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In-situ Spectroscopic Ellipsometry Study of SiC Oxidation at Low Oxygen-Partial-Pressures

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Abstract. We have investigated the oxidation process of SiC (000-1) C-face at low oxygen partial pressures using an in-situ spectroscopic ellipsometry. The oxide growth rate decreased steeply at the early stage of oxidation and then slowly decreased with increasing oxide thickness. The initial oxide growth rate was almost proportional to the oxygen partial pressure for both the polar directions. This result suggests that the initial interfacial reaction rate is constant regardless of the concentration of oxidants reaching the interface.

1. Introduction

SiC MOSFETs are expected to be high-performance power devices that operate at higher temperatures and have lower on-resistances compared to Si MOSFETs. It is true that SiC MOSFETs actually fabricated exceed Si MOSFETs, but the on-resistance is higher than that expected from the physical properties of SiC. This is attributed to high interface state density [1]. Thus, it is important to investigate the oxidation process of SiC, which is closely related to the interface structure and also to the formation of interface states.

We have so far observed the SiC oxidation process in real time using an in-situ spectroscopic ellipsometer [2], and found that the oxide growth rate in the thin oxide range decreases rapidly with increasing oxide thickness for both the Si- and C-faces [3, 4]. We have also investigated the oxygen partial pressure dependence of the oxide growth rate of SiC in the range from 0.1 to 1.0 atm, and have discussed the oxidation mechanism of SiC [4, 5]. Since the growth rate at the early stage of oxidation was considerably large, however, it was difficult to derive accurately the initial oxide growth rate at oxygen partial pressures higher than 0.1 atm, particularly for the C-face.

In this paper, we have studied the oxidation of SiC (000-1) C-face and (0001) Si-face at low oxygen partial pressures using *in-situ* spectroscopic ellipsometry in order to accurately derive the oxygen partial pressure dependence of the initial oxide growth rate.

2. Experiments

Epitaxial wafers of 4H-SiC with 0.5^{o} off oriented (000-1) C-face and 8° off oriented (0001) Si-face, n-type were used in this study. Immediately after RCA cleaning, the samples were placed into a furnace equipped with an in-situ spectroscopic ellipsometer. First, to determine the optical constants of SiC at the oxidation temperature, ellipsometric parameters (Ψ, Δ) were measured in the argon atmosphere. Then, the ellipsometric measurements were performed during oxidation at 1100 ^{o}C in a mixture of dry oxygen and argon. The partial pressure of oxygen was varied between 0.02 and 1.0 atm

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for C-face, and between 0.5 and 1.0 atm for Si-face. We derived the oxide and interface layer thicknesses, and optical constants (n, k) of the interface layer from the measured ellipsometric parameters assuming that the refractive index of the interface layer follows the Sellmeier's dispersion equation.

3. Results and discussion

Figure 1 shows the oxide growth rate X as a function of the oxide thickness for (000-1) C-face at various oxygen partial pressures. As can be seen from this figure, the oxide growth rate decreases steeply with oxide thickness at the early stage of oxidation, and then slowly decreases with increasing thickness for lower oxygen partial pressures.

In our previous studies, we had used the Deal-Grove model [7] and Massoud's empirical model [8] to analyze the oxide growth rate. In this study, however, we have applied another approximate expression to the oxide growth rate because the steep decrease in the growth rate can be explained by the suppression of the interface reaction due to the accumulation of interstitial Si and C atoms emitted during oxidation. According to Si-C emission model [9, 10] developed from Si emission model which explain well the experimental results for Si oxidation [11-13], the interfacial oxidation reaction rate k is expressed as a decreasing function for the concentration of interstitial Si and C atoms at the interface:

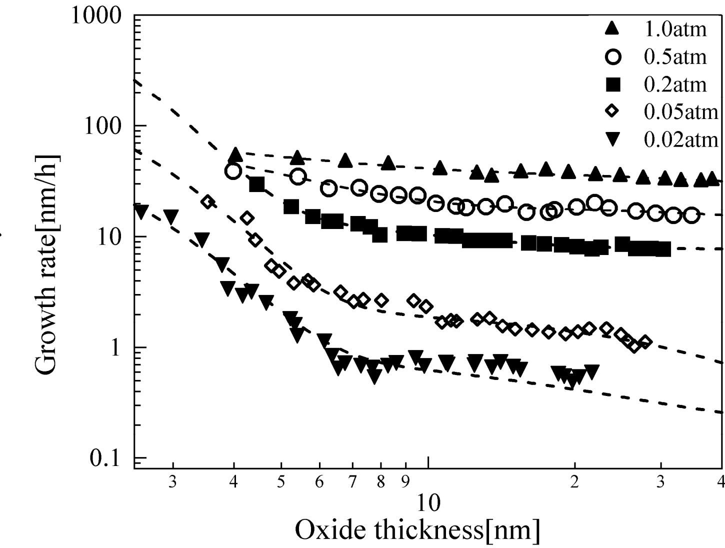

Fig. 1 Oxide growth rate of (000-1) C-face as a function of oxide thickness at various oxygen partial pressures. Dotted curves are fitted to the experimental data using eq. (2).

$$k = k_0\left(1-\frac{C_{\mathrm{Si}}^I}{C_{\mathrm{Si}}^0}\right)\left(1-\frac{C_{\mathrm{C}}^I}{C_{\mathrm{C}}^0}\right), \tag{1}$$

where C^{I} is the concentration of interstitial Si and C atoms at the interface, C^0 is the solubility limit of the corresponding interstitial atoms in the oxide. According to our previous study [9], the interfacial reaction rate decreases with oxide growth due to the accumulation of Si and C atoms, and the accumulation of C atoms is faster than that of Si atoms. Consequently, the accumulation of C atoms largely affects the decrease in the growth rate in the extremely thin oxide region, and then the concentration of interstitial C atoms approaches a quasi-steady state. On the other hand, the effect of Si-atom accumulation persists in the thicker oxide thickness region. Thus, after the C concentration becomes a quasi-steady state, the interfacial reaction rate decreases gently owing to a complex kinetics including the accumulation of Si atoms. In addition, since the influence of the oxidant-diffusion-limited process is negligible in the oxide thickness region we have studied in this work, the oxide growth rate should become constant after the concentration of Si atoms reach a steady state. Therefore, the oxide growth rate is approximated by the following double-exponential equation:

$$\frac{dX}{dt} = a_0 e^{-\frac{X}{L_0}} + a_1 e^{-\frac{X}{L_1}} + a_2 , \tag{2}$$

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Where L_0 and L_1 ($L_0 < L_1$) are characteristic lengths for the decrease in oxide growth rate, and the first and second terms represent the steep decrease mainly due to the accumulation of C atoms at the early stage of oxidation and the slow decrease partly due to the accumulation of Si atoms. The dotted curves shown in Fig. 1 are obtained by using eq. (2) and successfully reproduce the experimental growth rates.

Figure 2 shows the oxygen partial pressure dependence of the initial growth rate R_0 and quasi-steady growth rate R_1 for C-face, where R_0 is expressed by $a_0+a_1+a_2$, and R_1 calculated by a_1+a_2. Since the initial oxide growth rates R_0 at pressures higher than 0.2 atm was too fast, we could not accurately derive them, and thus the experimental data are not shown in this figure. As shown in this figure, the initial growth rate R_0 is nearly proportional to the oxygen partial pressure below 0.2 atm. The quasi-steady growth rate R_1 is not expressed by a power function all over the pressure range studied but is proportional to $p^{0.58}$ at higher oxygen partial pressures. This is in good agreement with our previous result that B/A, which corresponds to R_1 in this study, is proportional to $p^{0.58}$ in the oxygen partial pressure range from 0.1 to 1.0 atm for C-face [4]. Although the slope of R_1 increases with decreasing oxygen partial pressure, it is difficult to discuss the physical meaning because the quasi-state oxide growth rate R_1 is determined by the balance between many factors, such as the quasi-steady concentration of C atoms.

