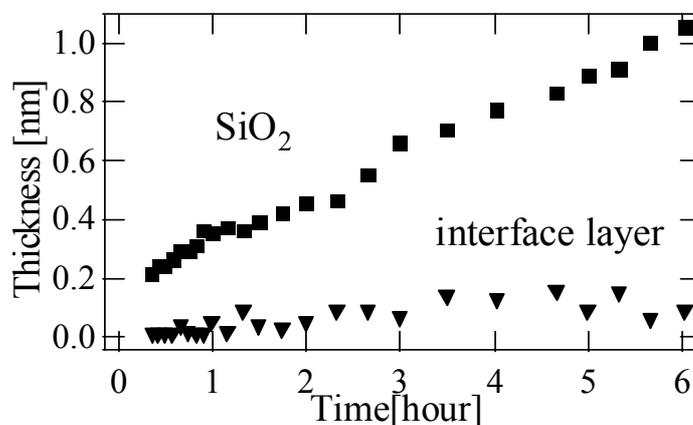


Fig. 2 Oxidation time dependences of the thickness of the interface and SiO_2 layers for the oxidation under an oxygen partial pressure of 0.01 atm at 850°C.

These results suggest that the interfacial layer is not formed or is extremely thin when the oxidation temperature is as low as 700°C or the SiO₂ layer is thinner than around 1 nm. That is to say, there are two possible conditions for realizing oxide layers on SiC with no interface layer, *i.e.*, low oxidation temperatures or/and oxide layers thinner than 1–2 nm. To determine which the important factor for no interface layer is, one way is to check whether an interface layer is formed at 850°C when the oxide layer is thinner than 1 nm. It is difficult to measure the thickness of the interface layer in the oxide thickness less than 1 nm regime at 850°C, however, because the time required to form SiO₂ of 1 nm is quite short. To clarify the formation process of the interface layer, we have studied more precisely the oxidation at 850°C by reducing the oxygen partial pressure down to 0.01 atm, where the oxidation rate is almost the same as that at 700°C and 1 atm.

Figure 2 shows the oxidation time dependence of the thickness of the interface and SiO₂ layers under oxygen partial pressure of 0.01 atm. When the SiO₂ layer thickness is smaller than ~1 nm, the interface layer thickness is extremely thin. This suggests that the formation of an interface layer is independent of oxidation temperature but depends on the SiO₂ layer thickness. However, to clarify the origin of the formation of interface layers more strictly, it is necessary to perform the experiment on the oxidation at low temperatures or under the reduced oxygen partial pressure for a long time enough to obtain the oxide thickness more than several nanometers.

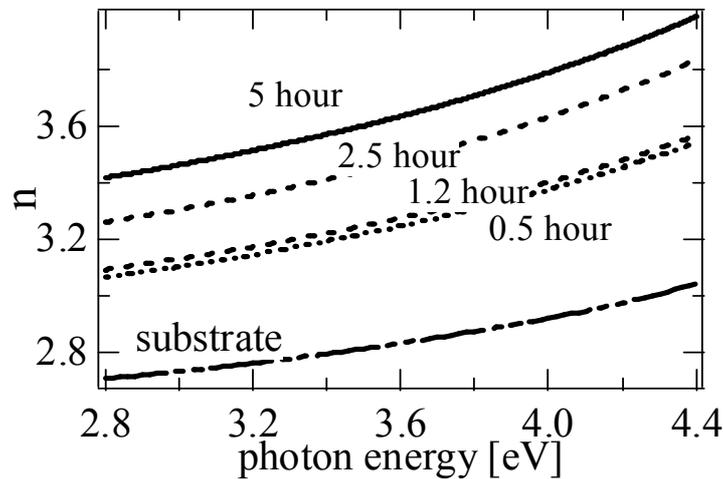


Fig. 3 Photon energy dependences of the refractive indices of the interface layers at various oxidation times at 850°C.

Figure 3 shows the refractive index of the interface layer at different oxidation time at 850°C an 1 atm. The refractive index of the interface layer increases with oxidation time, and is in the range from 3 to 4, which is larger than those of both SiC and SiO₂ (2.76 and 1.47, respectively, at 3.0eV). The extinction coefficient of the interface layer is almost zero in the photon energy range measured. Seki *et al.* [8] have studied the oxide thickness dependence of the interface layer by use of a deep ultraviolet spectroscopic ellipsometer in the photon energy range from 2.0 to 6.0 eV, and have reported the refractive index is about 3 and the extinction coefficient is almost zero in the visible and near ultraviolet spectral range and that in the deep ultraviolet region, the extinction coefficient starts rising up at about 5 eV, which is quite close to the direct transition energy (E_0) of SiC. That is, the interfacial layer has larger refractive index than SiC and the extinction coefficient which is close to that of SiC. These results suggest that the interfacial layer is not a transition layer between SiC and SiO₂, like as SiO_x, and/or SiO_xC_y but a layer composed of substance modified a little from SiC.

Recently, Hijikata *et al.* [9] have successfully reproduced the oxide growth rate of SiC C-face at the entire oxide thickness regime by using the Si atom emission model proposed originally for the explanation of Si oxidation [10]. In the model, Si atoms are considered to be emitted into the oxide layers accompanied by oxidation caused by a strain due to the expansion of Si lattices by oxidation.

In the case when the oxide thickness is thinner than about 20 nm, the emitted Si atoms reach the oxide surface and then are oxidized rapidly. However, when the oxide thickness is over 20 nm, the emitted Si atoms cannot reach the oxide surface but pile up near the interface between SiC and oxide, resulting in the suppression of the interfacial reaction rate. According to this model, Si atoms are emitted into SiC as well as into oxide layer, which may result in the formation of SiC layers containing Si interstitials near the SiC–oxide interface. The Si interstitials in SiC may bring about the increase of the refractive index due to the increase of atomic density, while they may cause only a little change in the band structure of SiC. Considering the experimental results that the interface layer has the refractive index larger than SiC and extinction coefficient just like SiC, the interface layer is supposed to a SiC layer with interstitial Si atoms emitted from the interface accompanied by the oxidation of SiC. It has been reported that the expansion of Si lattices due to oxidation generates the strained Si layers near the interface [11]. Since the strain brings about a red-shift of the E_0 gap energy [10], there exists an interface layer having a little different optical constants from Si near the interfaces. In the case of SiC, the strain due to the oxidation may change the optical constants of SiC near the interface. It has also been reported that the stress causes the polytype conversion to 3C-type in the case of 6H- and 4H-SiC, which also influences the optical constants of SiC near the interface.

Next, we discuss the conditions that the interface layer does not exist or slightly formed in terms of the Si-emission model. In general, when the oxide layer is very thin, the interfacial strain should be relaxed. In this case, a little amount of Si atoms are emitted from the interface, resulting in no or very thin interface layer formed. With increasing oxide thickness, the interfacial strain increases, and then a large amount of Si atoms are emitted, which bring about the noticeable increase of refractive index of SiC near the interface, as shown in Fig. 3. The experimental results might suggest that the critical thickness of the oxides at which an interface layer forms, or the noticeable changes of optical constants occur in the SiC layer near the interface, is around 1 nm.

Summary

We have studied the structures of oxide layers on SiC in the ultra-thin thickness regime grown at low temperatures in detail by performing *in-situ* and real time spectroscopic ellipsometry measurements. We found the interface layer thickness is extremely thin or no interface layer forms when the SiO₂ layer thickness is smaller than ~1 nm and that an interface layer having higher refractive index than that of SiC and extinction coefficient just like SiC forms when the oxide thickness exceeds around 1 nm. We have discussed the critical thickness at which an interface layer forms, and the physical meaning of the optical constants of the interface layer by applying the Si emission model.

References

- [1] Y. Hijikata, H. Yaguchi, M. Yoshikawa, S. Yoshida: Appl. Surf. Sci. Vol. 184 (2001), p. 161
- [2] T. Iida *et al.*: Jpn. J. Appl. Phys. Vol.41 (2002), p. 800
- [3] Y. Ishida *et al.*: Mater. Sci. Forum Vols. 389-393 (2002), p. 1013
- [4] S. Hino *et al.*: Technical Digest of ICSCRM2007 (2007), We-2A-2.
- [5] K. Kakubari *et al.*: Mater. Sci. Forum Vols. 527-529 (2006), p. 1031
- [6] T. Yamamoto, Y. Hijikata *et al.*: Jpn. J. Appl. Phys. Vol. 46 (2007), p. L770
- [7] T. Yamamoto, Y. Hijikata, H. Yaguchi, and S. Yoshida: Jpn. J. Appl. Phys, in press.
- [8] H. Seki, Y. Hijikata, H. Yaguchi, and S. Yoshida: submitted to this conference.
- [9] Y. Hijikata *et al.*: Mater. Sci. Forum Vols. 600-603 (2009), p. 663
- [10] H. Kageshima *et al.*: Jpn. J. Appl. Phys. Vol. 38 (1999), p. L971
- [11] N. V. Nguyen *et al.*: Appl. Phys. Lett. Vol. 64 (1994), p. 2688

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