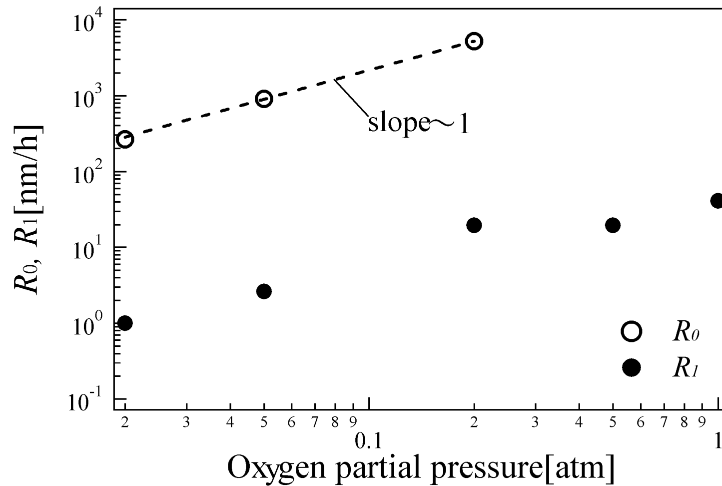

Fig. 2 Oxygen-partial-pressure dependence of the initial growth rate R_0 and quasi-steady growth rate R_1 of (000-1)C-face.

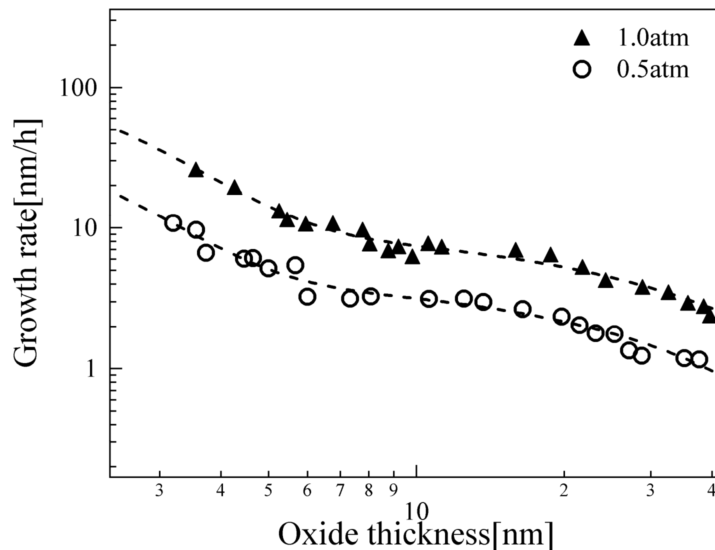

Fig. 3 Oxide growth rate of (0001)Si-face as a function of oxide thickness at various oxygen partial pressures. Dotted curves are fitted to experimental data using eq. (2).

Figure 3 shows oxide growth rates as a function of the oxide thickness for (0001)Si-face. The oxide growth rates are about 10 times slower than that for (000-1) C-face. The initial growth rate R_0 at 1.0 atm and 0.5 atm is 290 nm/h and 130 nm/h, respectively, which indicates that the initial growth rate R_0 is almost proportional to the oxygen pressure in the same way as for C-face.

The oxide growth rate is essentially proportional to the quantity of oxidants which reach the interface between the oxide and SiC. The initial growth rate R_0 is derived from the limit value of the

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growth rate when the oxide thickness X approaches 0, and thus is represented by the following expression:

$$R_0 \propto k_0 C_{O_2} , \quad (3)$$

where k_0 is the interfacial reaction rate when the oxide thickness X approaches 0, and C_{O2} is the concentration of oxidants at the SiC/SiO_2 interface. If k_0 is constant regardless of the concentration of oxidants, R_0 is always proportional to C_{O2}. In addition, C_{O2} is proportional to the oxygen partial pressure based on Henry's law. Therefore, the initial growth rate is proportional to the oxygen partial pressure, which is consistent with the result obtained both for C- and Si faces in this study.

4. Summary

We used *in-situ* spectroscopic ellipsometry to investigate the oxygen-partial-pressure dependence of oxidation process of SiC (000-1) C-face in the range from 0.02 to 1.0 atm and (0001) Si-face in the range from 0.5 to 1.0 atm. The oxide growth rate decreased steeply at the early stage of oxidation and then slowly decreased with increasing oxide thickness. We could derive accurately the initial oxide growth rate by the measurements at low oxygen partial pressure, and found that the initial oxide growth rate was proportional to the oxygen partial pressure for both the polar directions, which is reasonable if the interfacial reaction rate is constant regardless of the concentration of oxidants reaching the interface.

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